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A.S. Jensen & L. Wiesenfeld, organizers

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Preface

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The fourth international and interdisciplinary workshop

Critical stability of few-body quantum systems

was held at the Max-Planck Institute for the Physics of Complex Systems in Dresden from October 16 to 22, 2005. As for the previous workshops, at Trento in 1997 and 2003, and Les Houches in 2001, the main motivation was to discuss questions that are shared by specialists of different fields, and are formulated, tentatively solved and further developed using slightly different methods and languages. This interdisciplinary character, ranging from mathematical physics to quantum chemistry, via molecular, atomic, nuclear and hadron physics, was an essential ingredient of these workshops, and linked with the foundation of few-body physics. The present meeting increased slightly the emphasis on atomic and molecular physics and also on mathematical-statistical physics in the area of condensed matter. The following subjects were proposed in the call for abstracts and invitations:

1. Weakly Coulomb or gravitational-bound few-body states.
2. Weakly short-range-interaction bound few-body states.
3. Continuum structure and few-body decay properties.
4. Dynamical few-body problems near instability.
5. Correlation in boson-fermion and mixed condensates
6. Few-body correlation within many-body systems.
7. Exotic structures: Efimov, tango, Borromean and halo states.
8. Lower-dimensional systems.

We had 50 participants from 19 countries, mostly from Europe and North America but also from Japan and Brazil. The number was limited to optimize the interaction among the participants.

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We want to thank the Max-Planck-Institute for the generous financial support, the excellent organization, and the smooth and efficient running of the workshop. In particular we want to thank Jan-Michael Rost for his continuous support for this project and Mandy Lochar for taking care of all the logistics. In addition, we are grateful for the support of Few-Body Systems and its Editor in Chief B. Bakker for hosting the proceedings, thus ensuring a rapid and widespread diffusion. Last but not least, we want to thank the participants for the lively discussions after the talks and during the breaks, all in the genuine interdisciplinary spirit which is now the tradition of this series. Some more details about the workshop along with pictures of the participants can be seen on http://www.mpi-pks-dresden.mpg.de/~crit05
Structure of exotic three-body systems

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Abstract. The classification of large halos formed by two identical particles and a core is systematically addressed according to interparticle distances. The root-mean-square distances between the constituents are described by universal scaling functions obtained from a renormalized zero-range model. Applications for halo nuclei, $^{11}\text{Li}$ and $^{14}\text{Be}$, and for atomic $^{4}\text{He}_3$ are briefly discussed. The generalization to four-body systems is proposed.

1 Introduction

The properties of large three-body systems present universal behavior as the Thomas-Efimov limit is approached [1]. In this situation the sizes of the two and three body systems are much larger than the interaction range and the wave function almost everywhere is an eigenstate of the free Hamiltonian. Much of the physics of these systems can be studied using a zero-range interaction effective in s-wave. No scale is involved in this drastic situation and the momentum space Faddeev equations are scale invariant for vanishing two and three-body energies. The scale invariance is broken by finite values of two-body scattering lengths and three-body binding energy, which are the scales of the corresponding three-body systems [2]. Dimensionless ratios of three-body observables are then expressed by scaling functions which depends only on ratios of two (bound or virtual) and three-body energies [3]. The scaling functions can be obtained from the solution of regularized Faddeev equations.

The sizes of halo three-body systems (where two particles are identical) are functions of few physical scales. A classification scheme for these systems [4, 5, 6] ordered by their sizes is reviewed. For a given three-body binding energy the

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most compact system is the Borromean (single pairs are unbound) while the all-bound (all single pairs form bound states) is the largest one. The neutron-neutron mean square radius in examples of Borromean halo nuclei which are known experimentally [7] are briefly discussed. The extension of these ideas to four-body systems is proposed.

2 Scale invariance in three-boson systems

The collapse of a three-boson system when the two-body interaction range goes to zero (Thomas effect, see [1]) demands one new physical scale to stabilize the three-boson binding energy ($E_3$). The regulated trimer bound state integral equation in units of $\hbar = m = 1$ ($m$ is the boson mass) is written as

$$f(q) = 2\pi \tau(E_3 - \frac{3}{4}q^2) \int_0^\infty k^2 dk f(k) \int_{-1}^1 dz \left[G_0(E_3) - G_0(-\mu^2(3))\right],$$

(1)

where $G_0^1(E) = E - q^2 - k^2 - qkz$, and the renormalized two-boson scattering amplitude is $\tau^{-1}(x) = 2\pi^2 \left[|a| - \sqrt{-x}\right]$. Without regularization, Eq. (1) is the Skorniakov and Ter-Martirosian (SKTM) equation derived long ago [8] which is scale invariant when the scattering length $|a|$ tends to infinity and $E_3 = 0$. The second term in Eq. (1) brings the physical scale, $\mu(3)$, to the three-boson system [2] avoiding the Thomas collapse. The equivalence of Thomas and Efimov effects is seen in units of $\mu(3) = 1$, which means $|a|\mu(3) \rightarrow \infty$ either for $|a| \rightarrow \infty$ (Efimov limit) or for $\mu(3) \rightarrow \infty$ (Thomas limit).

The sensitivity of three-boson S-wave observables to the short-range part of the interaction in weakly bound systems is parameterized through the value of the trimer binding energy which corresponds to the scale $\mu(3)$. Three-boson S-wave observables are strongly correlated to the trimer energy in a general universal form [3, 9]:

$$\mathcal{O}_3(E, E_3, a) = |E_3|^\eta \mathcal{F}_3 \left(E/E_3, a\sqrt{|E_3|}\right),$$

(2)

where $\mathcal{O}_3$ can represent a scattering amplitude at an energy $E$ or an excited trimer energy (the dependence on $E$ does not appear in this case). The exponent $\eta$ gives the correct dimension to $\mathcal{O}_3$. Eq. (1) is renormalization group (RG) invariant with its kernel being a solution of a Callan-Symanzik differential equation as function of a sliding $\mu(3)$. In that way $E_3$ and three-body observables are independent of the subtraction point (see ref. [9] for a discussion of the RG invariance in three-body systems).

3 Classification of three-body halos and universal scalings

The sizes of halo three-body systems (with two identical particles ($\alpha$) and a distinct one ($\beta$)) are functions of few physical scales. A classification scheme for these systems as Borromean (single pairs are unbound), Tango (only the $\alpha\alpha$ pair form a bound state), Samba (only the $\alpha\beta$ pair is bound) and all-bound (all single pairs form bound states), ordered by their sizes is discussed below.
The typical lengths of the three-body halo systems are given by scaling functions for the mean-square separation distances written according to Eq. (2). The scaling functions for these radii are:

\[
\sqrt{\langle r_{\alpha\gamma}^2 \rangle} E_3 = R_{\alpha\gamma} \left( \pm \sqrt{E_{\alpha\alpha}/E_3}, \pm \sqrt{E_{\alpha\beta}/E_3}, A \right), \tag{3}
\]

\[
\sqrt{\langle r_{\alpha}^2 \rangle} E_3 = R_{\alpha}^{\text{cm}} \left( \pm \sqrt{E_{\alpha\alpha}/E_3}, \pm \sqrt{E_{\alpha\beta}/E_3}, A \right), \tag{4}
\]

where \( \langle r_{\alpha\gamma}^2 \rangle \) and \( \langle r_{\alpha}^2 \rangle \) are, respectively, the mean square relative and center of mass distances. The mass ratio is \( A = m_3/m_\alpha \) and \( \gamma = \alpha \) or \( \beta \). The + or - signs represent bound or virtual two-body subsystems, respectively. \( E_{\alpha\alpha} \) and \( E_{\alpha\beta} \) are the \( \alpha\alpha \) or \( \alpha\beta \) two-body energies.

For a given energy \( E_3 \) and identical particles, the effective interaction in Eq. (1) has a weaker strength for \( a < 0 \) (virtual two-body system) than for \( a > 0 \) (bound two-body system). Therefore, for a Borromean trimer Eq. (1) should have a larger value of \( \mu_3 \) than the corresponding one for an all-bound system, in order to keep the binding fixed with a weaker interaction. The spectator function, \( f(q) \), extends to large momentum for a Borromean system. The trimer wave function for zero total angular momentum is

\[
\Psi(q, p) = f(|q|) + f(|p + \frac{1}{3} q|) + f(|p - \frac{1}{3} q|) E_3 - \frac{3}{4} q^2 - p^2, \tag{5}
\]

which implies in a more compact spatial configuration for a Borromean trimer in comparison to the all-bound one. The Jacobi relative momenta are \( p \) for the pair and \( q \) for the spectator particle. In terms of the scaling functions the radii come as,

\[
R_{\alpha\alpha} \left( - \sqrt{E_{\alpha\alpha}/E_3} \right) < R_{\alpha\alpha} \left( \sqrt{E_{\alpha\alpha}/E_3} \right), \tag{6}
\]

and the separation distances obeys \( \sqrt{\langle r_{\alpha\alpha}^2 \rangle} E_3|_B < \sqrt{\langle r_{\alpha\alpha}^2 \rangle} E_3|_A \), where the labels \( B \) and \( A \) correspond to Borromean and All-bound systems, respectively. For the same reasons that led to Eq. (6), it is also valid that \( \sqrt{\langle r_{\alpha}^2 \rangle} E_3|_B < \sqrt{\langle r_{\alpha}^2 \rangle} E_3|_A \). The zero-range model applied to atomic \( ^4\text{He}_3 \) provides a qualitative understanding of the radii results of realistic calculations for the ground and excited states \([10]\) with an estimation of \( \sqrt{\langle r_{\alpha\alpha}^2 \rangle} = C \sqrt{\hbar^2/m_\alpha (|E_3 - E_{\alpha\alpha}|)} \) with \( 0.6 < C < 1 \) \([6]\). Also the excited trimer state energy of \( ^4\text{He}_3 \), \( E_3^* \), has a scaling behavior written as

\[
\sqrt{|E_3^* - E_{\alpha\alpha}|} = \sqrt{|E_3|} E \left( \pm \sqrt{E_{\alpha\alpha}/E_3} \right), \tag{7}
\]

which is consistent with results from realistic calculations (see \([3, 9]\) and references therein). The threshold for the appearance of an excited Efimov trimer state from the second energy sheet is \( |E_3| = 6.9/a^2 \) \([9, 11]\) in units of \( \hbar = m_\alpha = 1 \). The scaling behavior was extended to the complex energy plane and for three-boson Borromean systems, the excited Efimov state turns into a resonance when the virtual two-boson virtual state energy is decreased \([12]\).
The generalization of the reasonings leading to Eq. (6) to the $\alpha\alpha\beta$ system gives the qualitative classification of the different three-body systems in respect to sizes. The effective interaction is weaker when a pair has a virtual state than when the pair is bound, and the three-body system has to shrink to keep the binding energy unchanged if a pair which is bound turns to be virtual. Therefore it is reasonable to expect that

$$\mathcal{R}_{\alpha\gamma} \left( -\sqrt{E_{\alpha\alpha}/E_3}, -\sqrt{E_{\alpha\beta}/E_3}, A \right) < \mathcal{R}_{\alpha\gamma} \left( \sqrt{E_{\alpha\alpha}/E_3}, -\sqrt{E_{\alpha\beta}/E_3}, A \right)$$

$$< \mathcal{R}_{\alpha\gamma} \left( -\sqrt{E_{\alpha\alpha}/E_3}, \sqrt{E_{\alpha\beta}/E_3}, A \right) < \mathcal{R}_{\alpha\gamma} \left( \sqrt{E_{\alpha\alpha}/E_3}, \sqrt{E_{\alpha\beta}/E_3}, A \right),$$

which was checked numerically [6]. An analogous relation is valid for $\mathcal{R}_c^{em}$. The dimensionless products (we are using units of $\hbar = m_\alpha = 1$) $\sqrt{\langle r^2_{\alpha\beta} \rangle |E_3|}$ and $\sqrt{\langle r^2_{\alpha\alpha} \rangle |E_3|}$ increase from Borromean, Tango, Samba and to All-Bound configurations, systematizing the classification scheme proposed in Ref. [5] for weakly bound three-body systems.

A three-body model applied to light exotic nuclei [6] compares qualitatively well with the existent experimental data for the neutron-neutron separation distance in the neutron-halo of $^{11}$Li and $^{14}$Be [7]. Therefore, the neutrons of the halo have a large probability to be found outside the interaction range and the low-energy properties of the halo are, to a large extend, universal as long as few physical input scales are fixed in the model. An insight into the structure of halo nuclei can be found even considering the limitations of the model. The finite size of the core and consequently the antisymmetrization of the total nuclear wave function, are both missing in this simplified description. However, in examples where the neutrons in the halo tend to be more and more weakly bound with virtual or bound subsystems near the scattering threshold, the scaling relations apply for the halo properties, as the above limitations are less important.

4 Classification of four-body halos and universal scalings

The four-boson system has two Faddeev-Yakubovsky (FY) independent amplitudes and within a zero-range model, they are reduced to spectator amplitudes depending on two Jacobi momenta. The two spectator FY reduced amplitudes satisfy a coupled set of integral equations generalizing the SKTM equation for three bosons. The set of coupled integral equations needs regularization, and one recognizes that the resolvent of the immersed three-boson subsystem carries the scale $\mu_3$. Other terms are present and require regularization. We introduce a scale $\mu_4$ such that the four-body free Green’s function $G_0(E_4)$ are substituted by $G_0(E_4) - G_0(-\mu_4^2)$ [13] in a direct generalization of Eq. (1) as suggested by [2].

The momentum scales in the FY equations for the reduced amplitudes are only $a^{-1}$, $\mu_3$ and $\mu_4$. In this case, the tetramer binding energy depends on the momentum scales as

$$E_4 = \mu_3^2 \overline{E}_4 (\mu_4/\mu_3, a\mu_3).$$

(9)
For $a = \infty$ the trimer binding energy from the solution of Eq. (1) is $E_3 = -0.0093\mu^2_3$ [9], which simplifies Eq. (9) remaining only the dependence on the ratio $\mu_4/\mu_3$ in $E_4$:

$$E_4 = E_3 \mathcal{E}_4 \left( \frac{\mu_4}{\mu_3} \right).$$

(10)

If $\mathcal{E}_4$ is independent on the regularization scale $\mu_4$ for $\mu_4/\mu_3 \gg 1$ the four-body scale is not important. We solved numerically the FY equations up to large values of $\mu_4/\mu_3 \sim 20$ [13].

The tetramer ground state binding energy was calculated for different values of the ratio $\mu_4/\mu_3$ with $a = \infty$. The ratio $E_4/E_3$ depends strongly $\mu_4/\mu_3$. For equal three and four-body scales, i.e., $\mu_4/\mu_3 = 1$, the tetramer binding energy is $E_4 = 5E_3$, agreeing with the angular coefficient of the Tjon line [14], $E_4 = 4.72(E_3 + 2.48)$ MeV ($E_4$ is the $^4$He energy and $E_3$ the triton one). Also, a recent calculation [15] of the four-boson system with a two-body zero-range force and a repulsive three-body potential to stabilize the trimer against collapse, $E_4$ scales as $\sim 5E_3$. Our result for $\mu_4 = \mu_3$ agrees with both. However, for $\mu_4/\mu_3 = 20$ we found that the ratio between the tetramer and trimer energies is about 78, indicating the independent effect of the four-body scale.

The present results suggest that the general scaling of S-wave three-boson observables with the physical scales, Eq. (2), may be generalized to four-boson S-wave observables. The effect of the short-range dynamics in an observable comes through the values of the scattering length, trimer and tetramer binding energies, associated with $\mu_3$ and $\mu_4$, respectively. In this case, a S-wave four-boson observable will be strongly correlated to $a$, $E_3$ and $E_4$:

$$O_4(E, E_4, E_3, a) = |E_4|^\eta \mathcal{F}_4 \left( \frac{E}{E_4}, \frac{E_3}{E_4}, a\sqrt{|E_4|} \right),$$

(11)

where $O_4$ represents either a scattering amplitude at energy $E$, or an excited tetramer energy or some observable related to the tetramer (the dependence on $E$ does not appear in these cases). The exponent $\eta$ gives the correct dimension to $O_4$. For sizes one could think that the relation

$$R_{\alpha\alpha} \left( \sqrt{E_3/E_4}, -\sqrt{E_{\alpha\alpha}/E_4} \right) < R_{\alpha\alpha} \left( \sqrt{E_3/E_4}, \sqrt{E_{\alpha\alpha}/E_4} \right),$$

(12)

and the analogous for the distances of the particles to the center of mass would be valid. This indicates that is possible to envisage a generalized classification scheme based on sizes including weakly-bound four-body systems.

5 Outlook and Conclusions

The classification scheme of large halos formed by two identical particles and a core is reviewed and addressed systematically according to their sizes. The root-mean-square distances between the constituents are described by universal scaling functions. For a given three-body system and total energy, the Borromean configuration is the most compact. Applications to halo nuclei, $^{11}$Li and $^{14}$Be, and for atomic $^4$He$_3$ were briefly discussed.
The generalization of these concepts to four-body systems is proposed. We have shown that for a zero-range two-body interaction with an infinite scattering length and a fixed trimer ground state binding energy, a four boson momentum scale is evidenced in the calculation of tetramer binding energies in three-dimensions. The intensity of the effective interaction that composes the kernel of the reduced FY spectator equations depends on the dimer energy and trimer, therefore it is reasonable that a tetramer becomes more compact for a given four-body energy if the two and three-body binding are decreased. This effect indicates that it may be possible to generalize the classification scheme of weakly-bound three-body systems to four-body systems.

Acknowledgement. We thank the Brazilian funding agencies FAPESP and CNPq.

References

Variational Description of Bound States in Three- and Four-Nucleon Systems

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Abstract.

The hyperspherical harmonic basis is used to describe the bound states of the three and four nucleon systems. Modern nucleon-nucleon potentials plus three-nucleon interactions are considered in configuration space as well as in momentum space. The corresponding binding energies have been calculated with accuracy at the level of 1% or better. The convergence with respect to the number of states included in the expansion is much faster for the momentum space than for the momentum space potentials, due to a less repulsive core at short distances.

1 Introduction

The hyperspherical harmonic (HH) basis including correlation factors has been used to describe the $A = 3, 4$ nuclei considering modern nucleon–nucleon (NN) potentials plus three-nucleon forces[1, 2, 3]. The inclusion of correlation factors accelerates the convergence of the expansion since improves the description of the short range part of the wave function. The HH basis has also been used without the inclusion of correlation factors, showing the necessity of a very large basis in order to obtain a converged result for the binding energy[4, 5]. Here we explore the different rate of convergence of the uncorrelated HH expansion obtained using configuration space or momentum space potentials[6].

2 The three– and four–nucleon bound states using the Hyperspherical Harmonic basis

For four equal mass particles we can choose the following Jacobi coordinates:

$$z_p = \sqrt{\frac{3}{2}} \left( \frac{r_j + r_k + r_i}{3} - r_m \right)$$

1

---

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\[
\begin{align*}
\mathbf{y}_p & = \sqrt{\frac{4}{3}(\mathbf{r}_j + \mathbf{r}_k - \mathbf{r}_i)} \quad (2) \\
\mathbf{x}_p & = \mathbf{r}_j - \mathbf{r}_k, \quad (3)
\end{align*}
\]

where \( p \) specifies a given permutation corresponding to the order \( i, j, k, m \) of the particles. For four particles there are 12 even permutations whereas for three particles there are 3 even permutations and only the last two Jacobi vectors \( x_p, y_p \) exist.

The hyperspherical coordinates are given by the hyperradius \( \rho = \sqrt{x_p^2 + y_p^2 + z_p^2} \), which is independent of the permutation \( p \), and two hyperspherical angles defined from the relations

\[
\begin{align*}
x_p & = \rho \cos \theta_{1p} \quad (4) \\
y_p & = \rho \sin \theta_{1p} \cos \theta_{2p} \quad (5) \\
z_p & = \rho \sin \theta_{1p} \sin \theta_{2p}. \quad (6)
\end{align*}
\]

For three particles the hyperradius is \( \rho = \sqrt{x_p^2 + y_p^2} \) and there is only one hyperangle defined from the relations \( x_p = \rho \cos \theta_p, y_p = \rho \sin \theta_p \). The wave functions corresponding to the \( A = 3, 4 \) bound states can be written as a sum of amplitudes depending of the permutation \( p \) of the Jacobi coordinates

\[
\begin{align*}
\Psi_3 &= \sum_{p=1,3} \psi(x_p, y_p), \quad \Psi_4 = \sum_{p=1,12} \psi(x_p, y_p, z_p). \quad (7)
\end{align*}
\]

Each amplitude has total angular momentum \( JJ_z \), total isospin \( TT_z \) and definite parity. Using the \( LS \) coupling it is decomposed in partial wave amplitudes

\[
\psi(x_p, y_p, z_p) = \sum_{\alpha} \phi_{\alpha}(x_p, y_p, z_p) Y_{\alpha}^{(A)}(\Omega_p), \quad (8)
\]

and similarly for \( A = 3 \). Here \( \alpha \) denotes a channel and is a set of quantum numbers needed to specify the angular-spin-isospin function \( Y_{\alpha}^{(A)} \). \( N_c \) is the maximum number of channels considered. The set of hyperangular variables \( \Omega_p \) corresponds to \( \Omega_p \equiv [\theta_1, \theta_2, \hat{x}, \hat{y}, \hat{z}] \) in the case of \( A = 4 \) and reduces to \( \Omega_p \equiv [\theta, \hat{x}, \hat{y}] \) in the case of \( A = 3 \).

The two- and three-dimensional amplitudes \( \phi_{\alpha} \) can be expanded in terms of the HH basis and the final form for the \( A = 3, 4 \) bound state wave functions can be put in the form\cite{4, 5}

\[
\Psi_A = \rho^{-(3A-4)/2} \left[ \sum_{\alpha=1}^{N_c} \sum_{[K]} u_{[K]}^{\alpha}(\rho) B_{[K]}^{\alpha}(\Omega_A) \right], \quad (9)
\]

where \( B_{[K]}^{\alpha}(\Omega_A) \) is a complete antisymmetric spin-isospin HH function for \( A = 3, 4 \) and \([K]\) denotes a set of quantum numbers that define a HH basis element with \( K \) the grand angular quantum number. In general the hyperradial functions
can be expanded in a complete basis, as for example, Laguerre polynomials multiplied by an exponential factor

\[ u_{\alpha[K]} = \sum_{m} A_{m[K]}^{\alpha} L_{m}^{(n)}(\beta \rho) \ e^{-\beta \rho} \]  

(10)

with \( \beta \) a nonlinear parameter and \( n = 5, 8 \) for \( A = 3, 4 \). Therefore it is possible to define an antisymmetric basis element \( |\alpha m[K]\rangle \) and the description of the \( A = 3, 4 \) bound state can be obtained solving the following generalized problem

\[ \sum_{\alpha, m[K]} A_{m[K]}^{\alpha} \langle \alpha' m' [K'||H - E]|\alpha m[K]\rangle = 0 \]  

(11)

It is important to note that representation of the basis element \( |\alpha m[K]\rangle \) can be given in momentum space as well[6].

3 Results

In this section we present results obtained using the HH expansion for the \( A = 3, 4 \) systems described using modern NN potentials with and without the inclusion of three-nucleon forces. The NN configuration space potential of Argonne \( v_{18} \) (AV18)[7] has been considered as well as the momentum space potentials of CD-Bonn[8] and N3LO[9]. The three body force of Urbana (URIX)[10] has been added to the AV18 NN potential in the \( A = 3 \) case. The results for the binding energy, mean value of the kinetic energy and occupation probabilities of the \( P \) and \( D \) states are collected in Table 1 and compared to those obtained by other techniques as the solutions of the Faddev equations (FE) and the Faddeev-Yakubovsky (FY) equations in momentum space[11, 12] or configuration space[13], the Green Function Monte Carlo (GFMC) method[14] and the no-core shell model (NCSM) approach[15] for \( A = 4 \).

The last column of Table 1 shows the maximum grand angular quantum number \( K \) used to truncate the expansion using the criterion of a converged value for the binding energy within 1 KeV for \( A = 3 \) and 10 keV for \( A = 4 \). For \( A = 3 \) all antisymmetric HH basis states have been included up to the maximum \( K \) considered. For \( A = 4 \) a selection of the antisymmetric HH states has been made as explained in Ref.[4]. In this case the final number of HH states considered was around 8000 for AV18, 3000 for CD-Bonn and 1200 for N3LO. It is interesting to note that the non-local potentials have a much faster convergence due to a less repulsive core in the short range region, in particular the N3LO potential. This observation suggests the possibility of an extension of the HH expansion to describe heavier systems without encounter severe convergence problems.

References

### Table 1. The HH results for binding energies, mean values of the kinetic energy and occupation probabilities obtained with different potential models are compared to different techniques.

<table>
<thead>
<tr>
<th>Potential</th>
<th>Method</th>
<th>(B) (MeV)</th>
<th>(T) (MeV)</th>
<th>(P_P) (%)</th>
<th>(P_D) (%)</th>
<th>(K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(A = 3)</td>
<td>AV18</td>
<td>HH</td>
<td>7.624</td>
<td>46.73</td>
<td>0.066</td>
<td>8.51</td>
</tr>
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<td></td>
<td>FE[11]</td>
<td>7.621</td>
<td>46.73</td>
<td>0.066</td>
<td>8.51</td>
<td></td>
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<tr>
<td></td>
<td>CD-Bonn</td>
<td>HH</td>
<td>7.998</td>
<td>37.63</td>
<td>0.047</td>
<td>7.02</td>
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<td></td>
<td>FY[12]</td>
<td>7.997</td>
<td>37.62</td>
<td>0.047</td>
<td>7.02</td>
<td></td>
</tr>
<tr>
<td></td>
<td>N3LO</td>
<td>HH</td>
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<td>34.55</td>
<td>0.037</td>
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<td>FY[12]</td>
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<td>(A = 4)</td>
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<td>HH</td>
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<td>97.84</td>
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<td>13.74</td>
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<td>97.77</td>
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<td>GFMC[14]</td>
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<td>110.7(7)</td>
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<td>NCSM[15]</td>
<td>25.36</td>
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</tr>
</tbody>
</table>

How To Classify 3-Body Forces – And Why∗

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Abstract. For systems with only short-range forces and shallow 2-body bound states, the typical strength of any 3-body force in all partial-waves, including external currents, is systematically estimated by renormalisation-group arguments in the Effective Field Theory of Point-Like Interactions. The underlying principle and some consequences in particular in Nuclear Physics are discussed. Details and a better bibliography in Ref. [1].

1 Introduction

The Effective Field Theory (EFT) of Point-Like Interactions is a model-independent approach to systems without infinite-range forces in Atomic, Molecular and Nuclear Physics at very-low energies with shallow real or virtual 2-body bound-states (“dimers”), see e.g. [2, 3] for reviews. When the size or scattering length \(a\) of a 2-body system is much larger than the size (or interaction range) \(R\) of the constituents, a small, dimension-less parameter \(Q = \frac{R}{a}\) allows to classify the typical size of neglected corrections at \(n\)th order beyond leading order (\(N^\infty\)LO) as about \(Q^n\). For example, \(a \approx 104\ \text{Å} \) and \(R \approx 10\ \text{Å}\) in the \(^4\text{He}_2\) molecule, i.e. \(Q \approx \frac{1}{10}\), while \(a \approx 4.5\ \text{fm}\) and \(R \approx 1.5\ \text{fm}\) in the deuteron, i.e. \(Q \approx \frac{1}{3}\) in the “pion-less” EFT, EFT(\(\#\)), where pion-exchange between nucleons is not resolved as non-local. Thus, the detailed dynamics on the “high-energy” scale \(R\) can vary largely: For example, attractive van-der-Waals forces \(\propto \frac{1}{r^6}\) balance in \(^4\text{He}_2\) a repulsive core generated by QED; but in Nuclear Physics, one-pion exchange \(\propto \frac{1}{r^{1-3}}\) is balanced by a short-range repulsion whose origin in QCD is not yet understood. It is a pivotal advantage of an EFT that it allows predictions of pre-determined accuracy without such detailed understanding – as long as one is interested in low-energy processes, i.e. Physics at the scale \(a\), and not \(R\). Even when possible (as in QED – at least at scales \(\geq 1\ \text{fm}\)), EFTs reduce numerically often highly involved computations of short-distance contributions to low-energy

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observables by encoding them into a few simple, model-independent constants of contact interactions between the constituents. These in turn can be determined by simpler simulations of the underlying theory, or — when they are as in QCD not (yet) tenable — by fit to data. Universal aspects of few-body systems with shallow bound-states are manifest in EFTs, with deviations systematically calculable. In 2-body scattering for example, the EFT of Point-Like Interactions reproduces the Effective-Range Expansion, but goes beyond it in the systematic, gauge-invariant inclusion of external currents, relativistic effects, etc.

Take 3-body forces (3BFs): They parameterise interactions on scales much smaller than what can be resolved by 2-body interactions, i.e. in which 3 particles sit on top of each other in a volume smaller than $R^3$. Traditionally, they were often introduced \textit{a posteriori} to cure discrepancies between experiment and theory, but such an approach is of course untenable when data are scarce or 1- and 2-body properties should be extracted from 3-body data. But how important are 3BFs in observables? The classification in EFTs rests on the tenet that a 3BF is included if and only if necessary to cancel cut-off dependences in low-energy observables. I outline this philosophy and its results in the following, finding that — independent of the underlying mechanism — 3BFs behave very much alike in such disparate systems as molecular trimers and 3-nucleon systems, but do not follow simplistic expectations.

2 Construction

In the Faddeev equation of particle-dimer scattering without 3BFs, Fig. 1, the S-wave 2-body scattering amplitude is given by the LO-term of the Effective-Range Expansion. This dimer and the remaining particle “interact” via $\mathcal{K}_l$, the one-particle propagator projected onto relative angular momentum $l$. Even for small relative on-shell momenta $k$ between dimer and particle, we need the scattering amplitude $t^{(l)}_{\lambda}(p)$ for all off-shell momenta $p$ to determine its value at the on-shell point $p = k$, and hence in particular for $p$ beyond the scale $\frac{1}{a}$ on which a description in terms of point-like constituents is tenable. It is therefore natural to demand that all low-energy observables on a scale $k \sim \frac{1}{a}$ are insensitive to details of the amplitude at $p \gg \frac{1}{R}$, namely to form and value of the regulator, form-factor or cut-off chosen. If not, a 3BF must soak up the dependence. In an EFT, this is the fundamental tenet: Include a 3BF \textit{if and only if} it is needed as counter-term to cancel divergences which can not be absorbed by renormalising 2-body

![Figure 1](image-url)
interactions. Thus, only combinations of 2- and 3BFs are physically meaningful. With the cut-off variation of the 3BF thus fixed, the initial condition leads to one free parameter fixed from a 3-body datum or knowledge of the underlying physics. 3BFs are thus not added out of phenomenological needs but to guarantee that observables are insensitive to off-shell effects.

A Mellin transformation \( t_\lambda^{(l)}(p) \propto p^{-s_\lambda(\lambda)^{-1}} \) solves the equation for \( p \gg k, \frac{1}{a} \).

The spin-content is then encoded only in the homogeneous term: \( \lambda = -\frac{1}{2} \) for 3 nucleons with total spin \( \frac{3}{2} \), or for the totally spin and iso-spin (Wigner-)antisymmetric part of the spin-\( \frac{1}{2} \)-channel; \( \lambda = 1 \) for 3 identical spin-less bosons and the totally spin and iso-spin (Wigner-)symmetric part of the spin-\( \frac{1}{2} \)-channel. The asymptotic exponent \( s_\lambda(\lambda) \) has to fulfil \( \text{Re}[s] > -1 \), \( \text{Re}[s] \neq \text{Re}[l \mp 2] \), and

\[
1 = (-1)^l \frac{2^{1-l} \lambda}{\sqrt{3\pi}} \frac{\Gamma\left[\frac{l+s+1}{2}\right]}{\Gamma\left[\frac{2l+3}{2}\right]} \frac{\Gamma\left[\frac{l-s+1}{2}\right]}{\Gamma\left[\frac{2l-1}{2}\right]} \, _2F_1\left[\frac{l+s+1}{2}, \frac{l-s+1}{2}; \frac{2l+3}{2}; \frac{1}{4}\right].
\] (1)

This result was first derived in the hyper-spherical approach by Gasaneo and Macek \[4\]. The asymptotics depends thus only but crucially on \( \lambda \) and \( l \). Relevant in the UV-limit are the solutions for which \( \text{Re}[s + 1] \) is minimal.

At first glance, we would expect the asymptotics to be given by the asymptotics of the inhomogeneous (driving) term: \( t_\lambda^{(l)}(p) \propto \frac{k^l}{p^{l+2}} \), i.e. \( s_\lambda(\lambda) \equiv l + 1 \). However, we must sum an infinite number of graphs already at leading order. As Fig. 2 shows, this modifies the asymptotics considerably.

![Figure 2](image_url)

**Figure 2.** The first two solutions \( s_\lambda(\lambda) \) at \( \lambda = 1 \) (left) and \( \lambda = -\frac{1}{2} \). Solid (dotted): real (imaginary) part; dashed: simplistic estimate. Dark/light: first/second solution. Limit cycle and Efimov effect occur only when the solid line lies below the dashed one, and \( \text{Im}[s] \neq 0 \).

How sensitive are higher-order corrections to the UV-behaviour of \( t_\lambda^{(l)}(p) \)? The 2-body scattering-amplitude is systematically improved by including the effective range, higher partial waves etc. Corrections to 3-body observables (including partial-wave mixing) are found by perturbing around the LO solution as in Fig. 1. Most sensitive to unphysically high momenta is each correction at \( N^\text{LO} \) which is proportional to the \( n \)th power of loop momenta. The question when it becomes cut-off sensitive is now rephrased as: When does the correction diverge as the

\[\text{My apologies to the authors that I found this reference only after [1] was published.}\]
cut-off is removed, i.e. when is its \textit{superficial degree of divergence} non-negative? The answer by simply counting loop momenta in the diagram:

\[
\text{Re}[\mu - s_l(\lambda) - s_{l'}(\lambda')] \geq 0 . \tag{2}
\]

We therefore find at which order the first 3BF is needed just by determining when a correction to the 3-body amplitude with only 2-body interactions becomes dependent on unphysical short-distance behaviour.

It is instructive to re-visit these findings in position space. The Schrödinger equation for the wave-function in the hyper-radial dimer-particle distance \(r\),

\[
\left[ -\frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{s_l^2(\lambda)}{r^2} - ME \right] F(r) = 0 , \tag{3}
\]

looks like the one for a free particle with centrifugal barrier. One would thus expect \(s_l = l + 1\) (hyper-spherical co-ordinates!). It had however already been recognised by Minlos and Faddeev that the centrifugal term is for three bosons (\(\lambda = 1\)) despite expectations attractive, so that the wave-function collapses to the origin and seems infinitely sensitive to very-short-distance physics. In order to stabilise the system against collapse – or, equivalently, remove dependence on details of the cut-off –, a 3BF must be added – or, equivalently, a self-adjoint extension be specified at the origin i.e. a boundary condition for the wave-function must be fixed by a 3-body datum. On the other hand, 3BFs are demoted if \(s_l > l + 1\): The centrifugal barrier provides more repulsion than expected, and hence the wave-function is pushed further out, i.e. less sensitive to details at distances \(r \lesssim R\) where the constituents are resolved as extended. Birse confirmed this recently by a renormalisation-group analysis in position-space \([5]\).

3 Consequences

About half of the 3BFs for \(l \leq 2\) are weaker, half stronger than one would expect simplistically, see Table 1. The higher partial-waves follow expectation, as the Faddeev equation is then saturated by the Born approximation. The S-wave 3BF of spin-less bosons is stronger, while the P-wave 3BF is weaker.

That the first S-wave 3BF appears already at LO, first described by Bedaque, Hammer and van Kolck, leads to a new renormalisation-group phenomenon, the “limit-cycle”. It explains the Efimov and Thomas effects, and universal correlations e.g. between particle-dimer scattering length and trimer binding energy (the Phillips line), see the reviews \([2, 3]\). In general, it appears whenever the kernel of the integral equation not compact, i.e. \(\text{Im}[s] \neq 0\) and \(|\text{Re}[s]| < \text{Re}[l+1]|.\) We finally note that the power-counting requires a new, independent 3BF with 2\(l\) derivatives to enter at \(N^2\)LO and provides high-accuracy phase-shifts in atom-dimer and nucleon-deuteron scattering, and loss rates close to Feshbach resonances in Bose-Einstein condensates, see e.g. \([2, 3, 6]\) for details.

Demotion might seem an academic dis-advantage – to include some higher-order corrections which are not accompanied by new divergences does not improve the accuracy of the calculation; one only appears to have worked harder
Table 1. Order of the leading 3BF in particle-dimer scattering, indicating if actual values from eqs. (1/2) are stronger (“prom.”) or weaker (“dem.”) than the simplistic estimate. Last column: typical size of 3BF in EFT(\(\pi\)), in parentheses size from the simplistic estimate.

<table>
<thead>
<tr>
<th>partial-wave: in–out</th>
<th>bosons</th>
<th>fermions</th>
<th>naive dim. analysis (\Re[s_i(\lambda) + s_v(\lambda')])</th>
<th>simplistic (l + l' + 2)</th>
<th>typ. size if (Q^n \sim \frac{1}{L})</th>
</tr>
</thead>
<tbody>
<tr>
<td>S–S</td>
<td>2S–2S</td>
<td>(N^2)LO</td>
<td>(N^4)LO</td>
<td>prom.</td>
<td></td>
</tr>
<tr>
<td>2S–4D</td>
<td>(\lambda)</td>
<td>(N^4)LO</td>
<td>prom.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>P–P</td>
<td>2P–2P</td>
<td>(N^{\ast})LO</td>
<td>(N^4)LO</td>
<td>dem.</td>
<td></td>
</tr>
<tr>
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<td>(N^4)LO</td>
<td>(N^4)LO</td>
<td>dem.</td>
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<tr>
<td>2P–4P</td>
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<td>(N^4)LO</td>
<td>dem.</td>
<td></td>
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</tr>
<tr>
<td>2P–2P</td>
<td>(N^4)LO</td>
<td>(N^4)LO</td>
<td>dem.</td>
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<tr>
<td>4S–2S</td>
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<td>(N^4)LO</td>
<td>dem.</td>
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<td>4S–2D</td>
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<td>(N^4)LO</td>
<td>dem.</td>
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<td>4S–4D</td>
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<td>(N^4)LO</td>
<td>dem.</td>
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<td>higher</td>
<td>(\sim) as simplistic</td>
<td>(N^4)LO</td>
<td>(\sim) as simplistic</td>
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</table>

The cross-section of triton radiative capture \(nd \rightarrow t\gamma\) at thermal energies provides another example [7]. Nuclear Models give a spread of [0.49 . . . 0.66] mb, depending on the 2-nucleon potential, and how the \(\Delta(1232)\) as first nucleonic excitation is included. On the other hand, a process at 0.0253 eV [sic] incident neutron energy and less than 7 MeV photon energy should be insensitive to

\[
a(4S_\frac{1}{2}) = [5.09(LO) + 1.32(NLO) - 0.06(N^2LO)] \text{ fm} = [6.35 \pm 0.02] \text{ fm} , \quad (4)
\]

(here taken from [6]), it converges nicely at \(N^2\)LO and agrees very well with experiment, \(6.35 \pm 0.02\) fm. The theoretical accuracy by neglecting higher-order terms is here estimated conservatively by \(Q \approx \frac{1}{4}\) of the difference between the NLO- and \(N^2\)LO-result. Table 1 predicts that the first 3BF enters not earlier than \(N^4\)LO. Indeed, if the theoretical uncertainty continues to decreases steadily as from NLO to \(N^2\)LO, an accuracy of \(\pm (\frac{1}{3})^3 \times 0.02 \text{ fm} \lesssim \pm 0.001 \text{ fm}\) with input only from 2-nucleon scattering can be reached in calculations. This is comparable to the range over which modern high-precision potential-model calculations differ: \([6.34 \ldots 6.347]\) fm. If the 3BF would occur at \(N^4\)LO as simplistically expected, the error by 3BFs would be \((\frac{1}{3})^1 \times 0.02 \text{ fm} \approx 0.007 \text{ fm}\), considerably larger than the spread in the potential-model predictions. Differential cross-sections and partial-waves are also in excellent agreement with much more elaborate state-of-the-art potential model calculations at energies up to 15 MeV, see e.g. [6].
details of the deuteron wave-function and of a resonance with an excitation energy of 300 MeV. Indeed, the power-counting of 3BFs applies equally with external currents, only that the higher-order interaction in Fig. 1 includes now also the momentum- or energy-transfer from the external source as additional low-energy scales. As no new 3BFs are needed up to $N^2$LO to render cut-off independence, the result is completely determined by simple 2-body observables:

$$\sigma_{\text{tot}} = [0.485(\text{LO}) + 0.011(\text{NLO}) + 0.007(N^2\text{LO})] \text{ mb} = [0.503 \pm 0.003]\text{ mb} \quad (5)$$

It converges and compares well with the measured value, $[0.509 \pm 0.015]\text{ mb}$. The cross-section relevant for big-bang nucleo-synthesis ($E_n \approx 0.020 \ldots 0.4 \text{ MeV}$) is also in excellent agreement with data [8].

### 4 Conclusions

With these findings, the EFT of 3-body systems with only contact interactions is a self-consistent, systematic field theory which contains the minimal number of interactions at each order to render the theory renormalisable. Each 3-body counter-term gives rise to one subtraction-constant which is fixed by a 3-body datum. Table 1 sorts the 3BFs by their strengths, their symmetries and the channels in which they contribute at the necessary level of accuracy. Amongst the host of applications in Nuclear Physics are triton and $^3\text{He}$ properties, reactions in big-bang nucleo-synthesis, neutrino astro-physics, the famed nuclear $A_y$-problem, and the experimental determination of fundamental neutron properties.

The method presented here is applicable to any EFT in which an infinite number of diagram needs to be summed at LO, e.g. because of shallow-bound states. One example is Chiral EFT, the EFT of pion-nucleon interactions. Only those local $N$-body forces are added at each order which are necessary as counter-terms to cancel divergences at short distances. This mandates a careful look at the ultraviolet-behaviour of the leading-order, non-perturbative scattering amplitude. It leads at each order and to the prescribed level of accuracy to a cut-off independent theory with the smallest number of experimental input-parameters. The power-counting is thus not constructed by educated guesswork but by rigorous investigations of the renormalisation-group properties of couplings and observables using the methodology of EFT.

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### References

5. M. C. Birse, nucl-th/0509031.

On the uniqueness of the solution to the three-body problem with zero-range interactions*

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Abstract. We consider uniqueness of the solution to a three-body problem with zero-range Skyrme interactions in configuration space. With the lowest, \( k^0 \), two-body term alone the problem is known to have no unique solution as the system collapses – the variational estimate of the energy tends towards negative infinity, the size of the system towards zero. We argue that the next, \( k^2 \), two-body term removes the collapse and the three-body system acquires finite ground state energy and size. The three-body interaction term is thus not necessary to provide a unique solution to the problem.

Introduction. The zero-range interaction is an approximation to a short-range interaction in the case when the range of the interaction is significantly less than the typical wavelength of interest. Zero-range interactions have a long history in nuclear physics where they have been used in the form of the effective-range theory [1] where the short-range potential is substituted by a boundary condition at zero, and also in the form of Skyrme \( \delta \)-function interaction [2] used in the variational Skyrme-Hartree-Fock calculations of nuclei [3]. The Skyrme-Hartree-Fock approach has also been applied to bosonic atomic systems in the form of Gross-Pitaevskii equation [4].

Recently the zero-range model has also been reformulated in momentum space using the language of the effective field theory where the Lagrangian is represented as a series in terms of powers of the typical (low) momentum involved in the problem [5]. While extending the theory from two to three-body systems it turned out that due to the Thomas effect [6] the lowest order theory generally does not provide a unique solution. It appears that a three-body datum is necessary as an input for the theory to provide a unique solution to the three-body problem under constraints of EFT power counting [7, 8].

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However, there is a different view, formulated both in momentum [9] and coordinate space [10], that an additional two-body datum, e.g. the effective range, can as well provide a unique solution to the three-body problem with zero-range interactions. The three-body datum will then be a prediction of the theory, rather than its input. The asymptotic large-distance properties of the three-body solution are independent on whether a three- or a two-body datum is used to ensure its uniqueness.

In configuration space it has been shown that for the boundary-condition formulation of the zero-range interaction the effective-range term removes the Thomas collapse and provides a unique solution to the three-body problem [10]. We consider here another formulation of zero-range interaction in coordinate space, the Skyrme interaction model, and argue that in this model too the $k^2$ two-body term provides a unique solutions to the three-body problem.

**Skyrme interaction.** The Skyrme interaction [2] is a formulation of the zero-range model in configuration space, which explicitly contains $\delta$-functions and is designed to be used in variational calculations. A typical two-body interaction is

$$v(r) = t_0\delta(r) + t_1\left(\overrightarrow{k^2}\delta(r) + \delta(r)\overrightarrow{k}\right) + t_2\overrightarrow{k}^*\delta(r)\overrightarrow{k}, \quad (1)$$

where $t_0$, $t_1$, $t_2$ are the parameters of the model, $\overrightarrow{k} = -i\frac{\partial}{\partial r}$, and the left (right) arrow above the differential operator indicates that in the matrix element the operator acts on the left (right).

The idea of this approximation is that the matrix elements of the Skyrme potential between some smooth functions with the typical length parameter $\lambda$ should reproduce the lowest terms of the Taylor expansion of the corresponding matrix elements of the short-range potential in the small parameter $\frac{k^0}{\lambda} \ll 1$, where $r_0$ is the range of the short-range potential.

For example, the matrix element of the Skyrme potential (1) between plane waves is

$$\left< e^{ik'r} \left| v(r) \right| e^{ikr} \right> = t_0 + t_1(k^2 + k') + t_2 \overrightarrow{k}^*\overrightarrow{k} \quad (2)$$

The corresponding matrix element of a short-range potential $V(r)$ with the range $r_0$ in the limit $kr_0, k'r_0 \ll 1$ has the same form,

$$\left< e^{ik'r} \left| V(r) \right| e^{ikr} \right> \approx \int d^3r \left(1 - \frac{1}{2}\left[(\overrightarrow{k} - \overrightarrow{k'})^2\right]\right) V(r) = \quad (3)$$

$$= V_0 + V_1(k^2 + k^2) + V_2\overrightarrow{k}^*\overrightarrow{k} \quad (4)$$

where

$$V_0 = \int d^3r V(r), \quad V_1 = \frac{1}{2}V_2 = -\frac{1}{2}\int d^3r V(r)r^2 \cos^2\theta \quad (4)$$

The two-body Skyrme forces (1) can be supplemented by a three-body force

$$t_3\delta(r_1 - r_2)\delta(r_2 - r_3), \quad (5)$$

which provides a representation of many-body effects where the two-body interaction is modified in the presence of a third body. Although the three-body force improves the flexibility of the model by providing another free parameter, we shall show that it is not necessary to stabilize the system.
Variational estimate of the energy. Let us consider a system of three identical bosons with mass $m$ and coordinates $r_1, r_2, r_3$ interacting via the Skyrme interaction (1). This is the hardest case as the bosonic systems collapse much easier than the corresponding fermionic systems due to the absence of the positive pressure of the degenerate fermionic gas.

We shall concentrate on the relative motion which can be conveniently described by the relative Jacobi coordinates

$$x_i = \frac{1}{\sqrt{2}} (r_j - r_k), \quad y_i = \sqrt{\frac{2}{3}} \left( \frac{1}{2} (r_j + r_k) - r_i \right),$$

where $i, j, k$ is a cyclic permutation of $1, 2, 3$. In the following if the index of a Jacobi coordinate is omitted then any of the three can be equally well used.

The Hamiltonian of the system is

$$H = K + \sum_{i<j=1}^3 v(r_i - r_j), \quad K = \left( -\frac{\hbar^2}{2m} \right) \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right).$$

For the variational trial functions we shall use many-body Gaussians which provide a very flexible basis for many-body variational calculations [11].

First let us consider an uncorrelated Gaussian,

$$\Psi = e^{-\frac{1}{2} \alpha (x^2 + y^2)},$$

where $\alpha$ is the variational parameter with the dimension of length.

The expectation values of the different terms of the Hamiltonian (7) with this trial function are

$$\langle K \rangle = 3 \frac{\hbar^2}{2m} \alpha, \quad \left\langle \sum_{i<j=1}^3 t_0 \delta(r_{ij}) \right\rangle = 3t_0 \left( \frac{\alpha}{2\pi} \right)^{3/2},$$

$$\left\langle \sum_{i<j=1}^3 t_1 \left( -\frac{\partial^2}{\partial r_{ij}^2} \right) \delta(r_{ij}) + \delta(r_{ij}) \left( -\frac{\partial^2}{\partial r_{ij}^2} \right) \right\rangle = 12t_1 \alpha \left( \frac{\alpha}{2\pi} \right)^{3/2}.$$

The Skyrme $t_2$ force does not give a contribution with the function (8).

If only the kinetic energy ($\propto \alpha$) and an attractive $t_0$ force ($\propto t_0 \alpha^{3/2}$) are included in the model, the system collapses as the expectation energy diverges towards $-\infty$ at infinitely small distances, $\alpha \to \infty$.

However, a repulsive $t_1$-force, being one power of $\alpha$ stronger than the $t_0$-force, will apparently stabilize the system and provide a finite minimum of the expectation energy at finite $\alpha$.

Correlations. Let us check now that inclusion of correlations does not change our observation that the repulsive $t_1$-term can outweigh the attractive $t_0$-term for large $\alpha$. The fully correlated three-body Gaussian function is

$$\Psi = e^{-\frac{1}{2} \alpha x^2 - \beta xy - \frac{1}{2} \gamma y^2},$$
where $\alpha, \beta, \gamma$ are variational parameters satisfying the conditions $\alpha, \gamma > 0$, $\alpha \gamma - \beta^2 > 0$. The matrix element of the $t_0$-term with this correlated function is

$$\langle t_0 \delta(\sqrt{2x}) \rangle = t_0 \left( \frac{1}{2\pi} \frac{\alpha \gamma - \beta^2}{\gamma} \right)^{3/2}.$$  \hspace{1cm} (11)

The $t_1$-term has an additional factor $4\alpha$. The $t_0$-term can only be large in the limit $\alpha \to \infty$. In this limit, however, we recover the uncorrelated case – the $t_1$-term is one power of $\alpha$ higher than the $t_0$-term, and thus again the $t_1$-term wins over the $t_0$-term.

**Conclusion.** We have considered a system of three bosons with zero-range interaction in the form of the Skyrme potentials using the variational method with correlated Gaussians. The attractive $k^0$-term induces a collapse of the system – the ground state energy becomes infinitely large and the size of the system becomes infinitely small.

We have shown that the repulsive $k^2$ two-body term removes the collapse and provides a unique solution with finite ground-state energy and finite size of the system. This lends support to the point of view that for a three-body system with the zero-range interactions the three-body term is generally not necessary for the problem to have a unique solution.

**References**

Borromean bound states

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Abstract. The Hall–Post inequalities relating \(N\)-body to \((N - 1)\)-body energies of quantum bound states are applied to delimit, in the space of coupling constants, the domain of Borromean binding where a composite system is bound while the smaller subsystems are unbound.

1 Introduction

It is hardly necessary in front of this audience of the Workshop on “Critical Stability” to stress the importance of states at the edge between stability and instability. Two-body systems such as proton–proton, proton–neutron, \(D - D^*\) (a charmed meson and the spin excitation of its antiparticle), \(^4\text{He} - ^4\text{He}\) or \(^4\text{He} - ^3\text{He}\) are either tinily bound or miss binding by a small margin.

An intriguing question is whether it is easier to bind three or more components than to form a mere two-body bound state. An answer is provided by the study of halo nuclei, which contain peripheral neutrons. Consider for instance the \(^6\text{He}\) nucleus. It is stable against any dissociation, while the lighter \(^5\text{He}\) spontaneously decays into a neutron and a \(^4\text{He}\). In the (reasonable) approximation where the structure of the core is neglected, this means that the \((\alpha, n, n)\) three-body system is bound, while neither the \((\alpha, n)\) nor the \((n, n)\) has a discrete spectrum.

This property of 3-body binding without 2-body binding was astutely named Borromean [1], after the Borromean rings, which are interlaced in a subtle topological way (see the logo of the Workshop in Fig. 1) such that if any one of them is removed, the two other become unlocked. The adjective Borromean is nowadays broadly accepted in the field of quantum few-body systems.

Borromean binding is intimately related to two other fascinating properties of few-body quantum systems. The Efimov effect [2] indicates that when the two-body energy vanishes (e.g., by tuning the strength of the potential), a myriad of weakly-bound states

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Figure 1. Borromean rings

show up in the three-body spectrum. This implies that the three-body ground-state already exists at this point. Slightly above the onset of two-body binding, the ratio \( E_2/E_3 \) of two-body to three-body binding energies is very small. By rescaling, one can reach a situation with a finite 2-body energy, where the 3-body energy becomes infinite when the range of the potential is made shorter and shorter: this is the Thomas collapse [3].

### 2 Inequalities on binding energies

If an Hamiltonian \( H \) is split into subhamiltonians \( A, B, \ldots \), a lower bound on its ground-state energy \( E(H) \) is given by the sum of the lowest energies, namely

\[
H = A + B + \cdots \Rightarrow E(H) \geq E(A) + E(B) + \cdots .
\]

If, for instance, \( H = p^2 - 1/r + r^2/2 \) describes the motion of a particle feeling both a Coulomb and an harmonic potential, then \( E(H) \geq (-1/2) + (3/2) \), corresponding to an equal share of the kinetic energy. A slight improvement is obtained by writing \( H = [\alpha p^2 - 1/r] + [(1 - \alpha) p^2 + r^2/2] \), and optimising the parameter \( \alpha \).

This reasoning can be applied to obtain a lower bound on 3-body energies in terms of 2-body energies. This has been discovered independently by several authors working on the stability of matter [4] or baryon spectroscopy in simple quark models [5]. Let

\[
H_N(m,g) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + g \sum_{i<j} V(r_{ij}) ,
\]

be the Hamiltonian describing a system of \( N \) identical particles interacting with pairwise forces, and \( E_N(m,g) \) be its ground state energy. From the identity

\[
H_N(m,g) = \sum_i H_N^{(i)} \left( (N-1)m, \frac{g}{N-2} \right) ,
\]

where \( H_N^{(i)} \) does not include particle \( i \), one derives

\[
E_N(m,g) \geq N E_{N-1} \left( (N-1)m, \frac{g}{N-2} \right) \geq \frac{N(N-1)}{2} E_2(m(N-1),g) ,
\]

which can supplement any upper bound provided by a variational method, to frame the exact energy.

Numerical investigations show that the lower bound (4) is not very accurate and never reaches saturation. The relative wave function of particles 1 and 2 is of course modified by the presence of the third particle, and thus the three-body wave function
does not describe optimally the (1,2) subsystem. However, this is a small effect which
appears for the harmonic oscillator. The main source of inaccuracy in (4) is that the
contribution of the (1,2) subsystem is replaced by the rest energy of an isolated (1,2)
pair, although the (1,2) pair is not at rest in the whole system.

To overcome this difficulty, a better decomposition was written down by Hall and
Post [6], and rediscovered in Ref. [7]. It involves the translation-invariant part \( \tilde{H}_N \)
\[
\tilde{H}_N = H_N - \frac{(p_1 + p_2 + \cdots)^2}{2Nm},
\]
of each Hamiltonian \( H_N \) and reads
\[
\tilde{H}_N(m, g) = \sum_{i<j} \tilde{H}_{N-1}^{(i)} \left( m \frac{N(N-2)}{N-1}, g \frac{N}{N-2} \right).
\]
This leads to the new inequality
\[
E_N(m, g) \geq E_{N-1} \left( m \frac{N(N-2)}{N-1}, g \frac{N}{N-2} \right) \geq \frac{N(N-1)}{2} E_2 \left( \frac{mN}{2}, g \right),
\]
which is necessarily better than (4) since, \( mN/2 < m(N-1) \) for \( N \geq 3 \), and for
a given potential, the binding energy is a decreasing function of the constituent mass.
This inequality is optimal in the sense that it can be saturated: this occurs only for
the harmonic oscillator. The inequality (7) also holds for the variational approximation
\( E_N^{\text{var}} \) to the binding energy \( E_N \), provided the sets of trial functions \( \psi \) for \( N = 2 \) and
\( N = 3 \) are consistent. In particular, saturation, i.e., \( E_N^{\text{var}}(m, g) = 3E_2^{\text{var}}(3m/2, g) \), is
obtained if each variational energy is calculated with a single harmonic-oscillator func-
tion \( \psi_N \propto \exp(-\alpha_N \sum_i r_i^2) \). It happens rather often that (with minimal restrictions)
variational solutions share the properties of the exact ones. For the virial theorem this
was underlined by Fock and rediscovered by many authors [8].

The case of particles with unequal masses has revealed some surprises. The simple
extension of the decomposition (6), for, say \( H_3 \), in terms of 2-body Hamiltonians con-
taining the potential \( V_{ij} \) and a kinetic term proportional to \( (m_j p_i - m_i p_j)^2 \) does not
always give saturation for the harmonic oscillator. The remedy was found in Ref. [9] for
\( N = 3 \) particles and extended in Ref. [10] to \( N = 4 \): one should introduce more free-
dom in the decomposition of the Hamiltonian and find an optimal choice by suitable
adjustment. Namely, the kinetic-energy term associated to \( V_{12} \) contains a momentum
which is not necessarily \( m_2 p_1 - m_1 p_2 \), but \( \sum_i x_{12,i} p_i \), with \( \sum_i m_i x_{12,i} \) to ensure trans-
lation invariance, and \( x_{12,2} - x_{12,1} = 1 \) to make this momentum conjugate to \( r_2 - r_1 \).
The remaining parameters are adjusted to optimise the lower bound. See [7, 9, 10] for
details and numerical examples.

3 Borromean binding of bosons

The Hall–Post decomposition, used in the previous section to obtain inequalities on en-
ergies at given coupling constant \( g \), also provides relations between coupling constants
at given energy \( E \). In the case where this energy is \( E = 0 \), inequalities are obtained on
the critical couplings \( g_N \) required to achieve \( N \)-body binding.
In one- or two-dimensional quantum mechanics, any attractive potential supports at least one bound state [11]. More precisely, \( g_2 = 0 \) if the integral \( \int d^nxV(x) \) is negative. For \( n = 3 \) dimensions, the problem is more subtle [12]. A short-range attractive potential \( gV(r) \) needs a minimal strength \( g \) or a minimal constituent mass \( m \) to achieve binding, namely \( mg > g_2 \). A classic paper by Blatt and Jackson [13] gives estimates of \( g_2 \) for simple potentials such as Yukawa.

In this context, the phenomenon of Borromean binding is expressed by the property that the critical coupling \( g_3 \) required to bind three bosons is smaller than \( g_2 \). More generally, \( g_N \leq g_{N-1} \). Several questions can be raised: what is the typical range of values for \( g_3/g_2, g_4/g_3, \) etc.? Are there rigorous constraints on these ratios? Are these constraints saturated for some particular potentials? What can be said in the limit of large \( N \)?

Some results are given in Refs. [14, 15, 16], which contain references to the earlier papers. In particular, the decomposition (6) \( \tilde{H}_N \propto \sum \tilde{H}_{N-1} \) implies that \( \tilde{H}_N \) hardly explores the domain of binding with negative expectation values, if all \( \tilde{H}_{N-1} \) remain positive. Thus

\[
Ng_N \geq (N-1)g_{N-1} \geq \ldots g_2.
\]

For simple monotonic potentials, numerical estimates give \( g_3/g_2 \simeq 0.80 \), above the rigorous bound \( g_3/g_2 \geq 2/3 \), but still opening a remarkable window of about 20\% in the coupling constant, where three-body systems are bound without two-body binding. For four bosons, \( g_4/g_2 \simeq 0.67 \) is typically obtained, which, when compared to \( g_3/g_2 \simeq 0.80 \), reveals a window of about 13\% for four-body binding without three-body binding.

For bosons, the situation is rather simple. If a potential does not succeed in binding a pair of bosons, but is predominantly attractive, that is to say has a negative scattering length, it will bind a sufficiently large number of bosons.

We have seen that Hall–Post inequalities are saturated for harmonic potentials. A pure \( V(r) \propto r^2 \) does not give Borromean binding, as \( gV \) would confine even for very small \( g \). But a potential behaving like \( V \propto r^2 - C \) in the domain of the relevant wave functions, and vanishing at very large distances \( r \), would give \( g_3/g_2 \simeq 2/3 \), i.e., nearly saturate the inequality [16]. This corresponds to an attractive potential with an external barrier.

More important for physical applications are the potentials with an internal repulsive core. Their wave functions significantly depart from those of the harmonic oscillator and the ratio \( g_3/g_2 \) become closer to 1. Examples are given in [16].

4 Borromean molecules

Borromean binding as described in Sec. 3 seems at first hardly conceivable for a Coulomb potential, since changing the strength by an overall factor \( g \) simply results in a mere rescaling by \( g^2 \) of all binding energies \( E_N \). However, if the stability of ions and molecules does not depend on the overall strength of the interaction, it relies on an adequate balance between attraction and repulsion, and, for a given set of charges, on the ratios of the constituent masses which are involved.

Consider for instance a set of three masses \( \{m_i\} \) carrying charges \( \{q_i\} = \pm\{+1, -1, -1\} \), (times an overall factor). Systems with identical or nearly identical inverse masses \( m_2^{-1} \) and \( m_3^{-1} \), such as \( \text{H}_2^+ (e^-, p, p) \), \( \text{Ps}^- (e^+, e^-, e^-) \) or \( \text{H}^- (p, e^-, e^-) \), ...
or neighbouring configurations, are stable, while less symmetric systems such as \((e^-, p, e^+)\) or \((p, \bar{p}, e^-)\) spontaneously decay into an atom and an isolated charge [17]. Note that the stable systems with three unit charges are not Borromean, since there are always two stable atoms among the subsystems, \(\{1, 2\}\) and \(\{1, 3\}\) in our notation. This means that one can construct each stable system step by step: two charges form a stable atom, which attracts the third charge.

For \(N = 4\) unit charges \(\{q_i\} = +1, +1, -1, -1\), there are several possibilities: unstable configurations, such as \((p, e^+, \bar{p}, e^-)\), which spontaneously splits into a protonium and a positronium; stable systems, the simplest being the \(Ps_2\) molecule \((e^+, e^+, e^-, e^-)\), whose all three-body subsystems \(\pm(e^+, e^-, e^-)\) are stable; less stable systems, such as the positronium hydride \((p, e^+, e^-, e^-)\), which can be viewed as a stable \(H^-\) fixing a positron, or a stable \(Ps^-\) attached to a proton, or, more interestingly, as an unstable \((e^-, p, e^+)\) stabilised by the addition of a second electron.

More recently, a new category of four unit-charge systems was revealed [18]. They are stable, but all the three-body subsystems are unstable. Hence, they are Borromean, in the sense that they cannot be built by adding the constituents one by one. An example is \((p, d, \bar{p}, \bar{d})\), with a proton, a deuteron and their antiparticles. Indeed, a study by Mitroy [19], who uses Varga's stochastic variational method [20], indicates that asymmetric ions \((m^+, M^-, m^-)\) are stable in the range

\[
0.70 \lesssim \frac{M}{m} \lesssim 1.69, \tag{9}
\]

while other studies, such as the one by Bressanini et al. [21], who use a diffusion Monte-Carlo approach, or by Varga [22] with a stochastic search of the range coefficients of a Gaussian parametrisation, have established that \((M^+, m^+, M^-, m^-)\) remain stable for

\[
\frac{1}{2.2} \lesssim \frac{M}{m} \lesssim 2.2. \tag{10}
\]

Then, the four-body system \((M^+, m^+, M^-, m^-)\) for \(M/m \sim 2\), and the neighbouring configurations are stable while none of their three-body subsystems is stable.

5 Outlook

In molecular, nuclear, or hadronic physics, there are fragile and subtle quantum states, whose stability relies on the joint efforts of many subsystems, which by themselves do not contain enough attraction to be stable. The theoretical analysis is now well under control for system of bosons in their ground state. For fermions, much progress remains to be made, in spite of the existing contributions [23]. For molecules, more studies are also be desirable, to better understand the Borromean binding discovered in numerical calculations.

References


\(^{1}\) In this section, we consider Coulomb forces only, and annihilation, strong interaction, etc., are neglected.


A hyperspherical variational approach to the N fermion problem

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Abstract. A variational treatment in hyperspherical coordinates is developed to describe the two-component normal Fermi gas with two-body zero-range interactions. We adopt a variational trial function that is a Slater determinant of noninteracting oscillator functions, multiplied by an unspecified function of the hyperradius. Optimization of the hyperradial function approximately reduces the many-body problem to a linear, one-dimensional Schrödinger equation in the hyperradius R of the N-atom system. Results from this variational treatment are compared with more conventional descriptions based on mean-field theory.

1 Introduction

The physics of the degenerate Fermi gas consisting of fermions in two different spin states has emerged as a subject of particular interest recently, largely because it has been experimentally realized and because BCS-type pairing phenomena have been observed.\cite{1} This type of pairing occurs when the temperature becomes sufficiently low, $T \ll T_f$, when the interatomic scattering length $a$ is sufficiently attractive, and when the density is sufficiently high. The peak density in such a zero temperature Fermi gas can be expressed in terms of the Fermi wavenumber $k_F$, through the definition $\rho \equiv k_F^3/(3\pi^2)$. The negative scattering length portion of the BEC-BCS crossover regime is the range $k_F a < -1$. While the highly-correlated BCS-type pairing phenomena are highly interesting, we believe that the behavior of the normal Fermi fluid is deserving of further study in its own right, even in the absence of pairing physics. This is the topic of the present paper, which follows a recent study of this problem that was carried out from a different but related perspective.\cite{2}

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The starting point of our approach connects with the hyperspherical coordinate treatments that have been applied to finite nuclei. The formulation is a rigorous variational many-body calculation, aside from the usual limitations of the assumed pairwise Hamiltonian with zero-range interactions. For simplicity, we only consider fermionic systems with completely filled shells. This is done for analytical and computational simplification; the same approach should be equally applicable to open-shell fermi systems, with modest extensions.

Consider \( N \) identical fermions confined either magnetically or optically in a spherically symmetric harmonic oscillator trap with angular frequency \( \omega \). Half of the fermions are in one spin substate, while the other half are in a second spin substate. The full \( N \)-body time-independent Schrödinger equation for this system reads \( H \psi = E \psi \), with \( H \) given by:

\[
\sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} m \omega^2 r_i^2 \right) + \sum_{i>j} \frac{4\pi\hbar^2 a}{m} \delta(\mathbf{r}_i - \mathbf{r}_j),
\]

where \( m \) is the fermion mass, and where \( a \) is the two body s-wave scattering length. Next we transform to a set of hyperspherical coordinates. The hypersphere radius for this system of equal mass particles is the root mean square distance of the atoms from the trap center, \( R = (\sum r_i^2/N)^{1/2} \). The remaining \( 3N - 1 \) dimensions are described by a set of angular coordinates collectively denoted by \( \Omega \). These include the ordinary set of \( 2N \) spherical polar coordinates for each particle \( \{(\theta_i, \phi_i)\}_{i=1}^{N} \), and as in Ref. \([3]\), an additional set of \( N - 1 \) hyperangles \( \alpha_i, i = 1, 2, 3, ..., N - 1 \): \( \tan \alpha_i \equiv (\sum_{j=1}^{i} r_j^2)^{1/2}/r_{i+1} \). In these coordinates the kinetic energy is \([5]\)

\[
-\frac{\hbar^2}{2M} \left( \frac{1}{R^{3N-1}} \frac{\partial}{\partial R} R^{3N-1} \frac{\partial}{\partial R} - \frac{A^2}{R^2} \right),
\]

where \( M = Nm \) is the total mass of the system, and the squared grand angular momentum operator \( A^2 \) is defined as in the usual references. The trap potential is purely hyperradial, i.e. \( \sum_{i=1}^{N} \frac{1}{2} m \omega^2 r_i^2 = \frac{1}{2} M \omega^2 R^2 \). It is convenient to eliminate first-order radial derivative terms in the Hamiltonian that acts on \( \psi \) by separating out explicitly the factor \( R^{3N-1}/2 \). One factor in our variational approximation to the many-particle wavefunction \( \psi (R, \Omega) \) is chosen here to be the lowest antisymmetric eigenfunction of the operator \( A^2 \). These eigenfunctions, or “hyperspherical harmonics” (HHs, see \([3, 5]\)) are expressible in terms of Jacobi polynomials. The eigenvalue equation they obey is

\[
A^2 Y_{\lambda \nu} (\Omega) = \lambda (\lambda + 3N - 2) Y_{\lambda \nu} (\Omega) \quad \text{where} \quad \lambda = 0, 1, 2, \ldots \quad \text{is the order of the harmonic.}
\]

The second index, \( \nu \), represents the further set of \( N - 2 \) quantum numbers required to distinguish the set of degenerate states having each specified value of \( \lambda \). The full trial wave function is written as \( \psi (R, \Omega) = G (R) \Phi_{\lambda} (\Omega) \) where \( \Phi_{\lambda} (\Omega) \) is an antisymmetric linear combination of HHs (with appropriate spinors) having grand angular momentum \( \lambda \). \( G (R) \) is a variationally optimized hyper-radial function that will be determined later. The antisymmetrizing coefficients of this HH expansion are generally difficult to obtain. In some references, they are calculated recursively\([3, 6, 7]\) using a coefficient of fractional parentage (cfp)
expansion. We have seen, however, that the antisymmetrization can be handled quite simply, provided we restrict our treatment here to only magic numbers of particles, i.e., to filled energy shells of the noninteracting isotropic harmonic oscillator. Because the $N$-particle oscillator has a separable Schrödinger equation in either independent particle coordinates or hyperspherical coordinates, any nondegenerate, normalized, antisymmetric $N$-body state must be identical in the two coordinate systems. Consequently, any nondegenerate wavefunction for $n$ completely filled shells ($n = 1, 2, \ldots$) can be written as a Slater determinant of the independent particle states, whereby $\Phi_\lambda (\Omega)$ takes the form:

$$\frac{1}{\sqrt{N!}} F_\lambda (R) \sum_p (-1)^p P \prod_{i=1}^N R_{n_i} (r_i) y_{l_i m_i} (\omega_i) |m_{s_i}\rangle^i$$

(3)

Where the sum runs over all permutations $P$ of the $N$ spatial and spin coordinates. Here $R_{n_i} (r_i)$ is the radial solution to the independent particle harmonic oscillator for the $i$th particle given by $r R_{n\ell} (r) = Nn \exp \left(-r^2/2 \ell^2\right) (r/\ell)^{\ell+1} L_{n\ell} [r^2/\ell^2]$, where $L_{n\ell} (r)$ is a modified Laguerre polynomial with $l = \sqrt{\hbar/m\omega}$. $y_{l_i m_i} (\omega)$ is an ordinary 3D spherical harmonic with $\omega_i$ as the spatial solid angle for the $i$th particle, $|m_{s_i}\rangle$ is a spin ket that allows for two spin species of atoms, $|\uparrow\rangle$ and $|\downarrow\rangle$. $R^{(3N-1)/2} F_\lambda (R) = A_\lambda \exp \left(-R^2/2L^2\right) (R/L)^{\lambda+3(N-1)/2+1}$ is the nodeless hyperradial solution for $N$ noninteracting particles in an oscillator with hyperangular momentum $\lambda$ where $A_\lambda$ a normalization factor and $L = l/\sqrt{N}$. The method of expanding antisymmetrized hyperspherical harmonics in Slater determinants of oscillator spin-orbitals has been used before. [8, 9, 10, 11] With this trial wavefunction, the expectation value of the Fermi pseudopotential yields an $R$-dependent effective potential for the function $G(R)$.

Multiplication of $G(R)$ by $R^{(3N-1)/2}$ to remove first derivative terms gives the following form for $H_R$ in oscillator units, where $\hbar = 1$ and $\sqrt{\hbar/m\omega} = 1$,

$$H_R = -\frac{1}{2N} \frac{d^2}{dR^2} + \frac{(\lambda + (3N-3)/2) (\lambda + (3N-1)/2)}{2NR^2} + \frac{1}{2} \frac{N R^2}{N^{3/2} R^3}. \quad (4)$$

This effective hyperradial Hamiltonian, first derived for fermions in Ref. [2], resembles the similar result derived for $N$ identical bosons by the authors of Ref.[12]. BECs formed with $a < a_c$ were predicted to collapse by a number of studies [13, 14, 12], and the corresponding phenomenon of the bosenova was observed experimentally. [15, 16].

$$C_\lambda = \frac{\Gamma (\lambda + 3N/2)}{\Gamma (\lambda + 3(N-1)/2)} \sum_{k<k'} B_{kk'}, \quad (5)$$

where $B_{kk'}$ is an integral over the zero-interaction radial Laguerre polynomials,

$$B_{kk'} = \frac{\Gamma (2l_k + 1) (2l_{k'} + 1)}{2\pi} \int_0^\infty \frac{r^2 dr R_{n_k l_k} (r) R_{n_k l_{k'}} (r)^2}{R_{n_{k'} l_{k'}} (r)^2}. \quad (6)$$

Calculations of $C_\lambda$ up to the 100th filled shell, a shell with 343,400 atoms and $\lambda = 25, 497, 450$, have been carried out numerically. This number is large enough to
extract the leading order asymptotic behavior of \( C_\lambda \to 0.16802N^{7/2}\sqrt{2}/\pi^2 \). Note that the value of \( \lambda \) can be extracted simply by comparing the ground state energy in the two representations, giving \( \lambda = \sum_{i=1}^{N} (2n_i + l_i) \). It is convenient to express \( \lambda \) and \( N \) in terms of the filled shell index \( n \), i.e. \( \lambda = (n - 1)n(n + 1)(n + 2)/4 \) and \( N = n(n + 1)(n + 2)/3 \). In the large-\( N \) limit the leading order terms from these expressions are given by \( n \to (3N)^{1/3} \) and \( \lambda \to (3N)^{4/3}/4 \).

We now proceed to apply the variational principle to this Hamiltonian. For a trial wave function we will take a non-interacting 3\( N \) dimensional nodeless oscillator function for an oscillator with rescaled frequency \( \omega' = \zeta^{-2}\omega \) given by \( R^{(3N-1)/2}G(R) = N(\zeta)\exp\left(-NR^2/2\zeta^2\right)\left(\sqrt{NR}/\zeta\right)^{\lambda+3(N-1)/2+1} \). The dimensionless quantity \( \zeta \) is the ratio of an effective oscillator length to the non-interacting oscillator length in our Hamiltonian, and it is a variational parameter that we will optimize below. Note that this expression is still written in the oscillator units of the actual trap. \( N(\zeta) \) is a normalization factor used to ensure that \( \langle G(R) | G(R) \rangle = 1 \). This choice of trial wave function corresponds to the assumption that the net effect of the interactions is that of contracting (for \( a < 0 \)) or expanding (for \( a > 0 \)) the hyperradial wavefunction only. With this choice the expectation value of the Hamiltonian as a function of \( \zeta \) is given in oscillator units by

\[
E(\zeta) = \frac{(\lambda + 3N/2)}{2\zeta^2} + \frac{1}{2}(\lambda + 3N/2)\zeta^2 + \frac{\Gamma(K)}{\Gamma(K + 3/2)} \frac{4\pi aC_\lambda}{\zeta^3}. \tag{7}
\]

If we rescale this energy by the noninteracting oscillator energy \( E_{NI} = \lambda + 3N/2 \) we obtain

\[
\frac{E(\zeta)}{E_{NI}} = \frac{1}{2\zeta^2} + \frac{1}{2}\zeta^2 + \frac{\Gamma(K)}{\Gamma(K + 3/2)} \frac{4\pi aC_\lambda}{(\lambda + 3N/2)\zeta^3}. \tag{8}
\]

After multiplying above and below by \( k_f = \sqrt{2(n-1)/l} \) and taking the leading order behavior in the large \( N \) limit where \( k_f \to \sqrt{2}(3N)^{1/6} \) we see that

\[
\frac{E(\zeta)}{E_{NI}} \to \frac{1}{2\zeta^2} + \frac{1}{2}\zeta^2 + \sigma \frac{k_f a}{\zeta^3}, \tag{9}
\]

where \( \sigma = 0.16802 \left(64\sqrt{12}/81\pi\right) \). It is interesting to note that the only parameter in this large \( N \) behavior is the unitless quantity \( k_f a \). The behavior of \( \frac{E(\zeta)}{E_{NI}} \) is considerably different for \( k_f a > 0 \) and \( k_f a < 0 \), a graph of these two regions is shown in figure 1. For \( k_f a > 0 \), \( E(\zeta) \) has only one global minimum; as \( a \) increases, the minimum is pushed farther out and up in energy. Thus the effect of repulsive interactions is to increase the overall energy by shifting the effective oscillator level higher, while the interactions have the effect of “softening” the effective oscillator. As \( k_f a \) becomes negative there is an interesting behavior as the global minimum turns into a local minimum in the energy, while the global minimum moves to \(-\infty \) as \( \zeta \to 0 \). The presence of this local minimum implies the existence of a metastable state that is prevented from falling into the global minimum state by a tunneling barrier formed by the repulsive 3\( N \) dimensional centrifugal barrier in Eq.4. As \( k_f a \) is moved further negative, the height of the local maximum in \( E(\zeta) \) decreases. Eventually the interactions get so strongly
Figure 1. (a) Energy as a function of the effective oscillator length $\zeta$. For each curve (from the highest curve down) $k_f a = 0.7, 0$ (dotted), -0.7, $k_f a_c$ (bold) and $k_f a_c - 0.5$. (b) The ground state energy (solid line) and $\langle R^2 \rangle$ (dashed line) calculated using the hyperspherical variational method are compared with the Hartree-Fock results (circles and squares, respectively), as functions of $k_f a$. All calculations on this figure were carried out using 240 atoms.

Attractive that they overwelm the repulsive barrier and the local minimum disappears entirely. This translates into a loss of the metastable state at a critical value of $k_f a$ given by $k_f a_c = -1.21$. For values of $k_f a \leq k_f a_c$ there is no region where the Fermi gas can remain stable; hence the effective oscillator length collapses down to a considerably more compact geometry. This behavior is seen in figure 1 where $E(\zeta)$ has been plotted for several values of $k_f a$ above and below $k_f a_c$. Figure 1 compares the energy of the minimum (global for $k_f a > 0$ and local for $k_f a < 0$) of $E(\zeta)$ as a function of $k_f a$ compared to the ground state energy predicted using the Hartree-Fock method. Figure 1 also shows the expectation value of $R^2$ normalized by the non-interacting value $\langle R^2 \rangle_{NI} = l^2 \left( \frac{3}{2} + \lambda/N \right)$. Note that the variationally calculated values are very close to those predicted by Hartree-Fock.

In summary, we have developed a fully antisymmetrized, variational description of $N$ fermionic atoms, with zero-range interactions in a spherical harmonic trap. Truncation to the lowest antisymmetric hyperspherical harmonic reduces the problem to a linear, one-dimensional Schrödinger equation in the hyperradius with an effective potential. In the large atom number limit, it only depends on the quantity $k_f a$. The ground state energy and radius predicted from this linear quantum mechanical treatment map accurately onto those predicted with the Hartree-Fock method, while the breathing mode frequencies agree with the sum rule and are a qualitative improvement over the calculated HF frequencies. This picture predicts a ground state energy that collapses to $\infty$ at $k_f a < -1.21$, in a manner identical to the physics of the "bosenova". [12] But the full interrelationship between this phenomenon and the physics of pairing in the BEC-BCS crossover region goes beyond the scope of the present study and will be explored in a subsequent publication.

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Five-body calculation of resonance and scattering states of the \( uudd\bar{s} \) system

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Abstract. The scattering problem of the \( uudd\bar{s} \) system, in the standard non-relativistic quark model of Isgur-Karl, is solved for the first time, by treating the large five-body model space, including the \( NK \) scattering channel, accurately with the Gaussian expansion method and the Kohn-type coupled-channel variational method. The calculated \( NK \) scattering phase shift shows no resonance in the energy region of the reported pentaquark \( \Theta^+ \) (1540), that is, at 0–500 MeV above the \( NK \) threshold (1.4–1.9 GeV in mass). The phase shift does show two resonances just above 500 MeV: a broad \( \frac{1}{2}^+ \) resonance with a width of \( \Gamma \sim 110 \) MeV located at \( \sim 520 \) MeV (\( \sim 2.0 \) GeV in mass) and a sharp \( \frac{1}{2}^- \) resonance with \( \Gamma = 0.12 \) MeV at 540 MeV.

1 Introduction

The observation of a signal of a narrow resonance at \( \sim 1540 \) MeV with \( S = +1 \) by the LEPS group [1, 2], now called \( \Theta^+ \) (1540), triggered a lot of theoretical research on multi-quark systems [3], although further experimental reexamination is still needed to establish the state. The question whether or not the multi-quark baryon \( \Theta^+ \) (1540) really exists is then one of current issues in hadron physics. In order to answer the question theoretically, one has to nonperturbatively evaluate the mass and the decay width of \( \Theta^+ \) (1540), namely of the \( uudd\bar{s} \) resonance. All nonperturbative analyses made so far, however, did not impose any proper boundary condition on the \( NK \) scattering component of the pentaquark state. At the present stage, the non-relativistic quark model provides a nonperturbative framework which makes it possible to impose a proper boundary condition to the \( NK \) scattering component.

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In this paper, we consider the standard quark model of Isgur-Karl [4, 5]. The Hamiltonian consists of a confining potential of harmonic oscillator type and a color-magnetic spin-spin interaction. As shown later, the Hamiltonian satisfactorily reproduces observed properties of ordinary baryons and mesons. The same Hamiltonian is applied to the pentaquark with no adjustable parameter.

Resonant and non-resonant states of the $uudd\bar{s}$ system are nonperturbatively derived with the Kohn-type coupled-channel variational method [6] in which a proper boundary condition is imposed on the $NK$ scattering channel and the total antisymmetrization between quarks is explicitly taken into account. Reliability of the method for the scattering problem between composite particles was shown by one of the authors (M.K.) [6], and actually it was already applied to $qqq - qqq$ scattering [7].

The coupled-channel variational method is accurate, only when the five-body dynamics in the interaction region is solved precisely. To achieve this goal, we use the Gaussian expansion method (GEM) [8]. GEM is one of the most reliable few-body methods proposed by two of the present authors (E.H. and M.K.) and their collaborators. The method was successfully applied to various types of three- and four-body systems [8].

2 Model and Method

Hamiltonian of the standard non-relativistic quark model of Isgur-Karl [4, 5] is

$$H = \sum_i \left( m_i + \frac{p_i^2}{2m_i} \right) - T_G + V_{\text{Conf}} + V_{\text{CM}},$$

where $m_i$ and $p_i$ are the mass and momentum of $i$th quark and $T_G$ is the kinetic energy of the center-of-mass. In what follows, $u$ and $d$ quarks are labeled by $i = 1 - 4$, and $\bar{s}$ by $i = 5$. The confining potential $V_{\text{Conf}}$ is of harmonic oscillator type:

$$V_{\text{Conf}} = -\sum_{i<j} \sum_{\alpha=1}^{8} \frac{\lambda_i^\alpha \lambda_j^\alpha}{2} \left[ \frac{k}{2} (x_i - x_j)^2 + v_0 \right],$$

where $x_i$ is the position vector of $i$th quark, $v_0$ is a mass shift parameter, and $\lambda_i^\alpha$ are the Gell-Mann matrices for color; note that $\lambda_i^\alpha \to -\bar{\lambda}_i^\alpha$ for antiquark. The color-magnetic potential $V_{\text{CM}}$ is

$$V_{\text{CM}} = \sum_{i<j} \sum_{\alpha=1}^{8} \frac{\lambda_i^\alpha \lambda_j^\alpha}{2} \frac{\xi_\sigma}{m_i m_j} e^{-\frac{(x_i - x_j)^2}{\beta^2}} \sigma_i \cdot \sigma_j.$$  

Parameters of the Hamiltonian are fixed as follows. First we take standard values, $m_u = m_d = 330$ MeV and $m_s = 500$ MeV, for quark masses. And as for $k$ and $\beta$ we take the same values as in Refs. [4, 5], i.e. $k = 455.1$ MeV·fm$^{-2}$ and $\beta = 0.5$ fm. The remainder $\xi_\sigma$ and $v_0$ are so determined that the three-body calculation, done in the same manner as in Ref. [9], can reproduce $m_N = 939$ MeV and $m_\Delta = 1232$ MeV. The resultant values are $\xi_\sigma/m_u^2 = -474.9$ MeV and $v_0 = -428.3$ MeV. The parameters thus determined are assumed to be universal for all low-lying hadrons including the pentaquark.
The present Hamiltonian is tested on static properties of conventional baryons and mesons such as masses, magnetic moments and charge radii. It should be emphasized that the present set of parameters satisfactorily reproduces the observed data.

One may wonder whether a linear confinement potential should be used instead of the harmonic oscillator potential. The latter potential, however, has been used in many previous studies, since it is easy to handle. In our present analysis, rather than the practical advantage, we point out that as long as low lying states up to \( \hbar \omega \sim \) several hundreds MeV are concerned, their properties are rather insensitive to the type of the potential. For this reason, we adopt the harmonic oscillator confining potential for the first serious calculation of the five-body system. (Recently, we have applied linear-type confinement and color-magnetic potential of ordinary baryons and mesons to the pentaquark system, and have confirmed that our main conclusion of the absence of low-lying pentaquark resonances is unchanged in this more realistic calculation [10].)

We solve the five-body Schrödinger equation

\[
(H - E) \Psi_{J^*M} = 0,
\]

imposing the scattering boundary condition on the \( NK \) scattering component of the total wave function \( \Psi_{J^*M} \); here \( \Psi_{J^*M} \) is classified with the angular momentum \( J \), its \( z \)-component \( M \) and parity \( \pi \). The \( NK \) scattering component of \( \Psi_{J^*M} \) is expressed by

\[
\Psi_{J^*M}^{(NK)}(E) = A_{1234}\left[ \left[ \phi^{(N)}_0(123)\phi^{(K)}_0(45) \right] \frac{1}{2} \chi_L(R_1) \right]_{J^*M},
\]

where the operator \( A_{1234} \) antisymmetrizes particles 1–4 \((u,d\) quarks\) while particle 5 is \( \bar{s} \). Here, \( \phi^{(N)}_0 \) and \( \phi^{(K)}_0 \) are the color-singlet spin \( \frac{1}{2} \) and spin 0 intrinsic wave functions of \( N \) and \( K \), respectively, and \( \chi_L(R_1) \) is the wave function of the \( NK \) relative motion along the coordinate \( R_1 \) (cf. \( c = 1 \) of Fig. 1) with the angular momentum \( L \) and the center-of-mass energy \( E - E_{th} \), \( E_{th} \) being the \( NK \) threshold energy \((1422 \text{ MeV}) \) in the present model). The reported energy of \( \Theta^+(1540) \) is slightly above the \( NK \) threshold, it is then convenient to consider the pentaquark energy \( E \) with \( E - E_{th} \).

The interaction-region part of \( \Psi_{J^*M} \) should be described with a large model space. For this purpose, we take five Jacobi-coordinate sets, \( c = 1 \)–5 of Fig. 1, and construct \( L^2 \)-type basis functions, \( \Phi_{J^*M,\alpha}^{(c)} \), for each coordinate \( c \) as follows:

\[
\Phi_{J^*M,\alpha}^{(c)} = A_{1234}\left[ \xi_{1}^{(c)}(1234,5)\eta_{0(t)}^{(c)}(1234,5) \times \left[ \chi_{S(\bar{s}\bar{s})}^{(c)}(1234,5)\psi_{L[n]}^{(c)}(r_c,\rho_c,s_c,R_c) \right]_{J^*M} \right],
\]

where \( \xi_{1}^{(c)} \) is the color-singlet wave function, and \( \eta_{0(t)}^{(c)} \), \( \chi_{S(\bar{s}\bar{s})}^{(c)} \), and \( \psi_{L[n]}^{(c)} \) are the isospin, spin and spatial wave functions with the total isospin \( T = 0 \), the total spin \( S = \frac{1}{2} \) and the total orbital angular momentum \( L \), respectively. Here we have neglected \( S = \frac{3}{2} \), since it is decoupled from the \( N + K \) scattering channel.
with $S = \frac{1}{2}$; $t$ and $s, \bar{s}, \sigma$ are intermediate quantum numbers of isospin and spin coupling, respectively, and as shown in the next section the symbol $\{n\}$ specifies the radial dependence of the spatial wave functions. The suffix $\alpha$ in $\Phi_{J^\pi M, \alpha}^{(c)}$ specifies a set of $(t, S, s, \bar{s}, \sigma, L, \{n\})$.

The Hamiltonian is diagonalized within a model space spanned by a large number of $\Phi_{J^\pi M, \alpha}^{(c)}$ that is, $\sim 15,000$ basis functions in actual calculations. The resulting discrete eigenstates are called pseudostates, when the eigenenergies $E_\nu$ satisfy $E_\nu > E_{\text{th}}$. The pseudostates, $\{\hat{\Phi}_{J^\pi M}^{(n)}(E_\nu) ; \nu = 1 - \nu_{\max}\}$, are written in terms of $\Phi_{J^\pi M, \alpha}^{(c)}$ as

$$\hat{\Phi}_{J^\pi M}^{(c)}(E_\nu) = \sum_{c, \alpha} A_{J, \alpha}^{(c)}(E_\nu) \Phi_{J^\pi M, \alpha}^{(c)}(r_c, \rho_c, s_c, R_c).$$

(7)

It is possible to expand the interaction-region part of the total wave function in terms of those eigenfunctions since they are considered to form a complete set for each $J^\pi$ in the finite interaction region. The total wave function is then described as a superposition of the $NK$ scattering component and the $\hat{\Phi}_{J^\pi M}^{(n)}(E_\nu)$:

$$\Psi_{J^\pi M}(E) = \Psi_{J^\pi M}^{(NK)}(E) + \sum_{\nu=1}^{\nu_{\max}} b_\nu(E) \hat{\Phi}_{J^\pi M}^{(n)}(E_\nu).$$

(8)

The second term describes virtual excitations of $N$ and $K$ in $c = 1$ and other five-body distortions in $c = 2 - 5$ in the intermediate stage of the scattering. Unknown quantities $\chi_L(R_1)$ in $\Psi_{J^\pi M}^{(NK)}(E)$ and $b_\nu(E)$ are obtained by solving Eq. (4) with the Kohn-type variational method [6]. Inclusion of high-lying pseudostates in the model space do not change calculated values of the phase shift, when the energies $E_\nu$ are much larger than the $NK$ scattering energy. Hence, only a few tens of lowest-lying pseudostates contribute to the numerical result. In the present calculation, the $NK$ scattering energy should be smaller than an energy of the first spatial excited state of nucleon, i.e. the Roper resonance which is located at 675 MeV above the nucleon mass in the present model, because we consider only the $NK$ scattering component as an open channel where both $N$ and $K$ are in the ground state. The condition for our calculation to be valid is then $E - E_{\text{th}} < 675$ MeV.

Figure 1. Five sets of Jacobi coordinates among five quarks. Four $u, d$ quarks, labeled by particle 1–4, are to be antisymmetrized, while particle 5 stands for $\bar{s}$ quark. The $NK$ scattering channel is treated with $c = 1$. 
3 Results

Firstly, we calculate the $NK$ elastic scattering phase shifts for $J^\pi = \frac{1}{2}^-$ and $\frac{1}{2}^+$, by omitting the pseudostate terms in (8). In this calculation, $N$ and $K$ behave as particle with a frozen structure. The resulting phase shifts are shown in Fig. 2 as dash-dotted lines. There appears no resonance in the entire energy region.

Next, we do the full-fledged calculation including the pseudostate terms in (8). Calculated phase shifts are shown as solid lines. Up to the energy $E \sim 300$ MeV, the calculated phase shifts of $J^\pi = 1/2^-$ agree qualitatively well with the experimental data [12, 13] as well as with the previous quark model estimate [14].

No resonance is seen in the energy region $0 - 500$ MeV above the $NK$ threshold (1.4 – 1.9 GeV in mass), that is, in the reported energy region of $\Theta^+(1540)$. One does see two resonances around 530 MeV; one is a sharp $J^\pi = \frac{1}{2}^-$ resonance with a width of $\Gamma = 0.12$ MeV located at $E - E_{th} = 540$ MeV and the other is a broad $\frac{1}{2}^+$ resonance at $\sim 520$ MeV with $\Gamma \sim 110$ MeV. It should be noted here that our result on the absence of the low-lying pentaquark resonance is consistent with some recent lattice QCD results in Refs. [15, 17, 16], in which, in fact, no pentaquark resonance is observed below about 300 MeV with respect to the $N + K$ threshold.

Figure 2. Calculated phase shifts for a) $J^\pi = \frac{1}{2}^-$ and b) $J^\pi = \frac{1}{2}^+$ states. The solid lines are given by the full-fledged calculation, while the dash-dotted lines are by the approximate calculation with the elastic $NK$ channel alone (see (8)). Energies are measured from the $NK$ threshold. The arrow indicates the energy of $\Theta^+(1540)$ in $E - E_{th}$.

In summary, we solved the five-quark scattering problem by applying GEM [8] and the Kohn-type variational method [6] to a large model space including the $NK$ scattering component. We adopted the standard non-relativistic quark model of Isgur-Karl which satisfactorily reproduces experimental values of the two- and three-quark systems. The resultant $NK$ scattering phase shift showed no resonance in the reported energy region of $\Theta^+(1540)$; this is the most impor-
tant result of the present paper. At energies much higher (by \(\sim 400\) MeV) than the \(\Theta^+(1540)\) energy, we did find a broad \(J^\pi = \frac{1}{2}^+\) resonance with \(\Gamma \sim 110\) MeV at \(\sim 520\) MeV above the \(NK\) threshold and a sharp \(J^\pi = \frac{1}{2}^-\) resonance with \(\Gamma = 0.12\) MeV at 540 MeV. We have done the same calculation for other Hamiltonian proposed in [9] that also reproduces the observed properties of the ordinary hadrons and mesons. The result was qualitatively the same as in this paper; in particular resonances are absent in the low energy region up to 500 MeV from the \(NK\) threshold. The locations and the widths of the resonances at higher energies, however, depend on the details of the model hamiltonian. If the existence of the pentaquark is confirmed experimentally in the future, our results might suggest a limit of the constituent quark model with two-body potential. For this purpose, new many systematic data on five-body quark systems are desired in the future.

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An $\alpha$-particle model for $^{16}$O, is there a new 4-body scale? *

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Abstract. The $^{16}$O nucleus is modelled as a system of four $\alpha$-particles. It is shown that an Hamiltonian that includes established two- and three-body forces reproducing the $\alpha-\alpha$ phase shifts, the $^8$Be resonance and the first and second $0^+$ states of $^{12}$C overbinds the $^{16}$O nucleus. To rectify this a novel 4-body force is introduced, which then leads to a good agreement with the low-lying experimental spectrum of $^{16}$O.

1 Introduction

The formation of $\alpha$-particle like structures in various nuclei is a well known phenomenon dating to the early days of nuclear physics. Experimentally, the $\alpha$-decay process is the clearest evidence of this phenomenon in heavy nuclei, while clusterization and fragmentation are the evidence for such structures in light nuclei. The tendency of two protons and two neutrons to form an $\alpha$-particle stems from the fact that it is the smallest closed shell nucleus. Such a substructure of nuclei leads to large binding and polarization energies.

For symmetric even–even nuclei, like $^8$Be or $^{12}$C, it is most probable that the $\alpha$-cluster component is the dominant part of the nuclear wave function.

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Therefore a simplified description of those nuclei, as a system of interacting structureless α-particles, is called for. In fact in the past such α-cluster models have been employed to study the properties of \(^{8}\)Be [1] and \(^{12}\)C [2, 3, 4] as systems of two and three α-particles.

In a cluster approach the α-particles interact via effective forces, which in principle can be derived directly from the nuclear Hamiltonian. However, in practice the forces are usually fitted to reproduce a given set of observables. So far the cluster approach has been rather successful in the description of \(^{8}\)Be and \(^{12}\)C. Two-body forces fitted to the α-α phase shifts [1] reproduce the energy and width of the \(^{8}\)Be ground state. Adding a three-body force, also the energy of the ground state as well as energy and width of the first excited \((J^\pi = 0^+)\) states of \(^{12}\)C can be reproduced [2, 3].

In the current work we study the predictive power of such models when employed in the 4-α \((^{16}\text{O})\) and 5-α \((^{20}\text{Ne})\) sectors. To this end we use the Effective Interaction Hyperspherical Harmonics (EIHH) method [5] to solve the \(N\)-α-particle problem.

### 2 Formulation of the problem

Using the hyperspherical formalism and separating the center of mass motion the \(N\)-body Hamiltonian

\[
H = -\frac{\hbar^2}{2M_\alpha} \sum_i p_i^2 + \sum_{i,j} V^{(2)}(i,j) + \sum_{i,j,k} V^{(3)}(i,j,k) + \ldots \tag{1}
\]

is written in the following form

\[
H = -\frac{\hbar^2}{2M_\alpha} \left\{ \frac{\partial^2}{\partial \rho^2} + \frac{3N - 4}{\rho} \frac{\partial}{\partial \rho} - \frac{\hat{K}^2}{\rho^2} \right\} + \sum_{i,j} V^{(2)}(i,j) + \sum_{i,j,k} V^{(3)}(i,j,k) + \ldots , \tag{2}
\]

where \(\rho\) is the hyperradial coordinate which together with \(\Omega\) form the set of \(3N - 3\) hyperspherical coordinates and \(\hat{K}\) is the hyperangular momentum operator. The 2-body force is a sum of the long range Coulomb repulsion

\[
V_c(r_{ij}) = \frac{4e^2}{r_{ij}} \tag{3}
\]

and a short range nuclear force. For the nuclear part of the 2-body interaction it is customary to utilize the Ali–Bodmer force which reproduces the α-α phase shifts [1]. This force is expressed in each partial wave as a sum of two
Gaussians in the form
\[ V^{(2)}_{\alpha\alpha}(r_{ij}) = \sum_\ell \left[ V^{(2)}_\ell(r_{ij}) e^{-(\mu r_{ij})^2} - V^{(2)}_\alpha(\ell) e^{-(\mu_a r_{ij})^2} \right] |\ell\rangle\langle\ell|. \] (4)

The 3-body force, which we expand in 3-body partial waves, is expressed in terms of the hyperradial 3-body coordinate \( \rho_3 \)
\[ V^{(3)} = \sum_{L_3} V^{(3)}_{0}(L_3) e^{-(\mu_3 \rho_3)^2} |L_3\rangle\langle L_3| \] (5)

and is fitted to reproduce the low-lying states of \(^{12}\text{C}\). In order to solve the Schrödinger equation we expand the bosonic wave function using the symmetric hyperspherical harmonics basis functions [6, 7],
\[ \Psi_{LM}(\rho, \Omega) = \sum_{K\alpha} \sum_n C_{K\alpha n} \Phi_n(\rho) Y_{KLM\alpha}(\Omega), \] (6)

and replace the 2-body potential by an effective potential constructed through the Lee–Suzuki similarity transformation method [8], as explained in [5]. The first sum in the expansion, Eq. (6), runs over all the hyperspherical harmonics functions with hyperangular quantum number \( K \leq K_{max} \) and angular quantum numbers \( L, M \) that belong to the symmetric representation \( \Gamma = [N] \) of the permutation group \( S_N \). For the hyperradial basis states, \( \Phi_n(\rho) \), we use the generalized Laguerre functions.

3 Results

The free parameters in the force model of Eqs. (4,5) should be fixed through comparison to the available experimental data. In the current work we have used two parameter sets fitted by Fedotov et al. [2] to reproduce energy and width of the \(^8\text{Be}\) ground state as well as of the ground state and the first excited \((J^\pi = 0^+)\) states of \(^{12}\text{C}\). These sets, which we refer to as FKKM1 and FKKM2, include the 2-body parameters sets number 1 and 2 of table I in [2] and the 3-body parameters sets number \( N_1 = 3 \) for FKKM1 and \( N_1 = 1 \) for FKKM2 of table II in [2], see table 1.

Comparison of our results with the results of Fedotov et al. [2] for \(^{12}\text{C}\) are presented in table 2. We confirm that the potential models describe the ground and first excited \( J = 0^+ \) states of \(^{12}\text{C}\) very well, but our results with the FKKM2 parameter set slightly differ for the ground state energy from those reported in [2].
An α-particle model for $^{16}$O, is there a new 4-body scale?

Table 1. The parameters for the FKKM1 and FKKM2 two- and three-body forces [2]. Note that for the FKKM models $V_{r/a}(\ell) = V_{r/a}^{(2)}$ for all $\ell$. The strength parameters are given in [MeV] while the range parameters are given in [fm$^{-1}$].

<table>
<thead>
<tr>
<th></th>
<th>$V_r^{(2)}$</th>
<th>$\mu_r$</th>
<th>$V_a^{(2)}$</th>
<th>$\mu_a$</th>
<th>$V_0^{(3)}(L_3 = 0)$</th>
<th>$\mu_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>FKKM1</td>
<td>82.563</td>
<td>1/1.53</td>
<td>26.1</td>
<td>1/2.85</td>
<td>-24.048</td>
<td>$\sqrt{2}/4.6530$</td>
</tr>
<tr>
<td>FKKM2</td>
<td>279.206</td>
<td>1/1.53</td>
<td>40.0</td>
<td>1/2.85</td>
<td>-29.291</td>
<td>$\sqrt{2}/5.1213$</td>
</tr>
</tbody>
</table>

The corresponding results for $^{16}$O and $^{20}$Ne are presented in table 3. It can be seen that both models tend to overbind these two nuclei. Moreover, although the force models lead almost to the same results in the 3-body sector, their predictions differ quite substantially in the 4- and 5-body sectors.

In order to reproduce the binding energy of $^{16}$O we introduce a novel four-body force. As for the 3-body force we have used a simple gaussian form, namely $V^{(4)} = V_0^{(4)} e^{-(\mu_4 r)^2}$. Altogether the potential for the oxygen nucleus consists of the FKKM 2- and 3-body gaussian forces [2] and our additional 4-body force. It should be noted that when applying the FKKM models to the 4- and 5-body systems we find that the best results are obtained when the 3-body force is active only in relative 3-body $S$-waves (the $L_3 = 0$ subspace).

Since the work of reference [2] was limited to the $J^\pi = 0^+$ states of the carbon nucleus, this interpretation will not alter any of their results. The 4-body range and strength parameters ($\mu_4, V_0^{(4)}$), have been chosen to reproduce the ground state properties of $^{16}$O. For both models we have fixed the range parameter $\mu_4$ to the value $\mu_4 = 1/\sqrt{8}$ [fm$^{-1}$], which roughly corresponds to the matter radius of $^{16}$O. The strength parameter $V_0^{(4)}$ has been fitted to the binding energy. For the FKKM1 model we obtain $V_0^{(4)} = 177.0$ MeV, while for the FKKM2 model we find $V_0^{(4)} = 341.5$ MeV.

Having fitted the parameters of the 4-body force for the FKKM1 and FKKM2 models we can test the interactions by calculating the excitation spectrum of $^{16}$O. For the $J^\pi = 0^+_1$ level we get $E_{0_1^+} = -7.6 \pm 0.1$ MeV (FKKM1) and $E_{0_1^+} = -8.2 \pm 0.1$ MeV (FKKM2), while the experimental value is given by $E_{0_1^+} = -8.38724 \pm 0.001$ MeV [9]. One sees that both theoretical results are rather close to the experimental value with relative differences of about 10 % (FKKM1) and 2 % (FKKM2). For the $J^+ = 2_1^+$ state we have the following picture: $E_{2_1^+} = -7.51954 \pm 0.0006$ MeV [9] (experiment), $E_{2_1^+} = -7.45 \pm 0.2$ MeV (FKKM1), and $E_{2_1^+} = -8.2 \pm 0.1$ MeV (FKKM2). In this case the FKKM1 force is in good agreement with the experimental value (difference
about 1 %), whereas the FKKM2 model leads to a slight overbinding of about 10 %.

Table 2. Energies [MeV] and radii [fm] of the ground and first excited state of $^{12}$C with the FKKM1 and FKKM2 potentials. The nuclear radius is given by $R_i^{(3)} = \sqrt{R_\alpha^2 + R_i^2}$ where $R_\alpha = 1.47$ [fm] and $R_i$ is the rms matter radius for point like particles.

<table>
<thead>
<tr>
<th></th>
<th>$E_0$</th>
<th>$R_0^{(3)}$</th>
<th>$E_1$</th>
<th>$R_1^{(3)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>FKKM1 this work</td>
<td>-7.2738</td>
<td>2.547</td>
<td>0.367</td>
<td>3.92</td>
</tr>
<tr>
<td>FKKM1 [2]</td>
<td>-7.2747</td>
<td>2.55</td>
<td>0.3795</td>
<td>4.0</td>
</tr>
<tr>
<td>FKKM2 this work</td>
<td>-7.4987</td>
<td>2.816</td>
<td>0.367</td>
<td>3.92</td>
</tr>
<tr>
<td>FKKM2 [2]</td>
<td>-7.2747</td>
<td>2.82</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Experiment</td>
<td>-7.2747</td>
<td>2.47</td>
<td>0.3795</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 3. Ground state energies [MeV] for the $^{12}$C, $^{16}$O and $^{20}$Ne nuclei with the FKKM1, FKKM2 force models.

<table>
<thead>
<tr>
<th></th>
<th>$^{12}$C</th>
<th>$^{16}$O</th>
<th>$^{20}$Ne</th>
</tr>
</thead>
<tbody>
<tr>
<td>FKKM1</td>
<td>-7.2738</td>
<td>-31.15</td>
<td>-84.51</td>
</tr>
<tr>
<td>FKKM2</td>
<td>-7.2747</td>
<td>-25.08</td>
<td>-57.10</td>
</tr>
<tr>
<td>Experiment</td>
<td>-7.2747</td>
<td>-14.437</td>
<td>-19.17</td>
</tr>
</tbody>
</table>

4 Conclusions

In this work we employed an α-cluster model to study the low-lying energy spectra of the $^{12}$C, $^{16}$O and $^{20}$Ne nuclei. To this end, we have solved the Schrödinger equation for the $N$-body problem ($N = 3, 4,$ and 5 for $^{12}$C, $^{16}$O, and $^{20}$Ne, respectively) in the framework of the EIHH method.

The observations we draw from the application of the α-cluster model to the study of $^{16}$O and $^{20}$Ne are as follows: (i) local force models, which include only 2- and 3-body terms, overbind $^{16}$O and $^{20}$Ne, (ii) force models, which are essentially identical when dealing with the 3-body system, can lead to rather different predictions in the 4- and 5-body systems, (iii) by an introduction of a new 4-body force it is possible to reproduce the low-lying $^{16}$O spectrum. Observation (ii) suggests an interesting question: is it possible to introduce a force model where 2- and 3-body terms are sufficient for reproducing the 4-body system? Probably non-local force models can play an important role in answering this question.
As a matter of fact with the present models one is forced to introduce a new term, i.e. a new scale, with each α-particle added. Such a behaviour was claimed by Adhikari, Frederico, and Goldman [10] to be inherent to the low-energy expansion of the potential in the bosonic N-body problem. If indeed this is the case, then the α-cluster model exhibits an example where the importance of N-body force terms falls off very slowly. In this respect the 5-body Neon nucleus is a very interesting case study.

References

Molecular-nuclear transition $^{6}\text{LiD} \rightarrow ^{8}\text{Be}^\ast$: search with paired $\Delta E - E$ telescope

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Abstract. In the present report, results of new measurements of the probability of molecular-nuclear transitions $^{6}\text{LiD} \rightarrow ^{8}\text{Be}^\ast$ performed with improved technique are presented. The measuring system consisted of two $\Delta E - E$ telescopes, and it provided the identification of nuclear charge $Z$ for every detected event. During more than one month period of measurements only one event that could assumingly be ascribed to the searched effect was discovered. Lower limit for the half–life of the process is $3 \cdot 10^{19}$ y.

Recently, V. Belyaev and co-workers, the references [1, 2], paid attention at a possible increase of reaction probability of molecular-nuclear transitions in some few-atomic molecules due to the existence of nuclear resonances. If the energy and quantum numbers of molecular state and nuclear resonance coincide, then the above molecule and nucleus can be considered as two degenerate states of the same physical system. The long tail of nuclear wavefunctions is expected to lead to a noticeable overlap with the molecular functions, and hence to a measurable admixture of nuclear state in the corresponding molecules, or to the transitions between molecular and nuclear states, so-called molecular-nuclear transitions (MNT).

Thus, it is reasonable to search for a mixture of nuclear state in the molecular compound. Earlier, experiments for MNT effect were carried for $H_2O^\ast(1^-) \rightarrow ^{18}\text{Ne}^\ast(4.522;1^-)$ system. The result for lower limit of a half-life time of water decaying via the above channel was $T_{1/2} = 10^{19}$ y, ref. [3].

Another promising candidate for the effect of spontaneous molecular-nuclear transition is $^{6}\text{LiD} \rightarrow ^{8}\text{Be}^\ast$, where $^{8}\text{Be}$ is expected to be produced in a high excited state (22.28;2$^+$), identical in energy to some state of the $^{6}\text{LiD}$ molecule. Figure 1 shows the above situations for two mentioned systems $H_2O^\ast \rightarrow ^{18}\text{Ne}^\ast$ and $^{6}\text{LiD} \rightarrow ^{8}\text{Be}^\ast$. Following the work [2], the probabil-

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Molecular-nuclear transition can be presented in the form: 

\[ W(s^{-1}) = \omega(E_1) \exp[0.67\eta(E_2)] \cdot Q, \]

where \( \omega(E_1) \) is a frequency with which nuclei in a two-atomic molecule approach the barrier, \( E_1 \) is the binding energy of \( ^6\text{LiD} \) molecule (few eV), and \( Q \) is defined by the overlap integral between electronic configurations of \( ^6\text{LiD} \) molecule and \( ^8\text{Be} \) atom, \( 1 > Q > 0.01 \), and Zemmerfeld parameter \( \eta(E_2) = Z_1Z_2e^2/\hbar v \) where \( v \) is the relative velocity of the outgoing particles defined by the energy of transition between molecular and nuclear states of the system. This energy is approximately equal to the width of nuclear resonance.

The case of \( ^6\text{LiD} \) represents a good opportunity for high sensitive measurements, because the final high excited nucleus decays into two alpha–particles, each with energy \( E = 11.2 \text{ MeV} \). In our first experiments a background of double coincidences at a rate of several events per day was obtained, ref. [4].

In order to eliminate the background, a new technique based on a paired \( \Delta E-E \) telescope was implemented. For this system, detectors of specific ionization losses \( dE/dx \) were manufactured. A sample of \( ^6\text{LiD} \), in the form of a thin layer of fine crystalline powder deposited onto a thin maillar film, was positioned closely between two planar \( Si \) charged particle semiconductor detectors. Two \( \alpha\)-particles emitted simultaneously along the straight opposite directions are expected in the decay of highly excited \( ^8\text{Be} \) produced due to the molecular–nuclear transition \( ^6\text{LiD} \rightarrow ^8\text{Be}^* + 22.4 \text{ MeV} \). Thickness of \( \Delta E \) detectors was 9 \( \mu \), what provided the energy threshold for \( \alpha\)-particle detection as low as \( E_{\text{min}} = 2.6 \text{ MeV} \), thus, it was possible to maximize the thickness of \( ^6\text{LiD} \) layer and minimize losses of the detection efficiency at small angles to the detector plane. Measurement of \( \Delta E_i \) in combination with the total \( \alpha\)-particle energy \( E_i \), gave the exact identification of \( Z \) (atomic number) and \( A \) (atomic mass) of the detected charged particles. The total energy detectors \( E_i \) were 400 \( \mu \) thick. Behind, a pair of thick 750 \( \mu \)-detectors were placed. They served for exclusion of the background events produced by cosmic ray particles, penetrating all arrays, and yielding the coincidence signals.
in both detector telescopes of the array. The identification of the events and the exclusion of background were carried out during a subsequent off-line processing.

In Figure 2, results of calibration of the system with the use of $^{226}Ra$ source are shown. The insert in Figure 2 shows one-dimensional spectrum of $\alpha$-particles from this source. The most intensive $\alpha$-lines belong to $^{226}Ra$ ($E_\alpha = 4.78$ MeV), to radioactive nuclides $^{222}Rn$ ($E_\alpha = 5.49$ MeV), and to Po isotopes $^{218}Po$ ($E_\alpha = 6.00$ MeV), $^{214}Po$ ($E_\alpha = 7.68$ MeV), and $^{210}Po$ ($E_\alpha = 5.30$ MeV). At two-dimensional picture, separate regions of $(\Delta E, E)$-plane correspond to $^{226}Ra$, $^{218}Po$, and $^{214}Po$. The duplet line $E_\alpha = 5.49; 5.30$ MeV corresponds to $^{222}Rn$ and $^{210}Po$. In Figure 3, a two-dimensional $(\Delta E, E)$ spectrum from the measurements with $^6LiD$ sample is presented together with the results of simulation of the response of the system to $Z = 1$ and $Z = 2$ particles, emitted at various angles to the plane of $^6LiD$ sample with taking into account the thickness of the sample. The observed events are due to traces of the radon gas in the measuring chamber, which was emanating from a construction matter of the vacuum chamber elements, and from the $^6LiD$ sample.

In addition to $\alpha$-particles connected with the radon and its daughter products, a group of events with considerably lower values of energy and specific ionization power $dE/dx$ is observed in $(\Delta E, E)$ spectrum. Supposedly, these events corresponds to $Z = 1$ particles. An analysis showed that the above events correspond to $^3H$ nuclei produced in $^6Li + n_{therm} \rightarrow ^4He + ^3H$ reaction induced by thermal neutrons. The thermal neutrons are connected with the nearby heavy ion cyclotron, operated during the collection of the data. The effective cross section of $^6Li$ for thermal neutron capture is very high, $\sigma = 900$ b, thus, a thermal neutron background in the laboratory room might be sufficient for producing some amount of $^3H$ nuclei detected by the system.

Besides the events described above, which are due to the trace amount of radon in the measuring chamber, and to thermal neutron background from the cyclotron, no events were detected. An event marked by a circle in Figure 3 presents the only one exclusion. The values $\Delta E$ and $E$ for this event make it
Molecular-nuclear transition $^6\text{LiD} \rightarrow ^8\text{Be}^*$

Figure 3. Two-dimensional ($\Delta E, E$) spectrum from the measurements with $^6\text{LiD}$ sample.

Regions corresponding to $Z = 1$ and $Z = 2$ particles are indicated. Lines ab indicate location of points $(E_1, dE_1)$ for $\alpha$–particles incident onto the detectors at angles to the plane of detector in the range from $\theta = 90^\circ$ (points a) up to $\theta = 50^\circ$ (points b). A circle marks the only one possible candidate for the MNT effect in the system $^6\text{LiD} \rightarrow ^8\text{Be} \rightarrow \alpha + \alpha$. Events in $Z = 1$ region correspond to $^3\text{H}$ nuclei from $^6\text{Li} + n_{\text{therm}} \rightarrow ^4\text{He} + ^3\text{H}$ reaction induced by thermal neutrons in the environments due to operating HIC of NRL of JINR.

It is possible to ascribe this event to $\alpha$–particle with energy $E \approx 8.5$ MeV, which can be expected in the decay of excited $^8\text{Be}$ produced in the result of molecular–nuclear transition $^6\text{LiD} \rightarrow ^8\text{Be} \rightarrow \alpha + \alpha$, when two $\alpha$–particles are emitted with the energy $\sim 11.1$ MeV (if this event corresponds to the emission from inside layers of the sample). Certainly, with this low statistics it is impossible to make a definite conclusion about observation of the above process.

The obtained data allows to estimate the lower limit for the probability of the molecular-nuclear transition in the system $^6\text{LiD} \rightarrow ^8\text{Be}$.

For the half–life period $T_{1/2}$, the estimate is as follows:

$$T_{1/2} \geq \ln 2 \cdot \frac{\varepsilon \cdot A \cdot m}{dN/dT \cdot M} = 2.4 \cdot 10^{19} \text{ y}.$$  

Here, $A = 6.02 \cdot 10^{23}$ mole$^{-1}$ is Avogadro’s number, $\varepsilon$ detection efficiency of the telescopic $(E - \Delta E)$ assembly (defined by the geometry of detection for a distant detector of the assembly, i.e., the $E$ detector; under the experimental condition, $\varepsilon = 8.6\%$ (estimated by a simulation); $m$ mass of $^6\text{LiD}$ sample, $m = 50$ mg; $M$ molecular weight of $^6\text{LiD}$ compound, $M = 8$; $dN/dT$ counting rate.

Thus, the value $T_{1/2} \geq 2.4 \cdot 10^{19}$ y for the lower limit of the half–life time of the decay of $^6\text{LiD}$ via the channel $^6\text{LiD} \rightarrow ^8\text{Be}^* \rightarrow 2\alpha$, is obtained. The results of experiments with $^2\text{H}O$ and $^6\text{LiD}$ indicate that, probably, some factors slowing down the MNT processes exists, and that more detailed theory of the effect is needed. Moreover, more sensitive experiments are desirable.

One of new experiment, now in preparation, consists of detecting total $\alpha\alpha$–decay energy by a liquid scintillation counter with thin powdered $^6\text{LiD}$ introduced into the liquid scintillator in a form of emulsion. Special mechanism main-
tains permanent rotation and rocking of the counter for preventing sedimentation of the powder onto the walls of counter during lengthy measurements. The expected sensitivity is $T_{1/2} \approx 10^{21} \text{ y}$. Another experiment will use track detectors CR–39 with a large total area in back-to-back configuration. This type of detectors allows $Z$ and $A$ identification and determination of coordinates for every detected $\alpha-\alpha$ event. Estimated sensitivity of this experiments is $T_{1/2} = 10^{23} \div 10^{24} \text{ y}$ for the lower limit of half-life.

**References**

Tools for assigning resonance structures in collisions of few-body quantum systems

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Abstract. The complex dilated Mittag-Leffler, the T-matrix and the Siegert pseudostate methods are briefly reviewed. Their respective strengths and weaknesses and some recent results are discussed.

1 Introduction

Recent experimental development in atomic and molecular physics allows better energy resolution at relatively low collision energies. The atom-diatom experiments on the \(F + HD\) of Liu et al. [1] gave, for the first time, evidence for an isolated resonance as a triatomic reaction complex. The double electrostatic storage ring DESIREÉ [2], currently being constructed at Stockholm University, is expected to produce data on a variety of collisions between atomic and molecular systems. For example, it should be able to collide positive and negative ions, or ions and neutral atoms, or molecules with a very small relative kinetic energy (\(\sim 10 \text{ K}\)). The corresponding cross sections will most likely have peaks which may be the signature of resonances. Theoreticians therefore need to design tools that will be able to analyze these data.

Below we discuss the results of some recent [3, 4, 5, 6, 7, 8] Model potential studies, which may be instrumental in analyzing structures in a cross section and decide if a certain peak is the result of one or several resonances.
2 Three Theoretical Tools

All discussions below relate to the Schrödinger equation written as

\[ \left[ -\frac{1}{2} \frac{d^2}{dx^2} + V(x) - E \right] \phi(x) = 0, \tag{1} \]

where \( V(x) \) is a potential describing a single channel radial problem on a semiaxis \( x \in [0, +\infty) \), or a barrier transmission problem on entire axis \( x \in (-\infty, +\infty) \).

The complex dilation method applied to the radial problem defines the coordinate transformation \( x \to g(x) \) such that

\[ |g(x)| \to 0 \text{ when } x \to +\infty \text{ for real } \theta < \theta_{\text{crit}} \text{ and real } x_0 \geq 0. \]

This transforms a purely outgoing wave into a square integrable one. A similar transformation can be applied to the barrier transmission problem. Using these transformations we obtain a complex dilated Schrödinger equation, which, with similarly dilated boundary conditions, leads to a complex eigenvalue problem [3, 12].

2.1 Mittag-Leffler expansion and complex scaling – the CML method

The partial-wave \( S \)-matrix is normally defined by the two Jost solutions \( f_{\ell}^{\pm}(k, x) \), which in turn are expressed in terms of the Wronskian [9]. The standard Green’s formula for a second order differential operator \( H \) can now be generalized [3, 10] to the analytically continued Hamiltonian. This enables us to show that the Wronskians defining the Jost functions and therefore the partial-wave \( S \)-matrix \( S_\ell(z) \) can be continued analytically using the complex dilation technique. Thus \( S_\ell \) becomes a meromorphic function in a sector of the fourth quadrant of the complex momentum \( k = \sqrt{2E} \) plane (see Refs. [3, 10]). Now, let \( S_\ell(z) \) be analytic at the origin and meromorphic within the interior region bounded by a closed contour \( C \). Assuming that there are poles at \( k = k_j \) and using the Cauchy’s integral theorem, we can express \( S_\ell(k) \) as

\[
S_\ell(k) = S_\ell(a) + \sum_j \text{Res} \left[ S_\ell(k_j) \right] \left\{ \frac{1}{k - k_j} + \frac{1}{k_j - a} \right\} k - a \int_C \frac{S_\ell(z) dz}{(z - k)(z - a)}. \tag{2}
\]

This so-called Mittag-Leffler expansion of the partial wave \( S \)-matrix \( S_\ell(z) \) focuses our attention on the poles \( k_j \) and their residues \( \text{Res} \left[ S_\ell(k_j) \right] \). We have shown [3] that the residues can be calculated from the resonant wave function \( \varphi(k_j, \eta x) \) and the Jost solutions \( f^{-}(k, x) \) as

\[
\text{Res} \left[ S_\ell(k_j) \right] = i \left[ \frac{W[f_\ell^{-}(k_j, x), \varphi_\ell(k_j, x)]}{4 \eta_k} \right]^2, \]

which can be shown to be independent of the complex dilation. A generalization of Eq. (2) to a two-channel problem was recently studied in Ref. [7] where it was used together with the Argand plot technique for analyzing the role played by individual poles.
2.2 The T-matrix, Green function complex-scaling approach – the CT method

The S-operator $\hat{S}$ can be expressed in terms of the transition operator $\hat{T}$, which in turn can be expressed via the interaction potential $\hat{V}$ and Green operator $\hat{G}$

$$\hat{S} = 1 - 2\pi i \hat{T}; \quad \text{with} \quad \hat{T} = \hat{V} + \hat{V}\hat{G}\hat{V}. \quad (3)$$

This technique has been studied by Rescigno et al. [11] and Moiseyev [12]. All quantities in Eq. (3) can be expanded into partial waves. The partial-wave Green function can further be expanded in its eigenfunctions to obtain

$$T_{i}^{\ell f} = \langle \Phi_f | V | \Phi_i \rangle + \sum_{j} \frac{\langle \Phi_f | V | \varphi_{\ell}(k_j, x) \rangle \langle \varphi_{\ell}(k_j, x) | V | \Phi_i \rangle}{E - E_j}. \quad (4)$$

Now we can perform complex scaling and use Eq. (4) to obtain an expression for the S-matrix in the explicit form. In particular, for the orbital momentum $\ell = 0$, using $\Phi_f = \Phi_i = \sqrt{2/(\pi k)} \sin kx$ we obtain

$$S_{0}(k) = 1 - \frac{4i}{k} \int dx \sin^{2}(kx) V(x)$$

$$- \frac{2i}{k} \sum_{n=1}^{\infty} \frac{1}{E - E_n} \left( \int dx g'(x) \sin[kg(x)] V[g(x)] \varphi_{0}[k_n, g(x)] \right)^{2}. \quad (5)$$

Also here we are able to express the partial-wave S-matrix in terms of a background and its poles. In particular, we can study the influence of a single pole by omitting it in the sum in Eq. (5) and computing the remaining cross section.

2.3 Siegert pseudostate method – the SPS method

In recent papers [4, 6] we demonstrate the common features of barrier scattering on the interval $x \in (-\infty, +\infty)$ and the two-channel radial problem $[x \in [0, +\infty)]$ using the Siegert pseudostate method. A Siegert state $\phi(x)$ for a barrier potential $V(x)$ is defined as the solution of Eq. (1) with the boundary conditions

$$\left( \frac{d}{dx} + i k_1 \right) \bigg|_{x=a_1} \phi(x) = 0, \quad \text{and} \quad \left( \frac{d}{dx} - i k_2 \right) \bigg|_{x=a_2} \phi(x) = 0.$$

It is presumed that $V(x) = v_1$ for $x < a_1$ and $V(x) = v_2$ for $x > a_2$ with $v_2 > v_1$. The momenta are defined by $k_1 = \sqrt{2(E - v_1)}$ and $k_2 = \sqrt{2(E - v_2)}$. The solutions of this boundary problem exist only for discrete values of energy $E_n$; these eigenenergies are generally complex-valued and correspond to the poles of the S-matrix or the Green function.

Using this method we can express the S-matrix elements in terms of product functions containing the eigenmomenta $k_{1,2}^{(n)}$. The explicit expressions for the residues in terms of Siegert poles are as follows:

$$\text{Res} \left[ S_{11}(E_j) \right] = \exp \left( i 2k_1^{(j)} a_1 \right) \frac{1}{q} \left( k_1^{(j)} \right)^{2} k_2^{(j)} \prod_{n \neq j} \frac{1}{2q} \frac{k_1^{(j)} k_2^{(n)} + k_1^{(n)} k_2^{(j)}}{k_1^{(j)} - k_1^{(n)}}.$$

Assigning resonance structures
Table 1. Comparison of $\text{Res}[S_{12}(E_j)]$ with $M_j ≡ \sqrt{\text{Res}[S_{11}(E_j)] \text{Res}[S_{22}(E_j)]}$, using S-matrix element residues calculated numerically (Rakityansky and Elander [7]); $\zeta = 10^{-4}$.

<table>
<thead>
<tr>
<th>Resonance energy $E_j$</th>
<th>$\text{Res}[S_{12}(E_j)]$</th>
<th>$M_j$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.768197 – i 0.000710</td>
<td>(0.26429 – i 0.02943) × $\zeta$</td>
<td>(0.26288 – i 0.029206) × $\zeta$</td>
</tr>
<tr>
<td>7.241200 – i 0.755956</td>
<td>0.90478 + i 0.25589</td>
<td>0.901791 + i 0.254717</td>
</tr>
<tr>
<td>8.171217 – i 3.254166</td>
<td>–7.30357 – i 0.80750</td>
<td>–7.2852 – i 0.797861</td>
</tr>
<tr>
<td>8.072634 – i 9.572815</td>
<td>30.61007 + i 17.10104</td>
<td>30.5965 + i 17.0329</td>
</tr>
<tr>
<td>7.123813 – i 13.012669</td>
<td>–5.46659 + i 44.46505</td>
<td>5.39717 – i 44.437</td>
</tr>
</tbody>
</table>

\[
\text{Res}[S_{22}(E_j)] = \exp \left( -\frac{i 2k_2(j)}{q} \right) \left( \frac{1}{k_1(j)} \right)^2 \prod_{n \neq j} \frac{1}{2q} \frac{k_1(j)k_2(n) + k_1(n)k_2(j)}{k_2(j) - k_2(n)},
\]

\[
\text{Res}[S_{12}(E_j)] = \exp \left( \frac{i k_1(j) a_1 - i k_2(j) a_2}{q} \right) \left( \frac{1}{k_1(j)k_2(j)} \right)^{3/2} \prod_{n \neq j} \frac{1}{2q} \frac{k_1(j)k_2(n) + k_1(n)k_2(j)}{k_1(j) - k_1(n)}^{1/2} \left( k_2(j) - k_2(n) \right)^{1/2} \left( k_2(j) - k_2(n) \right)^{1/2},
\]

where $q = \sqrt{(v_2 - v_1)/2}$. These formulae are equivalent to the expressions presented in Ref. [6] in terms of the uniformization variable $u$. Basing on the Breit-Wigner formula for isolated resonances

\[
S_{\alpha\beta}(E) \approx e^{2i\delta_0} \delta_{\alpha\beta} - i e^{i(\delta_0 + \delta_\beta)} \frac{\sqrt{T_\alpha T_\beta}}{E - E_0 + i\Gamma/2},
\]

we find the relation between the S-matrix residues and partial widths $\Gamma_\alpha$:

\[
\sqrt{T_\alpha T_\beta} = |\text{Res}[S_{\alpha\beta}(E_m)]|.
\]

A universal relation exists between the residues, as seen from formula (6): $\text{Res}[S_{12}(E_m)]$ equals a geometric mean of $\text{Res}[S_{11}(E_m)]$ and $\text{Res}[S_{22}(E_m)]$,

\[
\text{Res}[S_{12}(E_m)] = \sqrt{\text{Res}[S_{11}(E_m)] \text{Res}[S_{22}(E_m)]}.
\]

Applying Eq. (7) to the two-channel problem studied in Ref. [7], we find, as seen in Table 1, a close agreement especially for the lower resonances, which implies that they were computed with a better accuracy than the higher ones.

3 Discussion

3.1 Formal aspects

The aim of the present contribution is to discuss various ways to assign quantum numbers and understand the origin of resonant structures in few-body collisions. In practice we need formally stable and computationally efficient methods. As
discussed above, it is meaningful to characterize a resonance through two complex quantities – its energy and its residue$^1$.

When the three methods are applied to one-dimensional problems, we find a particular difference. The CML and the SPS methods describe the contributions to the partial-wave S-matrix in terms of its residues at the corresponding poles. These contributions, apart from the $(k-k_n)$ in the denominator, are independent of the scattering energy. The CT methods, on the other hand, contain resonance contributions in terms of matrix elements which are dependent on the scattering energy [5]. A comparison of the results obtained from Eqs. (2) and (5), reported in Ref. [8], shows that the results are numerically identical. We can compare the CML and the CT methods by removing one and the same resonance from the two sums in Eqs. (2) and (5). When doing so, we still get good agreement between the cross sections obtained by these two techniques.

### 3.2 Numerical aspects

The numerical realization of the CML theory is computationally heavy, this is especially true for the contour integral in Eq. (2). For this reason numerical applications of this theory are limited to a few channels [7].

Our numerical realization of the CT and SPS methods is based on a one-dimensional finite element code [14] which is rather efficient. In particular, the SPS S-matrix is created from the Siegert pseudostates, which thus makes the present SPS S-matrix numerically stable. The CT method seems to be able to only converge for small complex dilation angles, $\theta$, and will therefore only reveal explicitly the influence of the more narrow resonances. This disadvantage may be compensated by the advantage that is easily extended from two channels to a realistic set of several (5 -10) channels.

### 4 Conclusions

We have here reviewed methods which show how the technique of analytic continuation can be used to compute the contributions of resonances and background to the cross sections. The idea behind this approach is based on a model-potential study [15] where it was shown how the spectral density can be decomposed into components from its poles, which are the same as the S-matrix poles, and a free-particle background (see also contribution by Matthias Back to this conference and [16]). The results obtained so far show that the residues of the CML and CT methods are numerically identical. The cross sections obtained with the two methods are also in close numerical agreement. The CML method allows us to separate the contributions of narrow as well as wide resonances from the background, which is set by the choice of the integration contour. The convergence of the contributions from the complex dilated continuum does on the other hand limit the applicability of the CT method to only separate narrow resonances from a background.

---

$^1$Generally, the entire S-matrix, including its residues, is expressible in terms of Siegert pseudostates [13], albeit this requires a complete set.
Since the SPS method is likely to be a stable method it can be expected to be able of describe the influence of wider resonances, as does the CML method. While the complex-dilation based Mittag-Leffler expansion (CML) and the Siegert pseudostate (SPS) methods are applicable only to one-dimensional problems, the complex-dilated T-matrix approach (CT) is originally formulated for three-dimensional systems. The need to describe wide resonances in realistic problems will finally influence the choice among the three techniques.

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References


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Abstract. We describe basic structure of the two- and three-body T-matrices, scattering matrices, and resolvents continued to the unphysical energy sheets. The description is based on the explicit representations that have been found for analytically continued kernels of the T-operators.

1 Introduction

Resonance is one of the most interesting and intriguing phenomena in quantum scattering. With a resonance one usually associates an unstable state that only exists during a certain time. The original idea of interpreting resonances in quantum mechanics as complex poles of the scattering amplitude (and hence, as those of the scattering matrix) goes back to G. Gamov (1928). For radially symmetric potentials, the interpretation of two-body resonances as poles of the analytic continuation of the scattering matrix has been entirely elaborated in terms of the Jost functions. Beginning with E. C. Titchmarsh (1946) it was also realized that the s-matrix resonances may show up as poles of the analytic continuation of the Green functions.

Another, somewhat distinct approach to resonances is known as the complex scaling (or complex rotation) method. The complex scaling makes it possible to rotate the continuous spectrum of the N-body Hamiltonian in such a way that resonances in certain sectors of the complex energy plane turn into usual eigenvalues of the scaled Hamiltonian. In physics literature the origins of such an approach are traced back at least to C. Lovelace (1964). A rigorous approval of the complex scaling method has been done by E. Balslev and J. M. Combes.
A link between the s-matrix interpretation of resonances and its complex rotation counterpart was established by G. A. Hagedorn (1979) who has proven that for a wide class of potentials the scaling resonances are also the scattering matrix resonances.

If support of the interaction is compact, the resonances of a two-body system can be treated within the approach created by P. Lax and R. Phillips (1967). An advantage of the Lax-Phillips approach is in the opportunity of giving an elegant operator interpretation of resonances. The resonances show up as the discrete spectrum of a dissipative operator which is the generator of the compressed evolution semigroup.

For more details on the history of the subject and other approaches to resonances, as well as for a bibliography we refer to paper [1]. Here we only notice that, in contrast to the “normal” bound and scattering states, the resonant ones are still a mysterious object and many questions related to resonances remain unanswered. In particular, it is still unknown how to describe (in an indisputable way) the scattering of a particle on a resonant state of two other particles. To say the truth, there is a problem even with definition of resonance since resonances are not a unitary invariant of a self-adjoint (Hermitian) operator. Moreover, following to B. Simon [2], one may conclude that no satisfactory definition can rely on a single Hamiltonian and always an extra structure is necessary. Say, an unperturbed dynamics (in quantum scattering theory) or geometric setup (in acoustical or optical problems). Resonances are always relative as the scattering matrix itself.

In our approach we follow the typical setup where the resonances arising due to an interaction $V$ are considered relative to the unperturbed dynamics described by the kinetic energy operator $H_0$. The resolvent $G(z) = (H - z)^{-1}$ of the total Hamiltonian $H = H_0 + V$ is an analytic operator-valued function of $z \in \mathbb{C} \setminus \sigma(H)$. The spectrum $\sigma(H)$ of $H$ is a natural boundary for holomorphy domain of $G(z)$ considered as an operator-valued function. However the kernel $G(\cdot, \cdot, z)$ may admit analytic continuation through the continuous spectrum of $H$. Or the form $\langle G(z) \varphi, \psi \rangle$ may do this for any $\varphi, \psi$ of a dense subset of the Hilbert space $\mathcal{H}$. Or the “compressed” resolvent $PG(z)P$ admits such a continuation for $P$ the orthogonal projection onto a subspace of $\mathcal{H}$. In any of these cases one deals with the Riemann surface of an analytical function.

In the simplest example with $H = H_0 = -\Delta$, the two-body kinetic energy operator in coordinate representation, we have

$$G(x, x', z) = \frac{1}{4\pi} \frac{e^{iz^{1/2}|x-x'|}}{|x - x'|},$$

where $x, x'$ are three-dimensional vectors. Clearly, $G(x, x', z)$ as a function of the energy $z$ has a two-sheeted Riemann surface which simply coincides with that of the function $z^{1/2}$.

In this way one also arrives with the concept of the unphysical energy sheet(s). The copy of the complex energy plane where the resolvent $G(z)$ is considered initially as an operator-valued function is called the physical sheet. The remainder of the Riemann surface is assumed to consist of the unphysical sheets (in general, an unphysical sheet may only be a small part of the complex plane).
Analytic function is uniquely defined by its values on an infinite set in \( \mathbb{C} \) having limiting point(s). Thus, if one knows the resolvent (\( T \)-matrix, \( S \)-matrix) on the physical sheet then one may, in principle, express it on unphysical sheets through its values in the physical sheet. In this case all the study of resonances would reduce to a work completely on the physical sheet.

In [1, 3] we have found just such expressions. More precisely, we have derived explicit representations for the two- and three-body \( G(z) \), \( T(z) \), and \( S(z) \) on unphysical energy sheets in terms of these quantities themselves only taken on the physical sheet. In particular, the representations obtained show which blocks of the scattering matrix are “responsible” for resonances on a certain unphysical sheet.

2 Two-body problem

In general, we assume that the interaction potential \( v \) falls off in coordinate space not slower than exponentially. When studying resonances of a two–body system with such an interaction one can employ equally well both coordinate and momentum representations. However in the three-body case it is much easier for us to work in the momentum space (for an explanation see [1], p. 149). This is one of the reasons why we proceed in the same way in the two-body case. Thus, for the two-body kinetic energy operator \( h_0 \) we set \( (h_0 f)(k) = k^2 f(k) \) where \( k \in \mathbb{R}^3 \) stands for the reduced relative momentum. In case of a local potential we have \( v(k, k') = v(k \square k') \) and \( v(k) = v(-k) \). For simplicity we assume that the function \( v(k) \) is holomorphic in \( k \) on the whole three-dimensional complex space \( \mathbb{C}^3 \).

The transition operator (t-matrix) reads
\[
t(z) = v - vg(z)v, \tag{1}
\]
where \( g(z) = (h - z)^{-1} \) denotes the resolvent of the perturbed Hamiltonian \( h = h_0 + v \). The operator \( t \) is the solution of the Lippmann-Schwinger equation
\[
t(z) = v - vg_0(z)t(z), \tag{2}
\]
that is,
\[
t(k, k', z) = v(k, k') - \int_{\mathbb{R}^3} dq \frac{v(k, q)t(q, k', z)}{q^2 - z} \tag{3}
\]
taking into account that \( g_0(k, k', z) = \delta(k - k')/(k^2 - z) \).

Clearly, all dependence of \( t \) on \( z \) is determined by the integral term on the r.h.s. part of (3) that looks like a particular case of the Cauchy type integral
\[
\Phi(z) = \int_{\mathbb{R}^N} dq \frac{f(q)}{\lambda + q^2 - z} \tag{4}
\]
for \( N = 3 \). Cauchy integrals of the same form but for both \( N = 3 \) and \( N = 6 \) we will also have below in three-body equations of Sec. 3.

Let \( R_\lambda, \lambda \in \mathbb{C} \), be the Riemann surface of the function
\[
\zeta(z) = \begin{cases} (z - \lambda)^{1/2}, & N \text{ odd}, \\ \log(z - \lambda), & N \text{ even.} \end{cases}
\]
If $N$ is odd, $R_{\lambda}$ is formed of two sheets of the complex plane. One of them, where $(z-\lambda)^{1/2}$ coincides with the arithmetic square root $\sqrt{z-\lambda}$, we denote by $\Pi_0$. The other one, where $(z-\lambda)^{1/2} = -\sqrt{z-\lambda}$, is denoted by $\Pi_1$.

If $N$ is even, the number of sheets of $R_{\lambda}$ is infinite. In this case as the index $\ell$ of a sheet $\Pi_{\ell}$ we take the branch number of the function $\log(z-\lambda)$ picked up from the representation $\log(z-\lambda) = \log|z-\lambda| + i2\pi\ell + i\phi$ with $\phi \in [0, 2\pi)$.

The following statement can be easily proven by applying the residue theorem (if necessary, see [3] for a proof).

**Lemma 1.** For a holomorphic $f(q)$, $q \in \mathbb{C}^N$, the function $\Phi(z)$ given by (4) is holomorphic on $\mathbb{C} \setminus [\lambda, +\infty)$ and admits the analytic continuation onto $R_{\lambda}$ as follows

$$
\Phi(z)|_{\Pi_{\ell}} = \Phi(z) - \ell \pi i(\sqrt{z-\lambda})^{N-2}\int_{S^{N-1}} d\mathbf{\tilde{q}} f(\sqrt{z-\lambda}\mathbf{\tilde{q}}),
$$

where $S^{N-1}$ denotes the unit sphere in $\mathbb{R}^N$ centered at the origin. (Position of the argument $z$ in the sheet $\Pi_0$ on the r.h.s. part of (5) is the same as that of the argument of $\Phi|_{\Pi_{\ell}}$ on the sheet $\Pi_{\ell}$.)

Now set $(g_0(z)f_1, f_2) \equiv \int_{\mathbb{R}^3} d\mathbf{q} \frac{f_1(q)f_2(q)}{q^2-z}$ where $f_1$ and $f_2$ are holomorphic. Then by Lemma 1

$$(g_0(z)f_1, f_2)|_{\Pi_1} = (g_0(z)f_1, f_2)|_{\Pi_0} - \pi i \sqrt{z} \int_{S^2} d\mathbf{\tilde{q}} f_1(\sqrt{z}\mathbf{\tilde{q}}) f_2(\sqrt{z}\mathbf{\tilde{q}}),$$

which means that the continuation of the free Green function $g_0(z)$ onto the unphysical sheet $\Pi_1$ can be written in short form as

$$g_0(z)|_{\Pi_1} = g_0(z) + a_0(z)j^\dagger(z)j(z), \quad (6)$$

where $a_0(z) = -\pi i \sqrt{z}$ and $j(z)$ is the operator forcing a (holomorphic) function $f$ to set onto the energy shell, i.e. $(j(z)f)(\mathbf{k}) = f(\sqrt{z}\mathbf{k})$.

Taking into account (6), on the unphysical sheet $\Pi_1$ the Lippmann-Schwinger equation (2) turns into

$$t' = v - v(g_0 + a_0 j^\dagger j)t', \quad t'|_{\Pi_1}.$$  

Hence $(I+v_g) t' = v - a_0 j^\dagger j t'$. Invert $I+v_g$ by using the fact that $t(z) = v - v_g t$ and, hence, $(I + v_g)^{-1}v = t$:

$$t' = t - a_0 t j^\dagger j t', \quad (7)$$

Apply $j(z)$ to both parts of (7) and obtain $jt' = jt - a_0 j t j^\dagger j t'$, which means

$$(I + a_0 j t j^\dagger) j t' = jt, \quad (8)$$

Observe that $I + a_0 j t j^\dagger$ is nothing but the scattering matrix $s(z)$ since the kernel of $s(z)$ reads

$$s(\mathbf{k}, \mathbf{k}', z) = \delta(\mathbf{k}, \mathbf{k}') - \pi i \sqrt{z} t(\sqrt{z}\mathbf{k}, \sqrt{z}\mathbf{k}', z).$$

Hence $jt' = [s(z)]^{-1}jt$. Now go back to (7) and get $t' = t - a_0 t j^\dagger [s(z)]^{-1}jt$, that is,

$$t(z)|_{\Pi_1} = t(z) - a_0(z) t(z) j^\dagger(z) [s(z)]^{-1} j(t(z) t(z). \quad (9)$$
Explicit Representations for the T-Matrix on Unphysical Sheets

All entries on the r.h.s. part of (9) are on the physical sheet. This is just the representation for the t-matrix on the unphysical sheet we looked for. From (9) one immediately derives representations for the continued resolvent,
\[ g(z)|_{\Pi_1} = g + a_0 (I - gv)j^\dagger [s(z)]^{-1}j(I - v), \]
and continued scattering matrix,
\[ s(z)|_{\Pi_1} = \mathcal{E} [s(z)]^{-1} \mathcal{E}, \]
where \( \mathcal{E} \) is the inversion, \((\mathcal{E}f)(\hat{k}) = f(-\hat{k})\). Hence, the resonances are nothing but zeros of the scattering matrix \( s(z) \) in the physical sheet. That is, the energy \( z \) on the unphysical sheet \( \Pi_1 \) is a resonance if and only if there is a non-zero vector \( \mathcal{A} \) of \( L^2(S^2) \) such that \( s(z)\mathcal{A} = 0 \) for the same \( z \) on the physical sheet.

The function \( \mathcal{A}(\hat{k}) \) is the breakup amplitude of the resonance state. This means that in coordinate space the corresponding “Gamov vector” (the resonance solution to the Schrödinger equation) has the following asymptotics
\[ \psi_{\text{res}}(x) \sim x^{-\infty} \mathcal{A}(-\hat{x}) \frac{e^{-i\sqrt{\varepsilon}|x|}}{|x|}. \]

3 Three-body problem

Let \( H_0 \) be the three-body kinetic energy operator in the center-of-mass system. Assume for simplicity that there are no three-body forces and thus the total interaction reads \( V = v_1 + v_2 + v_3 \) where \( v_\alpha, \alpha = 1, 2, 3 \), are the corresponding two-body potentials having just the same properties as in the previous section.

The best way to proceed in the three-body case is to work with the Faddeev components [4]
\[ M_{\alpha\beta} = \delta_{\alpha\beta}v_\alpha - v_\alpha G(z)v_\beta \quad (\alpha, \beta = 1, 2, 3) \]
of the T-operator \( T(z) = V - VG(z)V \) where, as usually, \( G(z) \) denotes the resolvent of the total Hamiltonian \( H = H_0 + V \). The components \( M_{\alpha\beta} \) satisfy the Faddeev equations
\[ M_{\alpha\beta}(z) = \delta_{\alpha\beta}t_\alpha(z) - t_\alpha(z)G_0(z)\sum_{\gamma \neq \alpha} M_{\gamma\beta}(z) \]
with \( G_0(z) = (H_0 - z)^{-1} \) and \( t_\alpha(P, P', z) = t_\alpha(k_\alpha, k'_\alpha, z - p^2_\alpha)\delta(p_\alpha - p'_\alpha) \) where \( k_\alpha, p_\alpha \) denote the corresponding reduced Jacobi momenta (see [1] for the precise definition we use) and \( P = (k_\alpha, p_\alpha) \in \mathbb{R}^6 \) is the total momentum.

Assume that any of the two-body subsystems has only one bound state with the corresponding energy \( \varepsilon_\alpha < 0, \alpha = 1, 2, 3 \). Assume in addition that all of these three binding energies are different. It is easy to see that the thresholds \( \varepsilon_1, \varepsilon_2, \varepsilon_3, \) and 0 are associated with particular Cauchy type integrals in the integral equations (12). By Lemma 1 the two-body thresholds \( \varepsilon_\alpha \) appear to be square-root branching points while the three-body threshold 0 is the logarithmic one. In order to enumerate the unphysical sheets we introduce the multi-index
\( \ell = (\ell_0, \ell_1, \ell_2, \ell_3) \) with \( \ell_0 = \ldots, -1, 0, 1, \ldots \) and \( \ell_\alpha = 0, 1 \) if \( \alpha = 1, 2, 3 \). Clearly, only encircling the two-body thresholds one arrives at seven unphysical sheets. The three-body threshold generates infinitely many unphysical sheets. (There might also be additional branching points on the unphysical sheets, in particular due to two-body resonances.)

It turns out that the analytically continued equations (12) can be explicitly (!) solved in terms of the matrix \( M = \{M_{\alpha\beta}\} \) itself taken only on the physical sheet, just like in the case of the two-body \( t \)-matrix. But, of course, now the result depends on the unphysical sheet \( \Pi_\ell \) concerned. More precisely, the resulting representation reads as follows

\[
M|_{\Pi_\ell} = M + Q_M L S_\ell^{-1} \tilde{L} \tilde{Q}_M. \tag{13}
\]

In the particular case we deal with, \( L \) and \( \tilde{L} \) are \( 4 \times 4 \) scalar matrices of the form \( L = \text{diag}(\ell_0, \ell_1, \ell_2, \ell_3) \) and \( \tilde{L} = \text{diag}(|\ell_0|, \ell_1, \ell_2, \ell_3) \), respectively; \( S_\ell(z) = I + L(S(z) - I)\tilde{L} \) is a truncation of the total scattering matrix \( S(z) \) and the entries \( Q_M, \tilde{Q}_M \) are explicitly written in terms of the half-on-shell kernels of \( M \) (see formula (7.34) of [1]). From (13) one also derives explicit representations for \( G(z)|_{\Pi_\ell} \) and \( S(z)|_{\Pi_\ell} \) similar to those of (10) and (11), respectively.

Thus, to find resonances on the sheet \( \Pi_\ell \) one should simply look for the zeros of the truncated scattering matrix \( S_\ell(z) \), that is, for the points \( z \) in the physical sheet where equation \( S_\ell(z)A = 0 \) has a non-trivial solution \( A \). The vector \( A \) will consist of breakup amplitudes of the resonance state into the various possible channels. Within such an approach one can also find the virtual states.

In order to find the amplitudes involved in \( S_\ell \), one may employ any suitable method, for example the one of Refs. [5, 6, 7] based on the Faddeev differential equations. In these works the approach we discuss has been successfully applied to several three-body systems. In particular, the mechanism of emerging the Efimov states in the \( ^4 \)He trimer has been studied [5, 6].

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\textbf{References}

Stability of charged exciton states in quantum wires

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\textbf{Abstract.} We show that the order of energies of negative ($X^-$) and positive trions ($X^+$) in quantum wires is determined by the relative electron and hole lateral confinements. For equal electron and hole confinement, $X^+$ has a larger binding energy, but a small imbalance towards a stronger hole localization changes the order of the $X^-$ and $X^+$ recombination lines in the photoluminescence spectrum.

\section{1 Introduction}

We study the exciton trions formed when an electron or a hole is bound to a neutral exciton ($X$). The binding energies of the complexes in nanostructures, i.e., in quantum wells \cite{1, 2, 3, 4} and quantum wires \cite{5, 6, 7} are measured in photoluminescence (PL) spectroscopy as shifts between the spectral lines of the complexes with respect to the exciton energy line. Due to the larger effective mass of the hole, in bulk \cite{8} as well as in strictly two-dimensional confinement \cite{2} the binding energy of positive trions ($X^+$) is larger than the negative trion ($X^-$) binding energy. However, in quantum wells the observed \cite{4} $X^-$ and $X^+$ binding energies are nearly equal, which is explained \cite{3, 4} by a stronger hole quantum-well localization enhancing the hole-hole interaction. In quantum dots the localization-related hole-hole interaction enhancement leads to the interchange of the order of the $X^-$ and $X^+$ recombination lines in the (PL) spectrum already for quantum dot diameters as large as 24 donor Bohr radii \cite{10}.

The present work is motivated by a recent experimental study \cite{7} on trions in V-groove GaAs/AlGaAs quantum wires. The $X^-$ was found to be distinctly more stable than $X^+$ (binding energies of $X^-$ and $X^+$ were determined as $-4.2$ and $-4.2$ respectively). \textsuperscript{*Article based on the presentation by F. Peeters at the Fourth Workshop on the Dynamics and Structure of Critically Stable Quantum Few-Body Systems, MPIPKS, Dresden, Germany, 2005. Received November 14, 2005, Accepted November 23, 2005

\textsuperscript{**E-mail address:} francois.peeters@ua.ac.be
-2.9 meV, respectively). In a previous theoretical study [5] of trions in quantum wires $X^+$ was found to be more stable than $X^-$, which was obtained in the case of equal hole and electron confinement. A crossing of $X^-$ and $X^+$ PL lines as function of the wire width has previously been obtained in a quantum Monte-Carlo study [6] of a quantum wire with a square well confinement potential. Here, we demonstrate that the observed [7] order of $X^-$ and $X^+$ energy lines is due to the enhanced hole localization.

2 Theory

We apply the single band model for the electron and the hole and consider a harmonic oscillator confinement potential in the directions perpendicular ("lateral") to the wire with $l_{e(h)}$ the oscillator length for the electron (hole) [9]. We assume that the lateral confinement is strong, so that only the lowest subband for the electron and hole is occupied. This assumption allows for a reduction of the Schrödinger equation to an effective two-dimensional form, which can be solved numerically with an exact inclusion of the interparticle correlations along the wire[9]. We adopt the donor units, i.e., donor Bohr radius $a_d = 4\pi\epsilon_0\epsilon/\hbar e^2$ for the unit of length and twice the donor Rydberg $2R_d = \hbar^2/m_e a_d^2$ as the unit of energy, where $m_e$ is the band electron effective mass and $\epsilon$ is the dielectric constant. The effective negative trion Hamiltonian after separation of the center of mass motion written with respect to the dissociated system is

$$H^{\text{rel}} = -\frac{1}{2\mu} \left( \frac{\partial^2}{\partial z_{eh1}^2} + \frac{\partial^2}{\partial z_{eh2}^2} \right) - \frac{1}{\sigma} \frac{\partial^2}{\partial z_{eh1} \partial z_{eh2}} + V^{\text{ef}}(l_{eh}; z_{eh1} - z_{eh2}) - V^{\text{ef}}(l_{eh}; z_{eh1}) - V^{\text{ef}}(l_{eh}; z_{eh2}),$$

with the reduced mass of an electron-hole pair $\mu = \sigma/(1 + \sigma)$, $\sigma = m_h/m_e$, and the coordinates of the relative electron-hole positions $z_{eh1} = z_h - z_{e1}$ and $z_{eh2} = z_h - z_{e2}$ along the wire. In Eq. (1) $l_{eh} = \sqrt{(l_e^2 + l_h^2)/2}$ and $V^{\text{ef}}$ is the effective one-dimensional interaction potential [5]

$$V^{\text{ef}}(l; z) = (\pi/2)^{1/2} \text{erfc}(|z|/\sqrt{2l}) \exp(z^2/2l^2)/l,$$

finite at the origin ($V^{\text{ef}}(l; 0) = 1/l$) and approaching the $1/z$ asymptotic at large $z$. Hamiltonian for $X^+$ has the form (1) but with $1/\sigma$ standing in front of the mixed derivative replaced by 1 [9].

3 Results

We consider a quantum wire made of GaAs ($m_h = 0.45m_0$, $m_e = 0.067m_0$, $2R_d = 11.9$ meV, $a_d = 9.8$ nm). Fig. 1 shows the wave function of $X^-$ (a) $X^+$ (b) trions for equal hole and electron oscillator lengths of the lateral confinement. The interaction potentials in the trion Hamiltonians have a minimum along $z_{eh1} = 0$ and $z_{eh2} = 0$ axis corresponding to an electron and a hole in the same position and a maximum along the diagonal $z_{eh1} = z_{eh2}$ corresponding to both electrons (for $X^-$) or both holes (for $X^+$) at the same position. Fig. 1 shows that the
electrons in $X^-$ with light effective masses tunnel easily through the diagonal barrier due to the interelectron repulsion. On the other hand the diagonal barrier is effectively much larger for the heavy-mass holes which leads to the appearance of the characteristic maxima separated by the minimum elongated along the diagonal [see Fig. 1(b)].

![Figure 1. Countour plots of the wave function for $X^-$ (a) and $X^+$ (b) trions for $l = L = 0.2$ with a mass ratio $\sigma = 6.72$ corresponding to GaAs.](image)

The $X^+$ and $X^-$ binding energies are plotted in Fig. 2. Both trions are equally stable for $l_h = 0.92 l_e - 0.38$ nm (see the black line in Fig. 2). For $l_h$ larger (smaller) than $0.92 l_e - 0.38$ nm $X^+$ is more (less) stable than $X^-$. The fit of the calculated $X^-$ and $X^+$ binding energies to the experimental data [7] is obtained at the crossing of the thick gray dotted lines, i.e., for $l_e = 2.95$ nm and $l_h = 1.3$ nm. The obtained fit corresponds to realistic values which give a general idea on the particle localization in the wire (the measurements [7] were performed on a V-groove GaAs/AlGaAs quantum wire with a thickness of the GaAs crescent of 3 nm at the center). Obviously, a more realistic model is required to extract details of the confinement from the experimental data.

4 Conclusions

We found that the order of the $X^-$ and $X^+$ PL lines is interchanged when the lateral confinement of the hole is stronger than the one for the electron due to the modification of the effective interactions in the trion complexes. The present results provide an explanation for the recently experimentally observed larger stability of the negative trion in quantum wires [7]. The magnetic field oriented parallel to the axis of the wire will tend to equalize the electron and hole localization enhancing stronger the $X^+$ binding energy, which can result in a crossing of the $X^+$ and $X$ lines [9].

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Figure 2. Contour plot of the binding energies for positive (blue lines) and negative (red lines) trions (in meV) as function of the electron and hole confinement lengths for GaAs material parameters. Below (above) the black line $X^- (X^+)$ trion is more stable. The dashed lines correspond to experimental [7] data, $E_B(X^-) = 4.2$ meV and $E_B(X^+) = 2.9$ meV.

References

On critical stability of three quantum charges interacting through delta potentials

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Abstract. We consider three one dimensional quantum, charged and spinless particles interacting through delta potentials. We derive sufficient conditions which guarantee the existence of at least one bound state.

1 Introduction

Denote by $x_i, m_i, Z_i e_i, i = 1, 2, 3$, the position, mass and charge of the $i$-th particle. Our system is formally described by the Hamiltonian

$$
\sum_{i=1}^{3} \frac{\hbar^2}{2m_i} \partial_{x_i}^2 + \sum_{1 \leq i < j \leq 3} Z_i Z_j e^2 \delta(x_i - x_j) \quad \text{acting in} \ L^2(\mathbb{R}^3) \ \text{which is defined as the unique self-adjoint operator associated to the quadratic form with domain} \ \mathcal{H}^1(\mathbb{R}^3):
$$

$$
\sum_{i=1}^{3} \frac{\hbar^2}{2m_i} \|\partial_{x_i} \psi\|^2 + \sum_{1 \leq i < j \leq 3} Z_i Z_j e^2 \int_{x_i = x_j} |\psi(\sigma_{i,j})|^2 d\sigma_{i,j}, \quad \psi \in \mathcal{H}^1(\mathbb{R}^3).
$$

Here $\sigma_{i,j}$ denotes a point in the plane $x_i = x_j$. We will consider the cases $m_1 = m_2 =: m > 0$, $m_3 =: M > 0$, $Z_1 = Z_2 = -1$, $Z_3 =: Z > 0$ and answer to the question: for what values of $m/M$ and $Z$ does this system possess at least one bound state after removing the center of the mass?

There is a huge amount of literature on 1-$d$ particles interacting through delta potentials either all repulsive or all attractive, but rather few papers deal with the mixed case. We mention the work of Rosenthal, [7], where he considered $M = \infty$. The aim of this paper is to make a systematic mathematical study of

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the Rosenthal results and extend them to the case $M < \infty$. It has been shown in [1] and [2] that these delta models serve as effective Hamiltonians for atoms in intense magnetic fields or quasi-particles in carbon nanotubes. As one can see in ([4], [5], [6], [3]), they also seem to be relevant for atomic wave guides, nano and leaky wires.

2 The spectral problem

Removing the center of mass. Using the Jacobi coordinates: $x := x_2 - x_1$, $y := x_3 - (m_1 x_1 + m_2 x_2)/(m_1 + m_2)$ and $z := \sum_i m_i x_i/\sum_i m_i$, we get the 2-d relative motion formal Hamiltonian $\tilde{H} = -\hbar^2/m(\partial_x^2 + 2m_3/M \hbar^2 \partial_y^2 + e^2\delta(x) - Ze^2\delta(y - \frac{\pi}{4}) - Ze^2\delta(y + \frac{\pi}{4})$. Define $\alpha^2 := (M + 2m)/4M$ and $\nu(\alpha) := \sqrt{1/4 + \alpha^2}$. Let $J$ be the Jacobian of the coordinate change $(x', y') = \{2\nu(\alpha)\hbar^2/(mZe^2)\}(x, y\alpha)$, and define the unitary $(U^{-1}f)(x, y) = \sqrt{J}f(x', y')$. Consider three unit vectors of $\mathbb{R}^2$ given by $A_1 := \frac{1}{\nu(\alpha)}(\alpha, -\frac{1}{2})$, $A_2 := \frac{1}{\nu(\alpha)}(-\alpha, -\frac{1}{2})$, and $A_3 := (0, 1)$. Define $A_i^\dagger$ as $A_i$ rotated by $\pi/2$ in the positive sense. Then $U\tilde{H}U^{-1} = \{mZ^2e^4\}/\{2\hbar^2\nu(\alpha)^2\} H$, where:

$$H := -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} - \delta(A_1^\dagger(x, y)) - \delta(A_2^\dagger(x, y)) + \lambda\delta(A_3^\dagger(x, y)), \quad \lambda := \frac{\nu(\alpha)}{Z}.$$

We denote by $\theta_{i,j}$ the angle between the vectors $A_i$ and $A_j$. We give some typical values of all these parameters (see fig. 1).

The skeleton Let $A$ be unit vector in $\mathbb{R}^2$. If one introduce the "trace" operator $\tau_A : \mathcal{H}^1(\mathbb{R}^2) \to L^2(\mathbb{R})$ defined as $(\tau_A \psi)(s) := \psi(sA)$ and if we let $\tau : \mathcal{H}^1(\mathbb{R}^2) \to \bigoplus_{i=1}^3 L^2(\mathbb{R})$ be defined as $\tau := (\tau_{A_1}, \tau_{A_2}, \tau_{A_3})$, we may rewrite the Hamiltonian $H$ as $H_0 + \tau^* g\tau$ where $2H_0$ stands for the free Laplacian and $g$ is the $3 \times 3$ diagonal matrix with entries $(-1, -1, \lambda)$. Denoting $R_0(z) := (H_0 - z)^{-1}$ and $R(z) := (H - z)^{-1}$ the resolvents of $H_0$ and $H$, one derives at once, with the help of the second resolvent equation, the formula for any $z$ in the resolvent sets of $H_0$ and $H$:

$$R(z) = R_0(z) - R_0(z)\tau^*(g^{-1} + \tau R_0(z)\tau^*)^{-1}\tau R_0(z). \quad (1)$$

Using the HVZ theorem (see [8] for the case with form-bounded interactions), we can easily compute the essential spectrum: $\sigma_{ess}(H) = [-\frac{1}{2}, \infty)$. Its bottom
is given by the infimum of the spectrum of the subsystem made by the positive charge and one negative charge.

From this and formula (1) it is standard to prove the following lemma:

**Lemma 1.** Let \( k > \frac{1}{\sqrt{2}} \). Define \( S := k^{-1}g + \tau R_0(-1)\tau^* \). Then \( E = -k^2 < -\frac{1}{2} \) is a discrete eigenvalue of \( H \) if and only if \( \ker(g^{-1} + \tau R_0(E)\tau^*) \neq \{0\} \). Note that up to a scaling this is the same as \( \ker S \neq \{0\} \). Moreover, \( \operatorname{mult}(E) = \dim(\ker S) \).

The spectral analysis is thus reduced to the study of \( S \), a \( 3 \times 3 \) matrix of integral operators each acting in \( L^2(\mathbb{R}) \). We call \( S \) the skeleton of \( H \). Let us denote by \( T_{A,B} := \tau A R_0(-1)\tau_B^* \), \( T_0 := T_{A,A} \), by \( \theta_{A,B} \) the angle between two unit vectors \( A \) and \( B \), and by \( \hat{T}_{A,B} \) the Fourier image of \( T_{A,B} \). Then the kernel of \( \hat{T}_{A,B} \) when \( \theta_{A,B} \not\in \{0, \pi\} \), and of \( \hat{T}_0 \) read as:

\[
|\hat{T}_{A,B}(p,q)| = \frac{1}{2\pi|\sin(\theta_{A,B})|} \left( \frac{p^2 - 2\cos(\theta_{A,B}) pq + q^2}{2\sin^2(\theta_{A,B})} + 1 \right), \\
|\hat{T}_0(p,q)| = \frac{\delta(p-q)}{\sqrt{p^2 + 2}} \tag{2}
\]

Then \( \hat{T}_0 \) is a bounded multiplication operator, and \( \hat{T}_{A,B} \) only depends on \( |\theta_{A,B}| \). Consequently we denote in the sequel \( T_{A_i,A_j} \) by \( T_{\theta_{i,j}} \) or \( T_{j,i} \).

**Reduction by symmetry.** \( H \) and \( S \) enjoy various symmetry properties which follow from the fact that two particles are identical. Let \( \pi : L^2(\mathbb{R}) \to L^2(\mathbb{R}) \) be the parity operator, i.e. \( \{\pi \varphi\}(p) = \varphi(-p) \) and denote by \( \pi_1 := \pi \otimes 1 \) and \( \pi_2 := 1 \otimes \pi \) the unitary symmetries with respect to the \( x \) and \( y \) axis. One verifies that for all \( i,j \in \{1,2\} \), we have \( [\pi_i, H] = 0 \) and \( [\pi_i, \pi_j] = 0 \). Thus if we denote by \( \pi_{i,\alpha} \), \( \alpha = +, -, \) the eigenprojectors of \( \pi_i \) on the even, respectively odd functions we may decompose \( H \) into the direct sum

\[
H = \bigoplus_{\alpha \in \{\pm\}, \beta \in \{\pm\}} H^{\alpha,\beta}, \quad H^{\alpha,\beta} := \pi_{\alpha}^0 \pi_{\beta}^0 H.
\]

Similarly let \( \Pi, \sigma : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3) \) defined by \( (\Pi \psi)(-p) := \psi(-p) \) and \( \sigma \psi = \sigma(\psi_1,\psi_2,\psi_3) := (\psi_2,\psi_1,\psi_3) \). They both commute with \( S \), and also \( [\Pi, \sigma] = 0 \).

Let \( I^{\alpha, \sigma} \), \( \alpha = +, -, \) denote the eigenprojectors of \( \Pi \) and \( \sigma \) symmetric and antisymmetric resp.. Then we can write \( S = \bigoplus_{\alpha \in \{\pm\}, \beta \in \{\pm\}} S^{\alpha,\beta}, \quad S^{\alpha,\beta} := \Pi^{\alpha} \sigma^{\beta} S \).

From the expression of \( \hat{T}_0(p,q) \) one also sees that \( [\pi, \Pi^\theta] = 0 \) so that \( T^\theta \) decomposes into \( T_+^\theta \oplus T_-^\theta \) where \( T^\theta \pm := \pi^\theta \mp T^\theta \). As usual we shall consider \( T^\theta \mp \) as operators acting in \( L^2(\mathbb{R}^+ \). Due to these symmetry properties we have \( \ker S = \bigoplus_{\alpha, \beta} \ker S^{\alpha,\beta} \), and each individual null-space can be expressed as the null-space of a single operator acting in \( L^2(\mathbb{R}^+ \) that we call effective skeleton. We gather in the following table the four effective skeletons we have to consider with their corresponding subspaces in \( L^2(\mathbb{R}^2) \):

<table>
<thead>
<tr>
<th>( S^{\alpha,\beta} )</th>
<th>effective skeleton</th>
<th>subspace in ( L^2(\mathbb{R}^2) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>++</td>
<td>( k - T_0 - T_{1,2}^\pm + 2 T_{2,3}^\pm (T_0 + k\lambda^{-1})^{-1} T_{2,3}^\pm )</td>
<td>Ran ( \pi_1^\pm \pi_2^\pm )</td>
</tr>
<tr>
<td>--</td>
<td>( k - T_0 - T_{1,2}^\pm + 2 T_{2,3}^\pm (T_0 + k\lambda^{-1})^{-1} T_{2,3}^- )</td>
<td>Ran ( \pi_1^\pm \pi_2^- )</td>
</tr>
<tr>
<td>+-</td>
<td>( k - T_0 + T_{1,2}^\pm )</td>
<td>Ran ( \pi_1^\pm \pi_2^\pm )</td>
</tr>
<tr>
<td>--</td>
<td>( k - T_0 + T_{1,2}^- )</td>
<td>Ran ( \pi_1^- \pi_2^\pm )</td>
</tr>
</tbody>
</table>

Table 1.
3 Sectors without bound states

**Properties of the** $T_\theta$ **operators.** From (2) we get $0 \leq T_0 \leq 1/\sqrt{2}$. Then $T_\theta$ is self-adjoint and has a finite Hilbert-Schmidt norm. The proof of the following lemma in not at all obvious, but will be omitted due to the lack of space.

**Lemma 2.** For all $\theta \in [\pi/2, \pi)$ one has $\pm T_\theta^\pm \geq 0$ and the mapping $[\pi/2, \pi) \ni \theta \mapsto \pm \inf T_\theta^\pm$ is strictly increasing.

**Absence of bound state in the odd sector with respect to $y$.** We have the following result:

**Theorem 3.** For all $Z > 0$ and all $0 < M/m \leq \infty$, $H$ has no bound state in the symmetry sector $\text{Ran} \pi_\theta^-$. 

**Proof.** The symmetry sector $\text{Ran} \pi_\theta^-$ corresponds to the second and third lines in Table 1. For the third line one uses that $T_{1,2}^+ \geq 0$ by Lemma 2, and that $k > 1/\sqrt{2}$ since we are looking for eigenvalues below $\sigma_{\text{ess}}(H) = [-\frac{1}{2}, \infty)$. Hence

$$k - T_0 + T_{1,2}^+ \geq k - \frac{1}{\sqrt{2}} > 0$$

thus $\ker(k - T_0 + T_{1,2}^+) = \{0\}$, and by Lemma 1 this shows that $H$ has no eigenvalues in $\text{Ran} \pi_\theta^-$. By the same type of arguments one has: $k - T_0 - T_{1,2}^- + 2T_{2,3}^-(T_0 + k\lambda^{-1})^{-1}T_{2,3}^- \geq k - \frac{1}{\sqrt{2}} > 0$. \[\Box\]

**Remark 4.** The above theorem has a simple physical interpretation. Wave functions which are antisymmetric in the $y$ variable are those for which the positive charge has a zero probability to be in the middle of the segment joining the negative charges. A situation which is obviously not favorable for having a bound state.

**Absence of bound state in the odd-even sector with respect to $x$ and $y$.** Looking at the fourth line of Table 1 we have to consider

$$S^{-\cdot}(k) := k - T_0 + T_{1,2}^- =: \sqrt{k - T_0} \left(1 + \tilde{T}_{1,2}^-(k)\right) \sqrt{k - T_0}$$

(3)

where $\tilde{T}_{1,2}^- := (k - T_0)^{-\frac{1}{2}}T_{1,2}^-(k - T_0)^{-\frac{1}{2}}$. Here we will only consider the case $M \geq m$, i.e. $\pi/2 \leq \theta_{1,2} \leq 2\pi/3$. Assume that we can prove that $\tilde{T}_{1,2}^-(2^{-\frac{1}{2}}) \geq -1$ for $\theta_{1,2} = 2\pi/3$, this will imply that $S^{-\cdot}(2^{-\frac{1}{2}}) \geq 0$ first for $\theta_{1,2} = 2\pi/3$ and then for all $\pi/2 \leq \theta_{1,2} \leq 2\pi/3$ by the monotonicity of $\inf T_{1,2}^-$ with respect to $\theta$ as stated in Lemma 2; finally looking at (3) this will show that $S^{-\cdot}(k) > 0$ for all $k > 1/\sqrt{2}$ and therefore that $\ker S^{-\cdot}(k) = \{0\}$. But $\tilde{T}_{1,2}^- := \tilde{T}_{1,2}^-(2^{-\frac{1}{2}})$ ( for $\theta_{1,2} = 2\pi/3$) is Hilbert-Schmidt since its kernel decay at infinity faster than the one of $T_{1,2}^-$ and it has the following behavior at the origin: $\tilde{T}_{1,2}^-(p,q) \sim -\frac{16\sqrt{2}}{3\sqrt{3}\pi} + \mathcal{O} \left((p^2 + q^2)\right)$. It turns out that $-1$ is an eigenvalue of $\tilde{T}_{1,2}^-$ with eigenvector

$$\mathbb{R}_+ \ni p \mapsto \left[\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{p^2 + 2}}\right]^{1/2} p \sim p^0 \frac{1}{32^{\frac{1}{4}}} + \mathcal{O}(p^2)$$
Critical stability of three quantum charges with delta self-interactions

and since the Hilbert-Schmidt norm of $\tilde{T}_{1,2}$ can be evaluated numerically to $||\tilde{T}_{1,2}||_{HS} \leq 1.02$, all the other eigenvalues of $\tilde{T}_{1,2}$ are above $-1$. Thus we have proved the

**Theorem 5.** For all $Z > 0$ and all $1 \leq M/m \leq \infty$, $H$ has no bound state in the symmetry sector $\text{Ran} \pi_1^- \pi_2^-$. 

4 The fully symmetric sector

According to Table 1, we need to find under which conditions one has $\text{ker} S^{+,+}(k) \neq \{0\}$ where

$$ S^{+,+}(k) := k - T_0 - K(k), \quad \text{with} \quad K(k) := T_{1,2}^+ - 2T_{2,3}^+(T_0 + k\lambda^{-1})^{-1}T_{2,3}^+. $$

The proof of the following lemma is an easy application of Fredholm and analytic perturbation theory:

**Lemma 6.** (i) $\{\text{Re} k^2 > 0\} \ni k \mapsto S^{+,+}(k)$ is a bounded analytic self-adjoint family of operators.
(ii) If $\inf \sigma\left(S^{+,+}(2^{-\frac{1}{2}})\right) < 0$, then there exists $k > 1/\sqrt{2}$ so that $\text{ker} S^{+,+}(k) \neq \{0\}$.

Denote by $K(p, q)$ the integral kernel of $K(2^{-\frac{1}{2}})$. Our last result is:

**Theorem 7.** For all $0 < M/m \leq \infty$, $H$ has at least one bound state in the symmetry sector $\text{Ran} \pi_1^+ \pi_2^+$ if $Z$ is such that $K(0, 0) > 0$.

**Proof.** We will now look for an upper bound on $\inf S^{+,+}(2^{-\frac{1}{2}})$ by the variational method. Let $j \in C_0^\infty(\mathbb{R}_+, \mathbb{R}_+)$ so that $\int_{\mathbb{R}_+} j(x)dx = 1$ and define two families of functions: $\forall \varepsilon > 0$, $\psi_\varepsilon(p) := \varepsilon^{-1} j(p\varepsilon^{-1})$, $\phi_\varepsilon := \frac{\varepsilon}{\sqrt{2\|j\|}} \psi_\varepsilon$, $\|\phi_\varepsilon\| = 1$. We know that $\psi_\varepsilon$ converges as $\varepsilon \to 0$ to the Dirac distribution. First one has

$$ ((2^{-\frac{1}{2}} - T_0)\phi_\varepsilon, \phi_\varepsilon) = \frac{1}{\varepsilon\sqrt{2\|j\|}} \int_{\mathbb{R}_+} [1 - (1 + \varepsilon^2 p^2 / 2)^{-1/2}]j^2(p/\varepsilon)dp $$

$$ \leq \frac{\varepsilon^2}{2\sqrt{2\|j\|}} \int_{\mathbb{R}_+} p^2 j(p)^2 dp. \quad (4) $$

Then one has $\langle K(2^{-\frac{1}{2}})\phi_\varepsilon, \phi_\varepsilon \rangle = \frac{\varepsilon^2}{\|j\|^2} \langle K(2^{-\frac{1}{2}})\psi_\varepsilon, \psi_\varepsilon \rangle = \frac{\varepsilon^2}{\|j\|^2} (K(0, 0) + O(\varepsilon))$ so that $\langle S^{+,+}(2^{-\frac{1}{2}})\phi_\varepsilon, \phi_\varepsilon \rangle = 2^{-\frac{1}{2}} - (T_0\phi_\varepsilon, \phi_\varepsilon) - (K(2^{-\frac{1}{2}})\phi_\varepsilon, \phi_\varepsilon)$ will be negative for $\varepsilon > 0$ small enough, provided $K(0, 0) > 0$. 

It is possible to compute $K(0, 0)$ analytically. It can be shown that there exists $Z_c^{\text{ub}}(M/m)$ such that for any $Z$ larger than this value, we have $K(0, 0) > 0$. If we now define the critical $Z$ as $Z_c(M/m) := \inf\{Z > 0, H = H(Z, M/m) \text{ has at least one bound state}\}$, it follows from our last theorem that $Z_c(M/m) \leq Z_c^{\text{ub}}(M/m)$.

The curve $Z_c^{\text{ub}}(M/m)$ is plotted on figure 2, where we used $\theta_{1,2}$ instead of the ratio $M/m$. 


Remarks 8. (a) Rosenthal found numerically $Z_{ub}^{uc}(\frac{\pi}{2})$, i.e. $Z_{ub}^{uc}$ for $M = \infty$ to be 0.374903. With our analytical expression of $K(0, 0)$ we know this value to any arbitrary accuracy: $Z_{ub}^{uc}(\frac{\pi}{2}) = 0.37490347747000593278...$

(b) The above curve shows that an arbitrarily small positive charge of mass $M < 0.48m$ can bind two electrons. However we believe that the exact critical curve will show that $M < m$ and $Z > 0$ is sufficient to bind these two electrons.

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Non-relativistic $H_2^+$-molecule in a strong magnetic field

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Abstract. We show that, under the influence of a strong uniform magnetic field, the energy of the $H_2^+$-ion at the 0-th order Born-Oppenheimer approximation goes over into that of the corresponding united atom limit, $He^+$.

1 Introduction

Atoms and molecules in a strong uniform magnetic field of strength $B$ will effectively behave like systems in one dimension, since the field will ‘freeze’ the motion of the electrons perpendicular to the field into Landau orbitals. The electrons will only be free to move along the field-direction, under the influence of one-dimensional effective potentials induced by the original Coulomb interactions. In the high field limit, these effective potentials are well-approximated by zero-range $\delta$-interactions, with a $B$-dependent coupling constant. This physical picture can be given a rigorous mathematical foundation for atoms and molecules having infinitely heavy nuclei aligned along the field direction, with the successive approximations holding true in the fairly strong sense of norm-convergence of resolvents, and explicit error bounds ([1] - [5]). This can be used to draw rigorous conclusions, for the original atomic or molecular Hamiltonian, from the $\delta$-model, which in one-electron cases is elementary solvable. We illustrate this by a detailed study of the $H_2^+$-molecule in a strong magnetic field, for which we

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prove that the equilibrium distance between the nuclei tends to 0 as the field strength tends to infinity, and the ground state energy tends to that of its united atom limit.

2 The Asymptotic Model

We consider a non-relativistic one-electron homonuclear diatomic molecule with fixed nuclei of charge $Z$ in a strong homogeneous magnetic field $\mathbb{B} = B\hat{z}$, where $\hat{z}$ is the unit vector in the $z$-direction. If the inter-nuclear distance is $R$, then the Pauli-Hamiltonian for the molecule, in atomic units, is:

$$H = \frac{1}{2} |p - \frac{1}{2} r \wedge \mathbb{B}|^2 + \sigma \cdot \mathbb{B} - V + \frac{Z^2}{R},$$

where $V$ is the electron-nuclei potential:

$$V(r) = \frac{Z}{|r - \frac{R}{2}\hat{z}|} + \frac{Z}{|r + \frac{R}{2}\hat{z}|},$$

and $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ the electron spin vector, given by the Pauli matrices. The conversion to the field strength in Gauss is done by multiplication of $B$ by $B_0 := m_e^2 e^3 / \hbar^3 = \approx 2.35 \times 10^9$ G. In [5], it was shown that atomic Hamiltonians in strong magnetic fields can be approximated, in norm-resolvent sense, by a hierarchy of effective Hamiltonians describing one-dimensional atoms on the line. The machinery of [5] is still applicable to the molecular case, provided the nuclear axes are taken parallel to $\mathbb{B}$, to ensure that total electron-angular momentum in the field direction is preserved (this is no longer true for arbitrary orientations). The simplest of the effective Hamiltonians of [5], [4], giving the lowest order approximation, is the $\delta$-Hamiltonian, which in the present case is given by

$$h_\delta = \frac{1}{2} p_z^2 - \sum_\pm Z L \delta \left( \frac{z \pm \frac{R}{2}}{R} \right) + \frac{Z^2}{R}.$$  

Here $L = L(B) := 2W(\sqrt{B}/2), W : [-e^{-1}, \infty) \to \mathbb{R}$ being the principal branch of the Lambert function, defined as the unique real solution of $W(x)e^{W(x)} = 1$ which is positive for positive $x$; see e.g. [6]. Note that $h_\delta$ still depends on $B$, through $L$. We have that $L(B) \simeq \log B$ as $B \to \infty$.

Under the reasonable assumption that the electron is in an $s$-state (this is not essential), $h_\delta$ will approximate $H$ in the following sense: let $\Pi_0$ be the orthogonal projection onto the lowest Landau band of the ‘free’ operator $\frac{1}{2} |p - \frac{1}{2} r \wedge \mathbb{B}|^2$ with $m = 0$, and let $\Pi_0^\perp$ be the projection onto the orthogonal complement; $\Pi_0$ commutes with $H$, and $h_\delta$ has a natural interpretation as an operator on $\text{Ran}(\Pi_0)$. Let $H_\delta := h_\delta \Pi_0 + H(B) \Pi_0^\perp$. Then:

**Theorem 1** (compare [5], thm. 1.5) If $d_\delta(\xi)$ is the distance of $\xi \in \mathbb{R}$ to the spectrum of $h_\delta$, then there exists positive constants $c_\delta$, $C_\delta$ and $B_\delta$, only depending on $Z$, such that if $B \geq B_\delta$ and $c_\delta L \leq d_\delta(\xi) \leq L^2 / 4$, then $\xi$ is in the resolvent set of $H$, and

$$||(H - \xi)^{-1} - (H_\delta - \xi)^{-1}|| \leq C_\delta \frac{L}{d_\delta(\xi)^2}. $$

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$$||(H - \xi)^{-1} - (H_\delta - \xi)^{-1}|| \leq C_\delta \frac{L}{d_\delta(\xi)^2}. $$
The spectrum of $HH_0^0$ turns out to be positive, and $d_\delta(\xi) > 0$ will imply that $\xi < 0$, since the essential spectrum of $h_\delta$ already contains $[0, \infty)$. Theorem 1 allows us to deduce information about the negative bound states of $H$ from those of $h_\delta$. Equation (4) may look strange as an approximation result, since the $L$ in the left hand side goes to $\infty$. However, the ground state energy of $h_\delta$ is of the order of $-cL^2$ in absolute value, and the same can then be shown to be the case for $H$, see below. In [1]-[3], as re-scaled version of theorem 1 was used.

The $\delta$-model is explicitly solvable, and $h_\delta$ can be shown to have two eigenvalues,

$$e_0 = e_0(R, L, Z) = -\frac{1}{2}(LZ)^2 \left(1 + \frac{W(xe^{-x})}{x}\right)^2 + \frac{Z^2}{R},$$

$$e_1 = e_1(R, L, Z) = -\frac{1}{2}(LZ)^2 \left(1 + \frac{W(-xe^{-x})}{x}\right)^2 + \frac{Z^2}{R},$$

(5)

where $x := RLZ$; note that $-xe^{-x} \geq -e^{-1}$, for all $x \geq 0$. The corresponding eigenfunctions can also be computed explicitly, cf. [1]. The ground state energy of $h_\delta$ is $e_0$, and the molecule will bind iff $\inf_R [e_0(R, L, Z) - e_{at}] < 0$, where $e_{at} = -Z^2L^2/2$, the ground state energy when the two nuclei are at infinite distance. The equilibrium distance $r_{eq}$ is the value of $R$ for which $e_0(R, L, Z) - e_{at}$ is minimized. The following theorem summarizes the situation for the $\delta$-model (numerical values are given to 4 decimal places):

**Theorem 2** (cf. [2]) The energy curve $e_0(R, L, Z) - e_{at}$ has: (i) a global strictly negative minimum if $Z/L \leq 0.3205$; (ii) a local minimum (corresponding to a resonance of the molecule) if $0.3205 < Z/L < 0.4398$ and (iii) does not have a local minimum if $Z/L > 0.4398$.

To find the equilibrium distance, one computes that $\partial_R e_0(R, L, Z) = R^{-2}LZ [G(x) - ZL^{-1}]$, where $G(x) := x^{-1}(1 + W)^{-1}(x + W)^2 W$, where $W = W(xe^{-x})$. The function $G(x)$ is found to be strictly increasing on the interval $[0, x_G]$ where $G(x_G) = 0.4398$. Hence $r_{eq} = G^{-1}(Z/L)$ for $Z/L < 0.4398$. The ground state energy of molecule in the $h_\delta$-model is $e_{min} = e(r_{eq}, L, Z)$. Their asymptotic behavior as $L \to \infty$ is given by:

$$r_{eq} = \frac{1}{2L^{3/2}Z^{1/2}} \left(1 + \frac{5}{4} \theta + \frac{45}{32} \theta^2 + O(\theta^3)\right),$$

(6)

$$e_{min} = -2Z^2L^2 \left(1 - 2\theta + \frac{5}{4} \theta^2 + O(\theta^3)\right),$$

(7)

where $\theta = \sqrt{Z/L}$. Although $h_\delta$ does not, by itself, provide numerically very good approximations for the ground-state energy and equilibrium distance of the real $H_2^+$-molecule for magnetic fields in the physically relevant range of $3 \times 10^9 - 4 \times 10^{13}$ Gauss, it can be used as the starting point of a perturbative calculation, as was done in [1]. The equilibrium distance and binding energy of the $H_2^+$ molecule computed there were found to be in good agreement with earlier variational calculations. One consequence of these computations is the
prediction of the existence, in fields $B \geq 10^{13}$ G, of $He_2^{3+}$, a new atomic system, and a further example of the binding-enhancing properties of strong magnetic fields.

3 Equilibrium nuclear separation for $H_2^+$

Using the arguments of [5], section 9, it can be shown that the ground state energy $E_0 = E_0(R, L, Z)$ of $H$ can be estimated in terms of that of $h_{\delta}$ by $|E_0(R, L, Z) - e_0(R, L, Z)| \leq c_{\delta} L$, uniformly in $R$ (recall that the constant $c_{\delta}$ of theorem 1 is independent of $R$). One encounters a technical difficulty due to the existence of the second eigenvalue $e_1$ of $h_{\delta}$ which, for large fields, becomes exponentially close to $e_0$, and prohibits a lower bound for the isolation distance of $e_0$ of the type required for theorem 1. However, all Hamiltonians under consideration commute with the $z$-parity operator $P_z : z \rightarrow -z$, and if we decide right from the start to work in the $P_z = 1$-eigenspace of even functions in $z$, then shows that $R_{1,2} = (2L^{3/2}Z^{1/2})^{-1} + O(L^{-7/4})$ (cf. [2], section 3).

Hence:

**Theorem 3** For sufficiently large $B$, ground state energy and equilibrium distance of the $H_2^+$-molecule (1) is given by, respectively

$$E_0(L, Z) = -2L^2Z^2 + 4Z^{5/2}L^{3/2} + O(L),$$

and

$$R_{eq} = \frac{1}{2L^{3/2}Z^{1/2}} + O\left(L^{-7/4}\right).$$

4 Discussion

By theorem 3, the internuclear distance tends to 0 as $B \rightarrow \infty$. Despite the electrostatic repulsion between the two nuclei, a single electron suffices, under the influence of a strong magnetic field, to bring them arbitrarily close to each other. This is again an example of the binding-enhancing effect of strong magnetic fields. Furthermore, as $B \rightarrow \infty$, $e_{\min} \rightarrow -2Z^2L^2$, which is the ground-state of $\frac{1}{2}p_z^2 - 2ZL\delta(z)$, a one-dimensional $He^+$-like ion with $\delta$-potentials. By [5], section 9, the ground-state $E_{0}^{He^+}(B)$ of the true $He^+$-ion in a strong magnetic field will lie within a distance of $O(L)$ of $-2Z^2L^2$. It follows therefore that

$$\frac{E_{0}^{H_2^+}(B)}{E_{0}^{He^+}(B)} \rightarrow 1, \quad B \rightarrow \infty.$$
The conclusion is that as field strength increases, the $H_2^+$-model goes over into its United Atom Limit, the $He^+$-ion. Several caveats are of course in order here. First of all, for values of $B \geq 4 \times 10^{13}$ Gauss, for which the electron's rest-mass becomes larger or equal than the lowest Landau level, our non-relativistic model should be replaced by a relativistic one (and ultimately of course nuclear effects will start to play a rôle). Next, the fixed-nuclei approximation is not realistic, and vibrational, and possibly also rotational, motions should be taken into consideration.

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References


Three Electrons in a Two-Dimensional Parabolic Trap: The Relative Motion Solution

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Abstract. In agreement with the Kohn theorem the relative motion (rel) of three electrons in a two-dimensional parabolic trap separates from the center-of-mass (CM) motion. By introducing new coordinates the Hamiltonian for relative motion in the approximation of non-interacting electrons can be taken to the normal form. The eigenstates of the normalized Hamiltonian are products of the Fock-Darwin states for normal modes. The energy levels for relative motion are obtained by diagonalizing the exact Hamiltonian in the eigenbasis for non-interacting case. In this basis the interaction matrix elements can be obtained in the analytical form. Since the rank of Hamiltonian matrix is significantly reduced the calculations are faster and more accurate than those for the full (CM+rel) motion. This advantage is especially important for the calculations of excited states and the analysis of energy spectra.

1 Introduction

The usual approach to solve quantum-mechanically the problem of few correlated electrons in a parabolic confinement (for example a few-electron quantum dot (QD)) is to diagonalize the Hamiltonian matrix in the eigen-basis of the same Hamiltonian but with non-interacting electrons. For the systems confined in a plane (2D approach – typical for QDs) the interaction matrix elements can be obtained in an analytical from [1]. This approach is applied in a number of papers (see e.g. [2]). The rank of Hamiltonian matrix, however, significantly reduces after separation of the centre-of-mass (CM) of electrons, what is ensured by the Kohn theorem [3]. An inconvenience is that the Hamiltonian for relative (rel) motion contains mixing terms both in the kinetic and the confining potential.
energy parts (except for the two-electron case) and it is not separable in original coordinates. For three-electron systems, in order to separate (at least approximately) the modes of collective dynamics, usually the transformations to Jacobi or hyperspherical coordinates are used [4]. Particularly, for special values of the effective frequency Taut [5] has found an analytical solutions for the systems with two and three electrons.

In this paper we solve the three-electron problem in two steps: (i) by finding appropriate coordinates which transform the Hamiltonian for non-interacting electrons (for the relative motion) to the normal form, and (ii) by diagonalizing the exact Hamiltonian (with correlated electrons) in this eigen-basis. Like in the case of full (CM + rel) motion [1], the interaction matrix elements for the relative motion can be expressed in the analytical form.

2 The Hamiltonian and separation of the CM motion

The Hamiltonian for three electrons moving in a two-dimensional parabolic trap including a perpendicular magnetic field reads

\[ H = \sum_{j=1}^{3} \left[ \frac{1}{2m^*} \left( \mathbf{p}_j - \frac{e}{c} \mathbf{A}_j \right)^2 + \frac{1}{2} m^* \omega_0^2 \mathbf{r}_j^2 \right] + V_C, \]  

where the Coulomb repulsion between electrons is determined by the potential

\[ V_C = \kappa \left( \frac{1}{r_{13}} + \frac{1}{r_{23}} + \frac{1}{r_{12}} \right), \quad \kappa = \frac{e^2}{4\pi \varepsilon_0 \varepsilon_r}. \]

Here \( \mathbf{r}_j \) and \( \mathbf{p}_j \) (\( j = 1, 2, 3 \)) are the positions and momenta of electrons, respectively, and \( r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| \). The constants \( c, e, m^*, \varepsilon_0 \) and \( \varepsilon_r \) are the speed of light, unit charge, effective electron mass, vacuum and relative dielectric constants (of a semiconductor, if we treat a QD), respectively. \( \hbar \omega_0 \) is the energy scale of the parabolic confinement.

Applying a perpendicular magnetic field (\( \mathbf{B} \parallel z\text{-axis} \)) and using symmetric gauge for the vector potential \( \mathbf{A}_j = \frac{1}{2} \mathbf{B} \times \mathbf{r}_j = \frac{1}{2} \mathbf{B}(-y_j, x_j, 0) \), it follows

\[ H = \sum_{j=1}^{3} \left( \frac{\mathbf{p}_j^2}{2m^*} + \frac{1}{2} m^* \Omega^2 \mathbf{r}_j^2 \right) + V_C - \omega_L L_z \]  

where \( \omega_L = eB/2mc \) is the Larmor frequency, \( L_z^{\text{tot}} = \sum_{j=1}^{3} l_j \) is the total angular momentum and \( \Omega = (\omega_L^2 + \omega_0^2)^{1/2} \) is the effective confinement frequency which depends through \( \omega_L \) on the magnetic field. In this way the magnetic field can be used to control the effective confinement of electrons.

Introducing the relative and CM coordinates: \( \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j, \mathbf{R} = \frac{1}{3} (\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3) \), the Hamiltonian (3), in agreement with the Kohn theorem[3], separates into the CM and relative-motion terms, \( H = H_{\text{CM}} + H_{\text{rel}} \), where

\[ H_{\text{CM}} = \frac{\mathbf{P}_R^2}{2M} + \frac{1}{2} M \Omega^2 \mathbf{R}^2 - \omega_L L_z^{\text{CM}}, \]  

\[ H_{\text{rel}} = \sum_{j=1}^{3} \left( \frac{\mathbf{p}_j^2}{2m^*} + \frac{1}{2} m^* \omega_0^2 \mathbf{r}_j^2 \right) + V_C, \]
Here $M = 3m^*$ and $L_{CM} + L_{rel}^z = L_{tot}^z$.

The CM term, essentially, has the form of the Hamiltonian for a single electron in an effective parabolic (2D) confinement (i.e. a single-electron QD). The only difference is in the mass $M$ (instead of $m^*$), but it does not affect the eigenergies which are well known Fock-Darwin energy levels [6] (see Fig. 1a)

$$E_{n,m} = \hbar \Omega (2n + |m| + 1) - \hbar \omega_L m,$$

where $n$, $m$ are the radial and magnetic quantum numbers, respectively. The levels with different $m$ for large $B$ converge asymptotically to Landau levels, $\hbar \omega_L (2n_L + 1)$, where $n_L = n + \frac{1}{2} (|m| - m)$ is the Landau index. Obviously, for $m \geq 0$, $n_L = n$ (see Fig. 1a).

In the following we focus our interest to the relative motion of three electrons described by the Hamiltonian (5).

3 The relative motion

3.1 Normal coordinates

The Hamiltonian (5) contains mixing terms both in the kinetic and the confining potential energy parts. This Hamiltonian for $V_C = 0$ (i.e. in the approximation of non-interacting electrons) can be transformed to the normal form if we write the relative positions $r_{13}$, $r_{23}$ as linear combinations of new coordinates $Q_1, Q_2$

$$r_{13} = a_1 Q_1 + a_2 Q_2, \quad r_{23} = a_2 Q_1 + a_1 Q_2. \quad (7)$$

The mixing terms in new variables disappear for $a_1 = (\sqrt{3}+1)/2$, $a_2 = (\sqrt{3}-1)/2$ and

$$H_{rel} = \sum_{i=1}^{2} \left( \frac{P_i^2}{2m^*} + \frac{1}{2} m^* \Omega^2 Q_i^2 \right) + V_C - \omega_L L_{rel}^z, \quad (8)$$

where $P_i = m^* \dot{Q}_i$. Obviously, the quasi-particles which dynamics is described by the canonical variables $\{P_i, Q_i\}$, $i = 1, 2$ have the same effective mass and charges and 'feel' the same effective confinement as the electrons in the Hamiltonian (3).

Using polar coordinates $(Q_1, \Phi_1; Q_2, \Phi_2)$ one has $P_i^2 = P_i^2 + L_{z_i}^2/Q_i^2$, where $L_{z_1} + L_{z_2} = L_{rel}^z$ and

$$H_{rel} = \sum_{i=1}^{2} \left( \frac{P_i^2}{2m^*} + \frac{L_{z_i}^2}{2m^*Q_i^2} + \frac{1}{2} m^* \Omega^2 Q_i^2 \right) + V_C - \omega_L L_{rel}^z. \quad (9)$$

3.2 The solution for non-correlated electrons

The eigenstates of the Hamiltonian (9) in the approximation of non-interacting electrons ($V_C = 0$) are products of the Fock-Darwin states,
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\[ \langle n_1, m_1; n_2, m_2|H_{\text{rel}}|n'_1, m'_1; n'_2, m'_2 \rangle = E_{n_1, n_2, m_1, m_2}^{(0)} \delta_{n_1, n'_1} \delta_{m_1, m'_1} \delta_{n_2, n'_2} \delta_{m_2, m'_2} + \langle n_1, m_1; n_2, m_2|V_C|n'_1, m'_1; n'_2, m'_2 \rangle, \]  

where \( \langle Q_1, Q_2|n_1, m_1; n_2, m_2 \rangle \equiv \psi_{n_1, n_2, m_1, m_2}^{(0)}(Q_1, Q_2) \). The interaction matrix elements are

\[ \langle n_1, m_1; n_2, m_2|V_C|n'_1, m'_1; n'_2, m'_2 \rangle = \kappa \sum \sum_{i=1}^{3} \sum_{j=i+1}^{3} \langle n_1, m_1; n_2, m_2|r_{ij}^{-1}|n'_1, m'_1; n'_2, m'_2 \rangle. \]  

Figure 1. (a) The energy levels for the CM motion for \( n = 0, 1, 2 \) as the functions of ratio \( \omega_L/\omega_0 \) (full lines) determined by Eq. (6) (Fock-Darwin energies). (b) The energy levels for the relative motion in the approximation of non-interacting electrons (Eq. (10)) for \( N_L = 0, 1, 2, 3 \) as the functions of ratio \( \omega_L/\omega_0 \) (full lines). The dotted lines in both cases represent the corresponding Landau levels.

\[ \psi_{n_1, n_2, m_2}^{(0)}(Q_1, Q_2) = \psi_{n_1, m_1}(Q_1) \psi_{n_2, m_2}(Q_2) \]  

(in this paper we do not consider the spin and symmetries related to the Pauli principle), and the eigenenergies are the sums

\[ E_{n_1, n_2, m_2}^{(0)} = \hbar E_{n_1, m_1} + \hbar E_{n_2, m_2} = \Omega(2n_1 + |m_1| + 1) + \hbar \Omega(2n_2 + |m_2| + 1) - \hbar \omega_L M, \]  

where \( M = m_1 + m_2 \) is a good quantum number.

The energy levels with different \( M \) for large \( B \) converge asymptotically to (double) Landau levels, \( 2\hbar \omega_L (N_L + 1) \) (see Fig. 1b), where \( N_L \) is the sum of Landau indices for two modes

\[ N_L = n_1 + n_2 + \frac{1}{2} (|m_1| + |m_2| - M) = n_{L1} + n_{L2}. \]  

3.3 Interaction matrix elements

Exact energy levels for the relative motion can be obtained by diagonalizing the Hamiltonian matrix which represents the full Hamiltonian (9) in the eigenbasis of the same Hamiltonian for non-interacting electrons. The corresponding matrix elements are
The relative distances $r_{13}$, $r_{23}$, $r_{12}$ expressed in terms of the normal coordinates $Q_1, Q_2$ can be written in the common form $r_{ij} = |b_1 Q_1 - b_2 Q_2|$, where $b_1 = a_1$, $b_2 = -a_2$ for $ij = 13$; $b_1 = a_2$, $b_2 = -a_1$ for $ij = 23$ and $b_1 = b_2 = 1$ for $ij = 12$.

Using the analytical forms for the Fock-Darwin functions $\psi_{n,m}$ [6, 1] and the relation $r_{ij}^{-1} = (2\pi)^{-1} \int q^{-1} e^{iq \cdot r_{ij}} d^2 q$ we obtain

$$\langle n_1, m_1; n_2, m_2 | r_{ij}^{-1} | n'_1, m'_1; n'_2, m'_2 \rangle = \delta_{m_1+m_2,m'_1+m'_2} \sqrt{\frac{m^* \Omega}{\hbar}} \times \left[ \frac{n_1! n'_1! n_2!}{(n_1 + |m_1|)! (n_2 + |m_2|)! (n'_1 + |m'_1|)! (n'_2 + |m'_2|)!} \right]^{1/2} \frac{(b_1 b_2)\bar{m}}{(b^2_1 + b^2_2)^{\bar{m}+1/2}} \times \sum_{k_1=0}^{n_1} \sum_{k_2=0}^{n_2} \sum_{k'_1=0}^{n'_1} \sum_{k'_2=0}^{n'_2} \frac{(-1)^{k_1+k_2+k'_1+k'_2} p_1! p_2!(n_1 + |m_1|)! (n_2 + |m_2|)!}{k_1! (n_1 - k_1)! (|m_1| + k_1)! k_2! (n_2 - k_2)! (|m_2| + k_2)!} \times \left( \frac{-b^2_2}{b^2_1 + b^2_2} \right)^{k_2} \left( \frac{-b^2_1}{b^2_1 + b^2_2} \right)^{k_1} \frac{p_1! p_2!(n'_1 - k'_1)! (|m'_1| + k'_1)! k'_2! (n'_2 - k'_2)! (|m'_2| + k'_2)!}{l_1! l_2! (p_1 - l_1)! (p_2 - l_2)! (l_1 + \bar{m})! (l_2 + \bar{m})!}, \tag{14}$$

where $\bar{m} = |m'_1 - m_1| = |m'_2 - m_2|$ and $p_i = k_i + k'_i + \frac{1}{2}(|m_i| + |m'_i| - \bar{m})$, $i = 1, 2$.

Applying a numerical diagonalization procedure the basis of functions $\psi_{n_1,m_1,n_2,m_2}^{(0)}$ have to be restricted to a finite number of elements: $n_i = 0, ... , n_{\text{max}}, m_i = m_{\text{min}}, ... , M - m_{\text{min}}$, where $n_{\text{max}}$ is a maximal value of the Landau index and $m_{\text{min}}$ is a minimal value of the magnetic quantum number for two modes ($i = 1, 2$). The rank of the Hamiltonian matrix is then: $(n_{\text{max}}+1)^2(M-2m_{\text{min}}+1)$.

4 Results and discussion

In Fig. 2a the lowest energy levels for the relative motion with $M = 1$ and zero magnetic field as functions of the relative strength of Coulomb interaction are shown. The relative strength of Coulomb interaction is measured by the Wigner parameter $R_W = (\kappa/l_0)/\hbar \omega_0$, where $l_0 = \sqrt{\hbar/m^* \omega_0}$ is the characteristic length of confining potential. The avoided crossings between the levels of the same symmetry indicate that the three-electron systems are non-integrable, in contrast to the two-electron case. The lowest levels (with different $M$) for the three-electron case as functions of the strength of magnetic field at a fixed value of $R_W$ are shown in Fig. 2b. Comparing to the case with $V_C = 0$, the levels are shifted upwards and, although the clustering associated to $n_L$ survives, there appear (exact) crossings between the levels with the same $n_L$ and different $M$.

These results are in agreement with previous calculations and experimental evidence for the lowest energies (ground state) [7]. The reduction of rank of the Hamiltonian matrix for relative motion comparing to that of the full Hamiltonian, however, accelerate and improves the accuracy of calculations, increasing the range of energy spectrum accessible for the analysis. The results shown in Fig. 2 are obtained by diagonalizing the Hamiltonian matrix with $n_{\text{max}} = 4$ and $m_{\text{min}} = -4$. For $M = 1$ the rank of this matrix is 250. For calculating the ground
state it is sufficient to take $n_{\text{max}} = 1$ or 2 and $m_{\text{min}} = -1$ or $-2$, what for $M = 1$ gives the matrices of rank 16 and 54, respectively. For the comparison, if we diagonalize the full Hamiltonian (3), in order to obtain the results with the same accuracy as for the relative motion solution, we have to restrict the three-particle basis to the same values of $n_{\text{max}}$ and $m_{\text{min}}$ but for all three electrons. Then, the rank of the corresponding Hamiltonian matrix is $(n_{\text{max}} + 1)^3(M - 2m_{\text{min}} + 1)^2$. To reproduce the results from Fig. 2a the rank in this case should be 12500.

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Level Density of the Hénon-Heiles System Above the Critical Barrier Energy

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Abstract. We discuss the coarse-grained level density of the Hénon-Heiles system above the barrier energy, where the system is nearly chaotic. We use periodic orbit theory to approximate its oscillating part semiclassically via Gutzwiller’s semiclassical trace formula (extended by uniform approximations for the contributions of bifurcating orbits). Including only a few stable and unstable orbits, we reproduce the quantum-mechanical density of states very accurately. We also present a perturbative calculation of the stabilities of two infinite series of orbits (R\textsubscript{n} and L\textsubscript{m}), emanating from the shortest librating straight-line orbit (A) in a bifurcation cascade just below the barrier, which at the barrier have two common asymptotic Lyapunov exponents χ\textsubscript{R} and χ\textsubscript{L}.

The two-dimensional Hénon-Heiles (HH) Hamiltonian

\[ H_{HH} = T + V_{HH}(x, y) = \frac{1}{2} (p_x^2 + p_y^2) + \frac{1}{2} (x^2 + y^2) + \alpha \left( x^2 y - y^3/3 \right) \]  

was introduced [1] to describe the mean gravitational field of a stellar galaxy. It describes an open system in which a particle can escape over one of three barriers with critical energy \( E_{\text{bar}} = 1/6\alpha^2 \) and has meanwhile become a textbook example [2, 3, 4] of a system with mixed dynamics reaching from integrable motion (for \( E \rightarrow 0 \)) to nearly fully chaotic motion (for \( E \gtrsim E_{\text{bar}} \)). Scaling coordinates and momenta with \( \alpha \) causes the classical dynamics to depend only on the scaled energy \( e = E/E_{\text{bar}} = 6\alpha^2 E \); the barrier energy then lies at \( e = 1 \).

The Hamiltonian (1) has also been used [5] to describe the nonlinear normal modes of triatomic molecules, such as \( \text{H}_3^+ \), whose equilibrium configuration has \( D_3 \) symmetry. Although this model may no longer be quantitative for large energies, it can qualitatively describe the dissociation of the molecule for \( e > 1 \).
In this paper we discuss the coarse-grained level density of the HH Hamiltonian (1) above the barriers, calculated both quantum-mechanically and semiclassically using periodic orbit theory. Since the potential $V_{HH}$ in (1) goes asymptotically to $-\infty$ like $r^{-3}$ ($r^2 = x^2 + y^2$) in some regions of space, the quantum spectrum of (1) is strictly speaking continuous. However, for sufficiently small $\alpha$ there are quasi-bound states for $E < E_{bar}$ whose widths are exponentially small except very near $E_{bar}$. For semiclassical calculations of the HH level density for $e < 1$, we refer to earlier papers [6, 7]. In [8] we have calculated the complex resonance energies $E_m - i\Gamma_m$ by the standard method of complex rotation, diagonalizing (1) in a finite harmonic-oscillator basis. The level density is, after subtracting the non-resonant part of the continuum, given by

$$\Delta g(E) = -\frac{1}{\pi} \text{Im} \sum_m \frac{1}{E - E_m + i \Gamma_m/2}.$$  \hspace{1cm} (2)

We define the coarse-grained level density by a Gaussian convolution of (2) over an energy range $\gamma$

$$\Delta g_{\gamma}(E) = \frac{1}{\gamma \sqrt{\pi}} \int_{-\infty}^{\infty} \Delta g(E') e^{-\frac{(E - E')^2}{\gamma^2}} \, dE',$$  \hspace{1cm} (3)

which can be done analytically [8]. Its oscillating part, which describes the gross-shell structure in the quantum-mechanical level density, is then given by

$$\delta g_{qm}(E) = \Delta g_{\gamma}(E) - \tilde{\Delta} g(E),$$  \hspace{1cm} (4)

where $\tilde{\Delta} g(E)$ is the smooth part of (2) which we have extracted by a complex version [8] of the numerical Strutinsky averaging procedure [9].

Semiclassically, the quantity $\delta g(E)$ can be approximated by Gutzwiller’s trace formula [10], which for a system with two degrees of freedom reads

$$\delta g_{scl}(E) = \frac{1}{\pi \hbar} \sum_{po} \frac{T_{po}(E)}{r_{po} \sqrt{\text{Tr} M_{po}(E) - 2}} e^{-\frac{(E - E_{po})^2}{4 \hbar^2}} \cos \left[ \frac{S_{po}(E)}{\hbar} - \frac{\pi}{2} \sigma_{po} \right].$$  \hspace{1cm} (5)

The sum goes over all isolated periodic orbits labeled ‘po’, and the other quantities in (5) are the periods $T_{po}$ and actions $S_{po}$, the Maslov indices $\sigma_{po}$ and the repetition numbers $r_{po}$ of the periodic orbits. $M_{po}(E)$ is the stability matrix obtained by linearization of the equations of motion along each periodic orbit. The Gaussian factor in (5) is the result of a convolution analogous to (3); it suppresses the orbits with long periods and hence yields the gross-shell structure in terms of the shortest periodic orbits, hereby eliminating the convergence problem characteristic of non-integrable systems [3]. This use of the trace formula to describe gross-shell quantum effects semiclassically has found many applications in different fields of physics (including interacting fermion systems in the mean-field approximation; see [4] for examples).

The shortest periodic orbits of the classical HH system (1) have already been extensively studied in earlier papers [11, 12, 13]. In [8] we have calculated all relevant orbits and their properties from the classical equations of motion and
computed the quantity \( \delta g_{\text{scl}}(E) \) in (5). Some of the shortest orbits are shown in the left part of Fig. 1, all evaluated at \( e = 1 \) (except for \( \tau_2 \) which is evaluated at \( e = 1.1 \)). Note that due to the \( D_3 \) symmetry of the HH potential, the orbits A_5, B_4, \( \tau_2 \) and L_6 (as well as all orbits R_n and L_m bifurcating from A, see below) have two symmetry partners obtained by rotations about \( \pm 2\pi/3 \). The orbit C_3 and all triplets of R_n orbits have a time reversed partner each.\(^1\)

In Fig. 2 we show a comparison of semiclassical (5) with quantum-mechanical (4) results, both coarse-grained with \( \gamma = 0.25 \) (units such that \( \hbar = 1 \)). At this resolution of the gross-shell structure, only 18 periodic orbits contribute to the semiclassical result; for the period-two orbit D_7 which is stable up to \( e \simeq 1.29 \) and involves to further orbits (E_8, G_7) in a codimension-two bifurcation scenario, we have used the appropriate uniform approximation [14] to avoid the divergence of the trace formula (5) (see [8] for details). We note that the agreement of

\(^1\)We use here the nomenclature introduced in [12, 13], where the Maslov indices \( \sigma_{po} \) appear as subscripts of the symbols (B_4, R_5, L_6, etc.) of the orbits.

Figure 1. Left: Contours of the HH potential and some of its shortest periodic orbits in the \((x, y)\) plane (see text). Right: Trace of the stability matrix of the A orbit and the three pairs of orbits \((R_5, L_6), (R_7, L_8), (R_9, L_{10})\) bifurcated from it, forming the beginnings of the 'HH fans'.

Figure 2. Comparison of quantum-mechanical (solid line) and semiclassical (dashed line) level density \( \delta g(E) \) of the HH potential versus scaled energy \( e \), coarse grained with Gaussian smoothing range \( \gamma = 0.25 \). Only 18 periodic orbits contribute to the semiclassical result [8].
semiclassics with quantum mechanics is excellent. Only near $e \sim 1$ there is a slight discrepancy which is mainly due to some uncertainties in the numerical extraction of $\Delta g(E)$. We can conclude that also in the continuum region above a threshold, the semiclassical description of quantum shell effects in the level density of a classically chaotic system works quantitatively.

In view of the importance of the level density close to the critical barrier energy $e = 1$ for the threshold behaviour of a reaction described by the HH model potential, we focus now on a particular set of periodic orbits existing at $e = 1$. The straight-line librating orbit $A$ reaches this energy with an infinite period after undergoing an infinite cascade of bifurcations for $e \to 1$. At these bifurcations, two alternating infinite sequences of rotational orbits $R_n$ ($n = 5, 7, 9, \ldots$) and librating orbits $L_m$ ($m = 6, 8, 10, \ldots$) are born; their bifurcation energies $e_n$ and $e_m$ form two geometric progressions converging to $e = 1$ with a 'Feigenbaum constant' $\delta = \exp(2\pi/\sqrt{3}) = 37.622367\ldots$; the shapes of these new orbits are self-similar when scaled with $\sqrt{\delta}$ in both $x$ and $y$ direction (see [12] for details). The stability traces of the first three pairs $(R_n, L_m)$ are shown in the right part of Fig. 1. As seen there, the curves $\text{Tr}M(e)$ of these orbits are nearly linear (at least up to $e \sim 1.02$) and intersect at $e = 1$ approximately at the same values for each type (R or L). For large $n$ and $m$, these values were found numerically [12] to be $\text{Tr}M_{L_m}(e = 1) \sim 8.183$ and $\text{Tr}M_{R_n}(e = 1) \sim -4.183$. This means that at $e = 1$, all L orbits have asymptotically the same Lyapunov exponent $\chi_L \simeq 2.087$, and all R orbits have the same Lyapunov exponent $\chi_R \simeq 1.368$. Based upon these numerical findings, we postulate the following asymptotic behaviour:

$$\text{Tr}M_{R_n,L_m}(e) \sim 2 \mp 6.183 \left( \frac{e - e^*}{1 - e^*} \right) \quad \text{for} \quad e \to 1, \ n, m \to \infty. \quad (6)$$

Here $e^*$ are the respective bifurcation energies of the orbits ($e_n$ or $e_m$), and the minus or plus sign is to be associated with the R or L orbits, respectively. The curves $\text{Tr}M_{R_n,L_m}(e)$ thus form two 'fans' spreading out from the values 8.183 and $-4.183$ at $e = 1$, the first three members of each being shown in the right part of Fig. 1. In the following we will sketch briefly how the qualitative features in (6) of these 'HH fans' can be obtained analytically from semiclassical perturbation theory. Details will be given in a forthcoming publication [15].

The idea is to start from the following 'separable HH' (SHH) Hamiltonian

$$H_0 = H_{SHH} = \frac{1}{2} (p_x^2 + p_y^2) + \frac{1}{2} (x^2 + y^2) - \frac{\alpha}{3} y^3 \quad (7)$$

and to include the term $\alpha x^2 y$ in first-order perturbation theory. Formally, we multiply it by a small positive number $\epsilon$ and write $H_{HH} = H_0 + \epsilon H_1$ with $H_1 = \alpha x^2 y = u^2 v/\alpha^2$, where $u = \alpha x$ and $v = \alpha y$ are the scaled coordinates. The Hamiltonian (7) is integrable; an analytical trace formula for it has been given in [7]. There is only one saddle at $(x, y) = (0, 1)$ with energy $e = 1$ and one librating A orbit along the $y$ axis which undergoes an infinite cascade of bifurcations for $e \to 1$. From it, an infinite sequence of rational tori $T_{lk}$ bifurcates, where $l$ is their repetition number and $k = 2, 3, \ldots$ counts the bifurcations (and the tori).
The \( v \) motion of the primitive A orbit \((l = 1)\), having \( u_A(t) = 0 \), is given by

\[
v_A(t) = v_1 + (v_2 - v_1) \sin^2(at, q), \quad a = \sqrt{\frac{v_3 - v_1}{6}}, \quad q = \sqrt{\frac{v_2 - v_1}{v_3 - v_1}} \tag{8}\]

in terms of the Jacobi elliptic function \([16] \text{sn}(z, q)\) with modulus \(q\). In (8), \( v_1 \leq v_2 \leq v_3 \) are the turning points of the motion along the \( v \) axis, defined by \( V_{HH}(u=0, v_i) = e \) \((i = 1, 2, 3)\). The tori bifurcating at the energies \( e_{lk} \) have the same \( v \) motion as the A orbit: \( v_T(t) = v_A(t) \). Their \( u \) motion is given by

\[
w_T(t) = \sqrt{(e - e_{lk})/3} \sin(t + \phi), \quad e \geq e_{lk}, \quad \phi \in [0, 2\pi). \tag{9}\]

The angle \( \phi \) describes the members of the degenerate families of tori.

According to semiclassical perturbation theory \([17]\), the actions \( S_{lk} \) of the tori are changed in first order of \( \epsilon \) by

\[
\delta_1 S_{lk}(\phi) = -\epsilon \int_{T_{lk}} H_1(u_T(t), v_T(t)) \, dt = -\frac{\epsilon}{\alpha^2} \int_{0}^{T_{lk}(0)} u_T^2(t) v_T(t) \, dt, \tag{10}\]

where \( T_{lk}(0) = 2\pi k \) are the periods of the unperturbed tori \([7]\). The integral in (10) takes the form \( \delta_1 S_{lk}(\phi) = A_{lk} + B_{lk} \cos(2\phi) \). In the asymptotic limit \( e \to 1 \), where \( q \to 1 \) and \( T_A \sim \ln[432/(1 - e)] \), the coefficients \( A_{lk} \) and \( B_{lk} \) can be given analytically \([15]\). Integrating the phase shift caused by \( \delta_1 S_{lk}(\phi) \) over the angle \( \phi \) (i.e., over the torus \( T_{lk} \)) yields a modulation factor \([17] \mathcal{M}_{lk} \)

\[
\mathcal{M}_{lk} = \frac{1}{2\pi} \int_{0}^{2\pi} e^{i\delta_1 S_{lk}(\phi)} \, d\phi = e^{i A_{lk}} J_0(|B_{lk}|/\hbar), \tag{11}\]

to be inserted under the sum of tori in the trace formula for the unperturbed SHH system given in \([7]\). Replacing the Bessel function in (11) by its asymptotic form \( J_0(x) \sim \sqrt{2/\pi x} \cos(x - \pi/4) \) yields two terms for each torus \( T_{lk} \), corresponding to the two isolated orbits R and L into which it is broken up by the perturbation. Reading off their overall amplitudes \( A_{R,L} \) in the perturbed trace formula and identifying them with their expression for isolated orbits given in (5), i.e. equating

\[
A_{R,L} = \frac{1}{\pi \hbar} \frac{T_{R,L}}{l \sqrt{|\text{TrM}_{R,L} - 2|}} \tag{12}\]

using the unperturbed periods \( T_{lk}(0) \) for \( T_{R,L} \), we can determine the perturbative expression for the stability traces. For the first repetitions \((l = 1)\) they become

\[
\text{TrM}_{R_n,L_m}(e) \sim 2 \mp 5.069 \left( \frac{e - e_{1k}}{1 - e_{1k}} \right) \quad \text{for} \quad e \to 1, \tag{13}\]

and thus have exactly the same functional form as in (6). Here \( e_{1k} \) are the bifurcation energies of the primitive A orbit \((l = 1)\); \( k = 2, 3, \ldots \) labels the pairs of \( R_m \) and \( L_n \) orbits with \( m = 2k + 1 \) and \( n = 2k + 2 \), and the signs are to be chosen as in (6). In (13) we have put \( \epsilon = 1 \) which is justified since even for this value the perturbations \( \delta_1 S_{lk} \) at \( e = 1 \) are sufficiently small.
Although the perturbative result (13) contains a too small value of the constant 5.069 (instead of 6.183) by 18%, it explains qualitatively correctly the numerical features of the 'HH fans' in (6), in particular the linear intersection of the curves $\text{Tr}M_{R,L}(e)$ at $e = 1$ at two values lying symmetrically to $\text{Tr}M = +2$.

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Wannier-type threshold laws for multifragmentation and Thomson’s problem

V. N. Ostrovsky1**, J. M. Rost2

Abstract. Wannier-type threshold theory for multiple break-up processes is based on the existence of special classical trajectories which represent partial fixed points of the equations of motion in a system of charged particles. These trajectories preserve the shape of the initial configuration while only changing its overall size in time. The relation between such scaling configurations and Thomson’s (or surface Coulomb) problem is analysed. In particular, it is shown that for eight electrons the twisted cube configuration solves Thomson’s problem and also governs the threshold break-up of eight electrons receding from a charged core. The relevant exponents for the threshold power law are evaluated.

1 Introduction

1.1 Scaling configurations

A variety of break-up processes is known in atomic, nuclear and cluster physics. The major difference between nuclear and atomic physics is that in the latter case generally the fragments have charges of different sign. A special fragmentation mechanism in atomic physics for total energies only slightly above the fragmentation threshold was introduced by Wannier [1]. Originally, he treated the case of three fragments, namely electron impact ionization of an atom.

Later the ideas were generalized to the situation with an arbitrary number $N$ of fragments (see Ref. [2] and bibliography therein). The key observation is that all the fragments have low velocities due to the small excess energy $E$ above threshold. Equally important is the notion, that most likely recapture occurs (into a bound excited, i.e., Rydberg state) among a pair of oppositely charged fragments if their distance increases with time more slowly than other relative

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distances. As a result, the desired complete fragmentation is not achieved. This can be avoided, if relative distances and orientations between the fragments are preserved. Indeed, modern non-linear dynamics methods allow one to describe this break-up processes entirely from the stability properties of a fixed-point for the equations of motion [3]. The seeming contradiction to describe a fragmentation process with particles leaving to infinite distance with a fixed point is resolved by using a scaling argument in excess energy $E$. Then any finite scaled distance $r/E$ tends to infinity if the excess energy approaches threshold $E \to 0$.

In a less abstract but essentially equivalent formulation the fragments form a scaling configuration (SC) in time [2]. It blows up while its shape is retained according to

$$r_j(t) = \phi(t)\rho_j,$$

where $r_j(t)$ are time-dependent vector of the ($j = 1, 2, \ldots N$) fragments with respect to the centre of mass (CM) of the system. Impling a classical description for the motion of the fragments, the Coulomb interaction, Eq. (1) reduces the multi-dimensional problem to that for a single degree of freedom, $\phi(t)$, with effective Hamiltonian [2]

$$H_0 = \frac{1}{2} M \left( \frac{d\phi}{dt} \right)^2 - \frac{Q_0}{\phi},$$

and initial condition $\phi(t_0) = 1$ and $\dot{\phi}(t_0)$ determined via Eq. (2) through energy conservation. Clearly, the dynamics of $\phi(t)$ must depend on the initial shape given by the $r_j(t_0) = \phi(t_0)\rho_j = \rho_j$. The initial shape determines parameters in the dynamic equation (2): the “effective mass” $M = \sum_{j=1}^{N} m_j \rho_j^2$ and the “effective charge” $Q_0 = -\sum_{i>j} q_i q_j |\rho_i - \rho_j|^{-1}$, where $m_j$ and $q_j$ are mass and charge of the $j$-th fragment, respectively. To remain shape-invariant the initial configurations $\{\rho_j\}$ need to satisfy a SC conditions [2]

$$\tilde{\alpha} \rho_j = -\frac{1}{m_j} \sum_{k \neq j} q_j q_k \frac{\rho_j - \rho_k}{|\rho_j - \rho_k|^3},$$

that ensure that acceleration of each particle $\ddot{r}_j$ is proportional to its CMS vector $r_j$, as follows from formula (1); $\tilde{\alpha} = Q_0/M$. An alternative, albeit equivalent formulation of the fixed-point condition is provided in the subsection 1.2.

It is universally known that the classical three- (or more) body problem does not allow analytical solution for a general initial condition. However this does not exclude possibility of SC analytical solutions (1) for some special initial conditions $r_j(t_0) = \rho_j$. Propagation along an expanding SC is the most efficient pathway to achieve full fragmentation given a small energy excess $E$. The actual trajectories leading to near–threshold fragmentation approach the SC configuration and their volume in phase space determines the cross section in the form the Wannier-type power law, $\sigma \sim E^\mu$. More precisely, the threshold exponent $\mu = \sum \mu_j$ is a sum of partial indices $\mu_j$ which characterize the instability of the SCs, for details, see [2, 3].
1.2 Scaling configurations and hyperspherical coordinate basis

Additional insight is obtained by considering the problem in hyperspherical coordinates where the SCs have an intuitive meaning [2, 4, 3]. In these coordinates the potential energy is cast in generalized Coulomb form

\[ V = \sum_{i<j} \frac{q_i q_j}{r_{ij}} = \frac{C(\Omega)}{R}, \quad (4) \]

where the hyperradius is defined by \( R^2 = \sum_j \rho_j^2 \). The hypercharge \( C(\Omega) \) depends on a set of hyperangles \( \Omega = \{\Omega_1, \Omega_2, \ldots, \Omega_{3N-7}\} \) which might be chosen in different ways (see, e.g., [5]). The set of hyperangles defines all geometrical angles in a configuration of particles and also all the ratios of distances between the fragments.

By definition, for an SC, all hyperangles have fixed values \( \text{in time} \), \( \Omega^{(0)} = \{\Omega_1^{(0)}, \Omega_2^{(0)}, \ldots, \Omega_{3N-7}^{(0)}\} \). Such a trajectory is possible only provided \( \Omega^{(0)} \) is stationary, i.e., a fixed point of \( C(\Omega) \) on the hypersphere,

\[ \left. \frac{\partial C(\Omega)}{\partial \Omega_j} \right|_{\Omega=\Omega^{(0)}} = 0, \quad j = 1, 2, \ldots, (3N - 7). \quad (5) \]

Note, that the stationary point cannot correspond to a stable equilibrium. This is the dynamic analogue [2] of the well known Earnshow theorem in electrostatics. The conditions (3) or (5) present two equivalent sets of non-linear equations; no systematic methods of solution are known.

It is easy to establish relation with parameters introduced in Section 1.1. With \( \phi(t_0) = 1 \), we find \( R(t_0)^2 = \sum_j \rho_j^2 = M, \ C(\Omega_0) = R(t_0) Q_0 = M^{1/2} Q_0 \). The partial threshold indices \( \mu_j \) characterize the instability of the saddle point \( \Omega^{(0)} \) on the hypersphere [2].

2 Scaling configurations and Thomson’s problem

2.1 Thomson’s problem

The problem of finding SCs is similar to Thomson’s famous problem (TP), also known as the surface Coulomb problem. It was put forward by J. J. Thomson in connection to his plum pudding model of an atom [6]. The problem belongs to electrostatics and implies to find the global minimum of potential energy for \( N \) identical point charges confined to the surface of a sphere, i.e. minimizing Eq. (4) under conditions \( q_j = 1, |\mathbf{r}_j| = 1 \) (hereafter a unit charge and a unit sphere are assumed). The related configuration of classical charged particles is referred to below as Thomson’s configuration (TC). Notwithstanding its elementary physical formulation, TP exhibits a variety of quite unexpected properties and serves as a testground for complexity studies. The literature on the problem (and its generalizations and extensions) is vast, ranging from mathematically rigorous studies to physical, chemical and biological applications; we give here only some representative references [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21].
Table 1. Comparison of Thomson’s problem and scaling configurations problem.

<table>
<thead>
<tr>
<th>Thomson’s problem</th>
<th>Scaling configuration problem</th>
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<tbody>
<tr>
<td>Charged particles confined to a sphere</td>
<td>Charged particles on a hypersphere</td>
</tr>
<tr>
<td>Search for a particle configuration that provides a minimum of interaction potential</td>
<td>Search for a particle configuration that provides a saddle point (minima do not exist)</td>
</tr>
<tr>
<td>Many configurations provide local minima</td>
<td>Many configurations provide saddle points</td>
</tr>
<tr>
<td>Global minimum is of interest</td>
<td>Scaling configuration that provides minimum threshold index $\mu$ is of interest</td>
</tr>
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2.2 Comparison of scaling and Thomson’s configurations

The objective of the present study is a comparative discussion of TCs and SCs, a summary is provided in table 1. For TCs one has to locate the \textit{minima} of potential energy for the charged particles confined to a sphere in real space. In distinction, for SCs the \textit{stationary points} (or saddle points) on a hypersphere are of interest. In simple terms this means that in the second case the particles are allowed to be at different distances from the center yet compatible with the fixed point condition Eq. (5).

In the TP the number of stationary points seems to increase exponentially with the number $N$ of particles [14]. The same applies to the SCs problem. There is no analytical solution to identify the \textit{global} minimum of the interaction energy $V$. For small $N$ the TCs can be found in different sources [14, 18, 21]. For large $N$ the problem is solved numerically by various trial and error methods; large-$N$ asymptotic expressions for the energy are discussed in [11, 14, 16]. Numerical finding of SCs is even more difficult, since the gradient methods do not work. When SCs are applied in the threshold law theory, one has to select the \textit{optimum scaling configuration} (OSC) that yields the minimum threshold exponent $\mu$ [2].

2.3 Special values of $N$

TCs and SCs are identical in case $N = 3$ (triangle) and $N = 4$ (tetrahedron, which is Platonic solid). The competing SCs with larger $\mu$, respectively, are a line (for $N = 3$) and a line and a square (for $N = 4$).

For $N = 5$ the TC and SC are different. In both cases they are bypyramids formed by equilateral triangles with the other two particles located symmetrically above and below the triangle. For the TP, when all charges lie on a sphere, the angle $\alpha$ at the pyramids vertices is equal to $45^\circ$. For the SC problem the angle $\alpha$ is a variable parameter to be defined from the SC conditions Eq. (5). The equation that governs $\alpha$ was derived in Ref. [2] for a more general situation when a charge $Z$ of opposite sign is placed in the centre of SC (such a charge does not influence TC). Table 2 lists values of $\alpha$ for different $Z$. They prove to be surprisingly close to $45^\circ$, albeit slightly less; they tend to $45^\circ$ as $Z$ increases. Hence, although for the SCs the particles are not forced to lie on a sphere, in fact for $N = 5$ the SCs
prove to be very close to spherical.

A similar situation emerges for \( N = 7 \) where both TC [18] and SC [22] are symmetrical bipyramids with a pentagon as a base. In this case the SC can also be characterized by a single angle \( \alpha \) [22]. It is slightly larger than 45° and approaches 45° for \( Z \to \infty \). For \( N = 6 \) both TC and SC are octahedron (Platonic solid). The case \( N = 8 \) is considered in the next section.

For some values of \( N \) the TCs correspond to the charge distributions with a non-zero dipole moment (the lowest value is \( N = 11 \)). Such a situation cannot occur for the SCs of identical particles, since the CM frame is pre-chosen.

### 3 Configurations with eight charges

For \( N = 8 \) equal charges the highly symmetrical cubic arrangement (Platonic solid) is an obvious candidate for the TC or SC. However, this configuration provides only a saddle point for the potential energy \( V \); the minimum is ensured by the twisted cube (known also as the compressed square antiprism). Transition from the cube to the twisted cube can be divided into two steps. First, upper plane with four charges is rotated by an angle \( \beta \) relative to the lower plane. The lowest energy is obtained for \( \beta = 45° \). Second, further energy lowering is achieved if the distance \( 2a \) between the planes is considered as a variable parameter (it is assumed that all the charges remain on a unit sphere whose centre lies symmetrically between the planes). The equation that governs \( a \) reads

\[
\frac{(2 + \sqrt{2})\sqrt{1 - a^2}}{[2 - \sqrt{2} + (2 + \sqrt{2})a^2]^{3/2}} + \frac{(2 - \sqrt{2})\sqrt{1 - a^2}}{[2 + \sqrt{2} + (2 - \sqrt{2})a^2]^{3/2}} - \frac{2\sqrt{2} + 1}{4(1 - a^2)} = 0. \quad (6)
\]

Its solution is \( a_c = 0.5604367652904 \), while the regular cube corresponds to \( a_c = 1/\sqrt{3} = 0.57735027 \). The twisted cube provides the global minimum for \( V \) [8, 18, 21] with a potential energy \( V_t = 19.67528786123277 \) which is by 0.33% lower than \( V_c = 19.74077407376279 \) for the regular cube. The surface of \( V \) as function of the collective coordinates \( \beta \) and \( a \) is shown in figure 1.

The fact that the twisted cube provides TC does not necessarily mean that it serves also as the OSC. Nevertheless, experience with the TC hints at considering the twisted cube as a competing candidate for OSC. The results of our calculations of partial \( \mu_j \) and total \( \mu_t \) threshold indices within the general framework

<table>
<thead>
<tr>
<th>( Z )</th>
<th>( \alpha_5 )</th>
<th>( \alpha_7 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>44.40165°</td>
<td>45.7899°</td>
</tr>
<tr>
<td>2</td>
<td>45.15762°</td>
<td>44.4655°</td>
</tr>
<tr>
<td>4</td>
<td>45.09672°</td>
<td>44.7121°</td>
</tr>
<tr>
<td>6</td>
<td>45.04479°</td>
<td>44.8789°</td>
</tr>
<tr>
<td>8</td>
<td>45.03799°</td>
<td>44.8985°</td>
</tr>
<tr>
<td>10</td>
<td>45.02610°</td>
<td>44.9317°</td>
</tr>
</tbody>
</table>

\( Z_5 \) for six-particle systems \( A^+ + 5e \) and \( \alpha_7 \) for eight-particle systems \( A^+ + 7e \); a – results from Ref. [2]; b – results from Ref. [22].

Table 2. Parameters of scaling configuration (bipyramids) \( \alpha \) for six-particle systems \( A^+ + 5e \) and \( \alpha_7 \) for eight-particle systems \( A^+ + 7e \); a – results from Ref. [2]; b – results from Ref. [22].
Table 3. Partial $\mu_j$ and total $\mu_t$ threshold indices for nine-particle systems $A^{+Z} + 8e$. The scaling configuration is twisted cube. The number in parentheses indicates degree of unstable mode degeneracy. $\mu_c$ is threshold index for regular cube as the scaling configuration [22].

<table>
<thead>
<tr>
<th>$Z$</th>
<th>$\mu_1$</th>
<th>$\mu_2$</th>
<th>$\mu_3$</th>
<th>$\mu_4$</th>
<th>$\mu_t$</th>
<th>$\mu_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>1.26687 (2)</td>
<td>1.24883 (2)</td>
<td>1.19876</td>
<td>1.19849 (2)</td>
<td>8.62711</td>
<td>8.65798</td>
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<tr>
<td>7</td>
<td>1.21226 (2)</td>
<td>1.19768 (2)</td>
<td>1.15719</td>
<td>1.15695 (2)</td>
<td>8.29096</td>
<td>8.31522</td>
</tr>
<tr>
<td>8</td>
<td>1.17628 (2)</td>
<td>1.16403 (2)</td>
<td>1.13002</td>
<td>1.12979 (2)</td>
<td>8.07022</td>
<td>8.09022</td>
</tr>
<tr>
<td>9</td>
<td>1.15075 (2)</td>
<td>1.14019 (2)</td>
<td>1.11086</td>
<td>1.11066 (2)</td>
<td>7.91406</td>
<td>7.93109</td>
</tr>
<tr>
<td>10</td>
<td>1.13170 (2)</td>
<td>1.12242 (2)</td>
<td>1.09663</td>
<td>1.09644 (2)</td>
<td>7.79774</td>
<td>7.81256</td>
</tr>
<tr>
<td>11</td>
<td>1.11693 (2)</td>
<td>1.08647 (2)</td>
<td>1.08563</td>
<td>1.08546 (2)</td>
<td>7.70770</td>
<td>7.72083</td>
</tr>
</tbody>
</table>

of Ref. [2] are shown in table 3 for different values of the central charge $Z$ (the SC parameters $\beta_t$ and $a_t$ do not depend on $Z$). Comparison with the results $\mu_c$ for the regular cube [22] reveal that the twisted cube is the OSC. Interestingly, not only total threshold index $\mu$, but also all partial indices $\mu_j$ for the twisted cube are smaller than for the regular cube.

The threshold indices $\mu_t$ in table 3 describe the electron impact fragmentation process

$$e + A^q \rightarrow A^{Z} + 8e , \quad Z = q - 7 , \quad (7)$$

or photofragmentation

$$\gamma + A^q \rightarrow A^{Z} + 8e , \quad Z = q - 8 . \quad (8)$$

Since these indices correspond to OSC, these indices are to be used instead of larger indices $\mu_c$ obtained in Ref. [22] for cubic configuration. The lowering of $\mu$ is relatively small and difficult to observe experimentally; still it is of principle interest. Concerning experimental observations of the Wannier-type threshold laws in electron impact ionization (or photoionization) of atoms it is worthy to indicate that they can be masked by the secondary threshold laws in case when the residual ion is a multielectron system [23]. However if the residual core is a bare atomic nucleus, then the resonance secondary mechanism is not operative.
4 Conclusion

We have discussed the analogy between the well studied Thomson problem and the threshold fragmentation of charged particles using the description of scaling configurations of the latter as a bridge. While there are specific differences, solutions of Thomson’s problem can guide the difficult search for optimal scaling configurations in high dimensions as demonstrated here with the twisted cube for 8-fold ionization of an atom or ion.

Possible generalizations include the threshold problem for fragments interacting by a dipole-like potential $\sim r_{ij}^{-2}$ [24]. A similar analogue of Thomson’s problem was studied by a number of authors [14]. In the quantum TP (not considered previously) one has to treat charges as quantum particles. Here an interesting feature is resonance tunnelling between equivalent minima (see Fig. 1) that leads to splitting of energy levels, similarly to internal rotation in molecules.

Acknowledgements

The authors are thankful to K. B. MacAdam for attracting their attention to Thomson’s problem.

References

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Mass-Related Dynamical Barriers in Triatomic Reactions

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Abstract. A methodology is given to determine the effect of different mass distributions for triatomic reactions using the geometry of shape space. Atomic masses are incorporated into the non-Euclidean shape space metric after the separation of rotations. Using the equations of motion in this non-Euclidean shape space, an averaged field of velocity-dependent fictitious forces is determined. This force field, as opposed to the force arising from the potential, dominates branching ratios of isomerization dynamics of a triatomic molecule. This methodology may be useful for qualitative prediction of branching ratios in general triatomic reactions.

1 Introduction

The roles played by atomic masses are of great interest in current chemical physics. Atomic-mass effects will be the most prominent in isotopic reactions such as the breakup dynamics of triatomic hydrogen ion H$_3^+$ and its isotopomers, D$_2$H$^+$, H$_2$D$^+$, and D$_3^+$ [1]. The anomalous isotope effect in ozone O$_3$ [2, 3] also provides intriguing problems that are related to the influence of atomic masses. Therefore, a general framework to describe the effect of atomic masses in triatomic reactions should serve many purposes.

Atomic masses are incorporated into the metric tensor of shape space on the basis of reduction theory [4] and gauge theory [5, 6, 7] that is used for the separation of rotational degrees of freedom. The metric tensor after reduction is generally non-Euclidean for three- and more-atom systems. As a result, the dynamical effects that have their origin in the non-Euclidean nature of the metric of shape space, should be important for understanding the effect of the masses. It should be noted that while the Born-Oppenheimer potential energy surface

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changes depending on the system, the geometry of shape space is rather intrinsic and independent of the system. Therefore, it is important to study the geometry of shape space of many-body systems.

Its non-Euclidean nature suggests that trajectories in shape space possess a certain directionality, even without the influence of the potential energy surface. This directionality is of importance in branching processes in multi-channel reactions. The behavior of geodesics signals this “preference” of motion in shape space. In this article, using suitable coordinates, an averaged field of “fictitious forces” is found that accounts for the directionality of geodesics. It is shown that this force field does, in fact, dominate mass-influenced branching ratios of isomerization dynamics of a triatomic molecule.

A prototypical model to study mass-related branching ratios of isomerization reactions is presented in §2, and §3 gives a theoretical explanation for the branching ratios via the geometry of shape space.

2 Model Reactions and Branching Ratios

This section investigates the isomerization dynamics of a molecular cluster composed of three atoms with different masses \((m_1, m_2, m_3) = (1, 1, 0.1)\) with the aim of determining the effects of the values of the masses. The total angular momentum of the system is taken to be zero for simplicity. The three atoms interact equally through a pairwise Morse potential. Because of the mass difference, this system is called a “modified” \(M_3\) cluster. The dimensionless Hamiltonian of the system is given by

\[
\mathcal{H} = \frac{1}{2} m_1 \dot{r}_1^2 + \frac{1}{2} m_2 \dot{r}_2^2 + \frac{1}{2} m_3 \dot{r}_3^2 + \sum_{i<j} \left[ e^{-2(d_{ij}-6)} - 2e^{-(d_{ij}-6)} \right],
\]

where \(r_i = (r_{ix}, r_{iy}, r_{iz})^T\) \((i = 1, 2, 3)\) is the three dimensional position vector of each atom. Here, \(\varepsilon\) represents the depth of the Morse potential and \(d_{ij}\) is the inter-particle distance between the \(i\)-th and \(j\)-th atoms. In what follows, our numerical results are presented in absolute units.

As shown in Fig. 1(a), this cluster has two local equilibrium structures (isomers) whose potential energy is \(V = -3.00\varepsilon\). These are equilateral triangle and permutationally distinct since motion of the system is confined to a plane because of the assumption of zero total angular momentum. The system has three saddle points with potential energy \(V \approx -2.005\varepsilon\), which correspond to collinear configurations. They are also permutationally distinct. Channel 1 and Channel 2 are essentially equivalent and only Channel 3 is different from the other two. The potential-barrier heights for these three channels are exactly the same since the three particles interact equally through the pairwise Morse potential. The difference lies in the effect that different masses have on the dynamics of the isomerization reactions.

Fig. 1(b) shows the energy dependence of the relative reaction frequencies for the respective channels. In this numerical experiment, the frequencies of reactions through respective channels are counted and normalized to 100. To avoid over-counting reactions due to recrossing, only the event in which the system leaves
Figure 1. (a) Two equilibrium configurations and three saddle configurations of the modified M₃ cluster. The curves are the steepest descent paths of the potential energy. The two equilibrium points are located at \((w₁, w₂, w₃) = (15.429, 0, ±13.607)\). The saddle point for Channel 1 is at \((10.277, 23.548, 0)\) while that for Channel 2 is located at \((10.277, -23.548, 0)\). The saddle point for Channel 3 is at \((71.939, 0, 0)\). Inset is the equi-potential surface at \(V = -1.4ε\). (b) Energy dependence of relative reaction frequency for each channel.

the vicinity of one of the equilibrium points and arrives at the vicinity of the other equilibrium point is counted. It is evident from Fig. 1(b) that the reaction through Channel 3 is much less frequent than those through Channels 1 and 2. In other words, the system prefers the reaction through heavy-heavy-light configurations rather than heavy-light-heavy configurations. Furthermore, this tendency is observed to become more prominent as the energy of the system increases. The bias in the reaction frequency in Fig. 1(b) cannot be explained simply by the potential energy barrier height since the barrier height for the three channels are the same. Instead, the bias must be related to the mass. In the next section, a possible explanation for this mass effect is given.

3 Geometry of Shape Space and Dynamical Barriers

A useful coordinate system for characterization of mass effect in triatomic reactions is the so-called “symmetrical coordinates” [6, 7], which is defined as follows. First, the mass-weighted Jacobi vectors are defined as

\[
\rho₁ = \sqrt{\mu₁} (r₁ - r₂), \quad \rho₂ = \sqrt{\mu₂} \left( \frac{m₁ r₁ + m₂ r₂}{m₁ + m₂} - r₃ \right),
\]

where \(\mu₁ = m₁ m₂ / (m₁ + m₂)\) and \(\mu₂ = (m₁ + m₂) m₃ / (m₁ + m₂ + m₃)\) are the reduced masses. Then the shape (internal) coordinates are defined as,

\[
w₁ = |\rho₁|^² - |\rho₂|^², \quad w₂ = 2 \rho₁ \cdot \rho₂, \quad w₃ = 2 \rho₁ \times \rho₂,
\]

where the sign of \(w₃\) specifies the permutational isomers of the modified M₃ cluster. Fig. 1(a) shows the steepest descent paths of the potential energy connecting
the two equilibrium points via the three saddle points. The inset shows the equi-
potential surface of the modified M$_3$ cluster at $V = -1.4\varepsilon$. The interior region
of the equi-potential surface is called “Hill’s region” in analogy with usage in
astrophysics. The structures in Fig. 1(a) have reflection symmetry with respect
to the $w_1$-$w_2$ plane and the $w_1$-$w_3$ plane.

The intrinsic metric tensor of shape space for the coordinates $(w_1, w_2, w_3)$
is known to be diagonal [6, 7] with $g_{11} = g_{22} = g_{33} = 1/4w$, where $w =
\sqrt{w_1^2 + w_2^2 + w_3^2}$ and $g_{ij} = 0 \ (i \neq j)$. Therefore the Lagrangian for the
triatomic system with zero-angular momentum is
\[
\mathcal{L} = \frac{1}{2} \left( \frac{1}{4w} \right) \dot{w}_1^2 + \frac{1}{2} \left( \frac{1}{4w} \right) \dot{w}_2^2 + \frac{1}{2} \left( \frac{1}{4w} \right) \dot{w}_3^2 - V(w_1, w_2, w_3). \tag{4}
\]

Then classical equations of motion derived from this Lagrangian are
\[
\frac{1}{4w} \ddot{w}_1 - \frac{w_1}{8w^3} \dot{w}_1^2 + \frac{w_1}{8w^3} \dot{w}_2^2 + \frac{w_1}{8w^3} \dot{w}_3^2 - \frac{w_2}{4w^3} \dot{w}_1 \dot{w}_2 - \frac{w_3}{4w^3} \dot{w}_1 \dot{w}_3 = -\frac{\partial V}{\partial w_1}, \tag{5}
\]
\[
\frac{1}{4w} \ddot{w}_2 + \frac{w_2}{8w^3} \dot{w}_1^2 - \frac{w_2}{8w^3} \dot{w}_2^2 + \frac{w_2}{8w^3} \dot{w}_3^2 - \frac{w_1}{4w^3} \dot{w}_2 \dot{w}_1 - \frac{w_3}{4w^3} \dot{w}_2 \dot{w}_3 = -\frac{\partial V}{\partial w_2}, \tag{6}
\]
\[
\frac{1}{4w} \ddot{w}_3 + \frac{w_3}{8w^3} \dot{w}_1^2 + \frac{w_3}{8w^3} \dot{w}_2^2 - \frac{w_3}{8w^3} \dot{w}_3^2 - \frac{w_2}{4w^3} \dot{w}_3 \dot{w}_2 - \frac{w_1}{4w^3} \dot{w}_3 \dot{w}_1 = -\frac{\partial V}{\partial w_3}. \tag{7}
\]

The terms from the 2nd to the 6th on the left hand sides of these equations are
quadratic in the velocity components $\dot{w}_i$. These terms are originated from the
non-Euclidean metric of shape space and can be regarded as velocity-dependent
“fictitious forces” in the coordinate chart depicted in Fig. 2. These terms char-
acterize the behavior of geodesics.

To extract the essential property of these velocity-dependent force terms,
their averages are considered. This is reasonable since these velocity-dependent
terms (forces) usually fluctuate rapidly in the chaotic dynamics of the system.
If the distribution of velocity vectors in the tangent space at each point is suffi-
ciently stochastic, then the equipartition law holds for the kinetic energy terms
in Eq. (4). As a result, one obtains, for the averages of the diagonal quadratic
terms, $\langle \dot{w}_1^2 \rangle = \langle \dot{w}_2^2 \rangle = \langle \dot{w}_3^2 \rangle = 8wK/3$, where $K = E - V(w_1, w_2, w_3)$ is the
kinetic energy at each point in the shape space. As for the cross terms, one gets
$\langle \dot{w}_i \dot{w}_j \rangle = 0 \ (\text{for } i \neq j)$, since one can assume $\dot{w}_i$ and $\dot{w}_j$ are independent in a
stochastic system. Applying these averages to the velocity-dependent terms in
Eqs. (5)-(7), an averaged force field is finally obtained as
\[
\left( -\frac{Kw_1}{3w^2}, -\frac{Kw_2}{3w^2}, -\frac{Kw_3}{3w^2} \right). \tag{8}
\]

This force field should be working effectively in the dynamics of the cluster.

Fig. 2(a) shows the field of Eq. (8) in the Hill’s region at $E = -1.4\varepsilon$. Ob-
serve that the averaged force works to block trajectories to get into the reaction
pathway of Channel 3 at the vicinity of the two equilibrium points. This is the
mass-related dynamical barrier originated from the geometry of shape space. To
quantify the effects of the averaged force, a “reaction-path potential” is intro-
duced, which is defined as the sum of the original potential and the line-integral
of the averaged force along a path. For simplicity, the steepest descent paths are chosen in Fig. 1(a) as the reaction paths. Fig 2(b) shows the original potential and the reaction-path potential as a function of arc-length of the path for respective channels. The height of original potential barrier is the same for all the channels. The barrier of reaction-path potential becomes higher and higher as the energy increases in Channel 3, while the energy dependence of the reaction-path potential is very weak for Channel 1 and 2. This explains why the isomerization reaction through Channel 3 becomes much less frequent as the energy increases.

In conclusion, a concise method to characterize the effect of different masses for triatomic reactions has been proposed. An averaged force field has been deduced using the non-Euclidean metric of shape space. This force field is shown to play a crucial role in determining the mass-related branching ratios of isomerization of the triatomic cluster. Since the geometry of shape space is independent of the system, the proposed methodology should be useful for varieties of triatomic reactions.

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References

Application of Tube Dynamics to Non-statistical Reaction Processes

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Abstract. A technique based on dynamical systems theory, is introduced for the computation of lifetime distributions and rates of chemical reactions and scattering phenomena, even in systems that exhibit non-statistical behavior. In particular, we merge invariant manifold tube dynamics with Monte Carlo volume determination for accurate rate calculations. This methodology is applied to a three degree of freedom model problem and some ideas on how it might be extended to higher degree of freedom systems are presented.

1 Introduction

Chemical reaction rates are usually computed using statistical methods, such as Rice-Ramsperger-Kassel-Marcus (RRKM) theory, also known as transition state theory (TST). TST is based on the identification of a transition state (TS) between regions of phase space that correspond to either “reactants” or “products.” TST yields rates based on a local study of the TS as well as the assumption that the phase space in each region is structureless. These values can be several orders of magnitude off of experimental values [1]. Despite its shortcomings, TST has been a workhorse of the chemistry community for decades. However, it is now well known that while the structureless assumption is useful in many situations, in general these regions (often defined by potential wells) are not structureless.

Many attempts have been made to remedy this situation. De Leon et al. [2] attempted to extend the local picture near the TS in two degree of freedom (dof) systems to a more global one and developed reaction island theory using cylindrical manifolds. Komatsuzaki and Berry [3] used perturbative methods to
study the transition near the saddle region. Uzer et al. [4] studied the local geometric structures of rank-one saddles that regulate reactions in systems with three or more dof. But a comprehensive theory of chemical reactions and efficient computational tools for reaction rate calculations in three or more dof systems which takes into consideration phase space structures still needs to be developed.

By merging tube dynamics of Koon el al. [6] and De Leon et al. [2] with Monte Carlo methods, [5] provides some enabling theoretical and computational tools for the computation of lifetime distributions and rates of chemical reactions and scattering phenomena. The standard RRKM assumption of an unstructured phase space fails to account for the dynamics of systems exhibiting significant non-statistical behavior. This difficulty is overcome by using the homoclinic and heteroclinic intersection structure of tubes in phase space developed in [6].

A main problem with the application of tube dynamics has been the computation of volumes of tube intersections in phase spaces of high dimension [2, 4]. The paper [5] provides a starting point for overcoming this hurdle with an algorithm that uses tube dynamics to provide the initial bounding box for a Monte Carlo volume determination. We apply the method to a model three dof problem in which the hypotheses of TST do not hold: namely, the full-scattering of electrons of Rydberg hydrogen atoms in crossed electric and magnetic fields. We use a variety of methods and software that have been developed for tube dynamics [6, 7] to better understand the transport between different regions of phase space. The numerical results obtained are a demonstration of accurate lifetime distribution and rate calculations which overcome some of the difficulties of the standard statistical methods. Moreover, we mention some of our current effort in extending the applicability of our computational methods.

2 Merge Tube Dynamics with Monte Carlo Methods

Many chemical reactions proceed through energetic barriers. Such situations are well described in phase space where the energy-fixed hyper-surface determines different regions connected by the energy barriers, specifically by structures related to rank-one saddles associated with the barriers. To simplify the discussion, we consider a two state system where one state is bound and the other is unbound. Figure 1(a) shows a planar projection of the Hill region for the Rydberg atom in crossed fields; this Hill region shows the region in configuration space where the motion of the electron is possible for a given energy level.

The ionization of a Rydberg hydrogen atom in external crossed electric and magnetic fields has been studied by other authors (such as [4]). To illustrate our method, we investigate the full-scattering problem, in which the system is prepared in an unbound initial state and we study the dynamics of formation of an excited Rydberg atom and its subsequent ionization. The dynamics of the outermost electron can be described by the following classical Hamiltonian:

\[
H = \frac{1}{2}(p_x^2 + p_y^2 + p_z^2) - \frac{1}{r} + \frac{1}{2}(xp_y - yp_x) + \frac{1}{8}(x^2 + y^2) - \varepsilon x,
\]

where \(r = \sqrt{x^2 + y^2 + z^2}\) is the distance from the electron to the center of the nuclear core and \(\varepsilon\) is the scaled electric field strength.
For an energy value just above that of a saddle, the bottleneck near the saddle opens (see Figure 1(a)) and the electron can move between the unbound and bound region. Specifically, in the bottleneck region, there exist 4 types of orbits: (i) a large number of bounded orbits which form a topological 3-sphere, i.e., instead of a periodic orbit $S^1$ in the 2dof case, we have a $S^3$ of bounded orbits in the 3dof case; it is an example of a normally hyperbolic invariant manifold (NHIM) where the stretching and contraction rates transverse to the NHIM dominate those tangent to the NHIM; (ii) 4 cylinders of asymptotic orbits that wind onto and off the NHIM; instead of 2-dimensional invariant manifold in the 2dof case, one has 4-dimensional invariant manifold: $S^3 \times \mathbb{R}$ in a 5-dimensional energy manifold; they act as separatrices for the trajectories through the bottleneck region; (iii) those inside the tubes are transit trajectories which the electron must use to transit from one region to another; (iv) those outside the tubes are non-transit trajectories where the electron bounces back to its original region. These tubes are the geometric structures that completely control the reaction between the bound and unbound regions.

To study the reaction mechanism and compute its corresponding rates, we use carefully chosen 4-dimensional Poincaré sections $\Sigma_h$. Any trajectory from an unbound state to a bound state must be in the interior of the stable tube $W^s_+$, and continues in the interior of the unstable $W^u_+$ tube. $W^s_+ \cup W^u_+$ which constitutes the capture reaction path from the unbound to bound state first pierces the Poincaré section in the entrance or first Poincaré cut $\tilde{C}_1$. See Figure 1(b). Similarly, $W^s_\square \cup W^u_\square$, constitutes the escape reaction path, and any trajectory from the bound state to the unbound state has to pass through the exit or first Poincaré cut $\tilde{C}_1^\square$ of this reaction path, just before reaction takes place. The intersection of the images of the entrance and the pre-images of the exit $f^{-1}(\tilde{C}_1) \cap f^{-(k-1)}(\tilde{C}_1^\square)$ under the Poincaré map $f$ on $\Sigma_h$ are what give rise to full-scattering reactions. The problem can be simplified by looking only at the intersections of the images of the entrance with the exit itself: $\tilde{C}_1 \cap \tilde{C}_1^\square = f^{l-1}(\tilde{C}_1) \cap \tilde{C}_1$ where $l = m + k - 1$. Any point inside the intersection $\tilde{C}_1 \cap \tilde{C}_1^\square$ is a trajectory that comes from the unbound state $R_U$, loops around the core and intersects $\Sigma_h$ $l$ times before escaping to $R_U$.

Since the system is Hamiltonian, the Poincaré map is volume preserving.
Assuming a uniform distribution of incoming reactants on $\bar{C}_1^+$, then the fraction of products escaping after executing $m$ loops around the bound region is $\frac{V(C_m^+ \cap \bar{C}_1^+)}{V(C_1^+)}$ where $V(A)$ is the volume of $A \subset \Sigma_h$. It is common to use Monte Carlo methods to compute numerically high dimensional volumes. We first choose a hyper-rectangle “bounding box” containing the Poincaré cuts of the stable and unstable manifolds of the NHIM. See Figures 1(b). For the method to be efficient, it is important that this box contains as tightly as possible the Poincaré cuts. It is then easy to obtain an oracle that distinguishes whether randomly chosen points inside this box belong to the targeted object: e.g., a point belongs to the $m$th overlap $C_m^+ \cap \bar{C}_1^+$ if it belongs to the exit $\bar{C}_1^+$ and its $(m-1)$th backward iterate by the Poincaré map belongs to the entrance. Given this oracle, we can use any standard Monte Carlo method to compute the desired volume.

![Figure 2](image)

**Figure 2.** (a) The electron scattering lifetime distribution for the Rydberg atom. (b) Isomerization of the modified $M_3$ cluster: a triatomic cluster of 2 heavy atoms and 1 light atom interacting through the pairwise Morse potential; the system has 2 permutationally distinct isomers, connected by 3 reaction pathways through 3 collinear saddles, each having the same potential barrier height.

In Figure 2(a), the percentage of reactants escaping from the bound state as a function of loops in the bound region is shown. The resulting scattering profile, computed from the 4D intersection volumes computed via the Monte Carlo method, is structured; i.e., it is not a simple exponential decay. The result implies that the phase space is not structureless, and we need to take into consideration the tube dynamics and non-RRKM effects in computing reaction rates.

3 Current Work on Isomerization in a Tri-Atomic Molecule

The method can be used in any system with rank-one saddles that separate phase space regions corresponding to different states of a chemical system, such as the isomerization of polyatomic clusters and bimolecular reactions. A primary concern is to develop a method that can be extended to higher dimensional systems. In [5], we construct the manifolds of the NHIM by computing an appropriate normal form of the Hamiltonian, which can be difficult in higher dimensions. Here, we outline some initial ideas that may be useful in extending the method that do not require the normal form (see [8] for another method).

The key point is that to compute the hyper-volumes of intersection of invariant manifolds that give rise to the reaction rates and life-time distributions,
one needs only to construct a hyper-rectangle “bounding box” in the $(2n - 2)$ space that contains the Poincaré cuts of the stable and unstable manifolds of the NHIM. Then a Monte-Carlo method can be used in this $(2n - 2)$-dimensional box to compute the volumes of interest. For energies close to that of a saddle, we can choose (i) the center of the box to be the intersection point of the stable (and unstable) manifold of the saddle point and the Poincaré section, and (ii) the size of the box to be the smallest box that circumscribes the $(2n - 2)$-dimensional ball with radius $R = \beta \sqrt{2\varepsilon / \min \{\omega_k\}}$, where $\varepsilon$ is the difference of the actual energy with that of the saddle, $\omega_k$ are the elliptic modes of the linear dynamics at the saddle (recall that the quadratic normal form at the saddle is given by $H_2 = \lambda q_1 p_1 + \sum_2^n \frac{\omega_k}{2} (q_k^2 + p_k^2)$), and $\beta > 1$ is a factor of enlargement, to ensure that the box contains the targeted object. We start with, e.g., $\beta = 2$, compute the volume of interest, and then increase $\beta$ and recompute the same volume; if the difference of these two volumes is smaller than our numerical error tolerance, we take this $\beta$; if not, we restart the process with a larger $\beta$ as an initial guess. This iterative process allows us to compute the intersection volumes of the stable and unstable manifolds of the NHIM, and therefore the reaction rate.

Currently we are applying this method to the modified $M_3$ cluster which has been introduced in [9] to study the mass effect in isomerization dynamics of triatomic molecules. See Figure 2(b). Despite the same flux across each dividing surface, a significant difference arises among the possibilities of occurrence of reactions through respective pathways. These observations are symptoms of breakdown of the statistical hypothesis behind TST, and more detailed investigation of transport mechanisms along the reaction paths is necessary. For multi-channel reactions such as isomerization of the modified $M_3$, the heteroclinic intersection structure is also needed; techniques for tube dynamics developed in [6] are useful. To study the structure of these intersections, the choice of a suitable set of Poincaré sections is important. The computation of the volumes of all these different intersections via the bounding box method is a key step in computing the reaction rates between the two isomers following different reaction channels.


References


Dynamical Hierarchy in Transition States of Reactions*

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Abstract. We present a partial normalization procedure of Lie canonical perturbation theory to elucidate the phase space geometry of the transition state in the multidimensional phase space for a wide range of energy above the threshold. State selectivity and dynamical correlation along the evolution of reactions will also be discussed.

1 Introduction

All reactions take place through the ‘edge of stability,’ which chemists have long envisioned as transition state (TS). The concept of TS has been much more widely utilized than just for the problems near instability in chemistry, e.g., atomic physics, cluster physics, celestial mechanics, and biology [1]. In 1930s, the TS is defined by Wigner as a no-return dividing hypersurface in the phase space through which reacting species passes only once on the way from the reactant to the product. In other terms, the no-recrossing condition requires that the ‘one dimensional’ motion normal to the TS (reaction mode) is separable from the motions tangent to the TS (bath modes). While the existence and the definability of such a no-return TS were well established in two degrees of freedom (dof) Hamiltonian systems, those dynamical problems in more than two dof has been an open problem until very recently [2, 3, 4, 5, 6]. For a N-dof Hamiltonian

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system, we can expand it near a saddle with index one (an equilibrium point
with one negative Hessian eigenvalue) as
\[ H = E_0 + \sum_{i=1}^{N} \left( \frac{p_i^2}{2} + \frac{\omega_1^2 q_i^2}{2} \right) + \sum_{n=3}^{\infty} H_n, \]  
where \( E_0 \) is the energy of the saddle point and \( H_n \) consists of terms of \( n \)-th degree in \((p_1, \cdots, p_N, q_1, \cdots, q_N)\). \((p_1, q_1)\) are the momentum and coordinate of the reactive normal mode, and \((p_b, q_b)(= (p_2, \cdots, p_N, q_2, \cdots, q_N))\) are those of the bath normal modes, respectively. The unperturbed frequency of the reactive mode \( \omega_1 \) is pure imaginary and those of the bath modes \( \omega_i(i \geq 2) \) are real.

In an energy regime slightly above the saddle point energy (i.e., quasi-regular regime [2]) where \( \omega_i(i \geq 2) \) do not satisfy the resonance condition \( \sum_{i=2}^{N} n_i \omega_i \cong 0 \) (for any integers \( \{n_i\} \) unless all \( n_i \)'s are zero), \( H \) can be fully normalized into the Birkhoff normal form \( H' \) (a classical analog of Dunham Hamiltonian in quantum mechanics) by a canonical transformation \((p, q) \rightarrow (p', q')\) in terms of the Lie canonical perturbation theory (LCPT).

\[ H'(p', q') = H'(J') = E_0 + \sum_{i=1}^{N} \omega_i J_i' + \sum_{i,j} a_{ij} J_i' J_j' + \sum_{i,j,k} a_{ijk} J_i' J_j' J_k' + \cdots, \]  
where \( J_i' = i(p_i^2/|\omega_1| - |\omega_1| q_i^2)/2 \) and \( J_i' = (p_i^2/\omega_1 + \omega_1 q_i^2)/2 \) are, respectively, the ‘action’ of the transformed reactive normal form coordinate \((p_i', q_i')\) and those of the bath normal form coordinates \((p_b', q_b')\). \( a_{ij}, a_{ijk}, \ldots \) are coupling constants among \( J' \). Note that the fully normalized Hamiltonian \( H' \) does not involve any ‘angle’ variable conjugated to \( J' \). Thus, all \( J' \) are invariants of motion (i.e., \( H' \) is integrable) and the crossing dynamics can be solved analytically in full.

As the energy of the system increases, nonlinear resonances among the bath modes become significant and the overlapping of these resonances gives rise to the transition to global chaos. Nevertheless, in the region of index one saddles, any resonance condition can never be satisfied among the pure imaginary frequency (associated with the reactive mode) and the real frequencies (with the bath modes) [10]. This leads to the existence of the following partial normal form \( H'' \) for a wide range of energy above the threshold (i.e., semi-chaotic regime [2, 5]);

\[ H''(J_1'', p_b'', q_b'') = E_0 + \omega_1 J_1'' + \sum_{i=2}^{N} \frac{p_i''^2 + \omega_i^2 q_i''^2}{2} + f_1(J_1'', p_b'', q_b'') + f_2(p_b'', q_b''), \]  
where \( J_1'' = i(p''^2/|\omega_1| - |\omega_1| q_1''^2)/2 \) and the functions \( f_1 \) and \( f_2 \) contain anharmonic terms in power of the partial normal form variables \((p'', q'')\). In particular, \( f_1 \) is defined so that \( f_1 = 0 \) when \( J_1'' = 0 \). Note that Eq. (3) does not involve the ‘angle’ variable conjugated to \( J_1'' \), resulting in that \( J_1'' \) is an invariant of motion. However, in \( f_1 \) and \( f_2 \), resonance terms can exist among the bath modes \((p_b'', q_b'')\) (i.e., \( H'' \) is non-integrable). Since solely the reactive dof is normalized, only \((p_1'', q_1'')\) should be called normal form coordinate while the bath modes \((p_b'', q_b'')\) remains to be “normal mode” coordinates. Note, however, that \((p_b'', q_b'')\)
are functions of the original normal mode momenta and coordinates \((p, q)\) and so they are different from the original set.

Most of the theoretical studies \([4, 6, 7, 8]\) have focused only on the quasi-regular regime. In this paper, by using a partial LCPT to normalize solely the reactive mode, we discuss how nonlinear resonances among the bath modes, which appear as energy increases above the threshold, affect the invariance of the normal form action of the reactive mode and the state selectivity of reactions.

### 2 The partial normal form in the region of index one saddles

First, let us briefly look into the equation of motion of the partial normal form \(H''\) in Eq. (3):

\[
\begin{align*}
\frac{dp''_1}{dt} &= -\frac{\partial H''}{\partial q''_1} = -\left(1 + \frac{1}{\omega_1 \partial J''_1}\right) \omega_1^2 q''_1 = -\omega_1'' \omega_1 q''_1, \\
\frac{dq''_1}{dt} &= \frac{\partial H''}{\partial p''_1} = \left(1 + \frac{1}{\omega_1 \partial J''_1}\right) p''_1 = \frac{\omega_1''}{\omega_1} p''_1; \\
\frac{dp''_b}{dt} &= -\frac{\partial H''}{\partial q''_b} = -\omega_2^2 q''_b = \frac{\omega_2''}{\omega_1} q''_b, \\
\frac{dq''_b}{dt} &= \frac{\partial H''}{\partial p''_b} = p''_b + \frac{\partial f}{\partial p''_b} + \frac{\partial g}{\partial p''_b}, \quad b = 2, \ldots, N
\end{align*}
\]

where \(\omega''(J''_1, p''_b, q''_b) = \partial H''/\partial J''_1 = \omega_1 + \partial f/\partial J''_1\) is the normalized frequency of the reactive dof. Note here that while \(\omega''_1\) in the full normal form \(H'\) is an invariant of motion, \(\omega''_1\) in \(H''\) varies in time through its dependence on the bath modes \((p''_b, q''_b)\). Nevertheless, the equation of motion of \((p''_1, q''_1)\) is formally the same as that of \((p'_1, q'_1)\) in \(H'\) [8], and preserves the hyperbolic structure on the \((q''_1, p''_1)\) plane (because \(J''_1 = \text{constant}\)). For instance, the condition \(p''_1 = q''_1 = 0\) (yielding \(dp''_1/dt = dq''_1/dt = 0\)) defines a \((2N - 3)\)-dimension normally hyperbolic invariant manifold (NHIM) on the \((2N - 1)\) dimension equienergy surface in the phase space \(\mathbb{R}^{2N}\). Normal hyperbolicity means that the stretching and contraction rates of the motion normal to the manifold (i.e., the ‘reactive’ dof) dominate those of the motions tangent to the manifold (i.e., the bath dof). Fig. 1 shows the geometrical structure in the multi-dimensional phase space in the region of an index one saddle of the partial normal form Hamiltonian.

Note that Eq. (4) tells us that the velocity \(dq''_1/dt\) does not change its sign if the sign of \(\omega''_1\) does not change during the crossing. This implies that the system never turns back to a hypersurface \(S\) defined by \(q''_1 = 0\) (except backward reactions). Therefore, the local no-return property of \(S\) in \(H''\) is guaranteed if \(\omega''_1\) does not change its sign while the system crosses the saddle. The change of sign of \(\omega''_1\) requires the passage of \(\omega''_1 = 0\), which corresponds to an “instantaneous” breakdown of normal hyperbolicity, that is, \((1 + 1/\omega_1 \partial f/\partial J''_1(J''_1, p''_b, q''_b))_{J''_1=0} = 0\). It was found [9] that, as the energy increases near to the breakdown of normal hyperbolicity, the system recrosses the hypersurface \(S\) much earlier than finding this condition. However, one of the most important feature of this condition is the dependency on \((p''_b, q''_b)\), implying that some portions of the “NHIM” start
Figure 1. The geometrical structure of the multidimensional phase space in the region of index one saddle (Eq. 4) and NHIM $M$, its stable/unstable invariant manifolds $W^-/W^+$ and the ‘local’ no-return TS $S$. $M$ and $W^-/W^+$, respectively, correspond to the origin, and the stable/unstable directions represented by $p''_i = q''_i = 0$, and $p''_i = \pm|\omega_1|q''_i$ on the $(q''_i, p''_i)$ plane with the same ‘internal’ structure composed of the bath dof represented by $H''(J''_1 = 0, p''_b, q''_b) = E$ (the dash box in the figure). $S$ for forward/backward reactions are denoted by the two bold lines along $q''_i = 0$ on the $(p''_i, q''_i)$ plane (0 < $p''_i <$ $p''_{i, max}/p''_{i, min}$) with the same internal structure of the bath dof represented by $H''(J''_1 = p''^2_i/(2\omega_1), p''_b, q''_b) = E$. As in the case of the full normal form, one can classify reactive/nonreactive trajectories in terms of the sign of $-iJ''_1$ [8].

to break the normal hyperbolicity, not globally at once but locally, as energy increases.

We apply the partial LCPT to the following 3-dimensional Hamiltonian, which is regarded as a prototype of isomerization reactions,

$$H = \frac{1}{2}(p_1^2 + p_2^2 + p_3^2) + a_1q_1^2 + a_2q_3^4 + \frac{1}{2}(\omega_1^2 q_1^2 + \omega_2^2 q_3^2)$$

$$+ \sum_{i=0}^{2} e^{-\alpha_i(q_{11}-q_{10})^2}(\beta_i q_2 q_3^2 + \gamma_i q_1^2(q_2^2 + q_3^2)).$$

(5)

The parameters were chosen as follows: $a_1 = -35/75$, $a_2 = 2/1875$, $\omega_2 = 1$, $\omega_3 = 0.809$, $q_{10} = 2$, $q_{11} = -q_{12} = 14.1421$, $\alpha_0 = 1/16$, $\alpha_1 = \alpha_2 = 1$, $\beta_0 = 8$, $\beta_1 = \beta_2 = 1$, $\gamma_0 = 0.75$, $\gamma_1 = \gamma_2 = 1$. The ratio between $\omega_2$ and $\omega_3$, approximately the golden mean, was chosen as being avoided from linear resonance. The imaginary frequency associated with $q_1$ at the saddle is estimated as $\omega_1 \simeq -0.924i$. The nonzero value of $q_{10}$ aims at avoiding specific symmetry of the potential energy function in $q_1$. The original Hamiltonian Eq. (5) is transformed to the full normal form $H'$ and the partial normal form $H''$ up to the fifteenth order.

In Fig. 2, we display the full and partial normal form actions of the reactive dof $J'_1(p, q)$ and $J''_1(p, q)$ evaluated by the full and partial LCPTs along three distinct classes of trajectories (namely, on a torus, in a stochastic layer and in a global chaotic sea) on the NHIM obeying the original Hamiltonian $H(p, q)$ at $E = +0.1$ above the threshold, at which the global chaotic regime appears. It is found that while the full normal form action $J'_1(p, q)$ only fairly persists as
Figure 2. $J'_1(p, q)$ (dashed line) and $J''_1(p, q)$ (solid line) at $E = +0.1$ above the threshold (a) on a torus, (b) in a stochastic layer and (c) in a global chaotic sea on the NHIM. The insets are the Poincaré surface of section defined by $q''_1 = 0$ and $p''_3 > 0$. The initial conditions were prepared by $q''_1(p, q) = p''_1(p, q) = 0$ at time $t = 0$ and the trajectories were propagated backward and forward in time by the original Hamiltonian $H$ (eventually at $t \to \pm$large the system leaves from the (approximate) NHIM because of the finiteness of the order of LCPTs). Note that at $E \approx +0.15$ the normal hyperbolicity of the NHIM starts to be ruined due to the nonlinear resonances between the reactive mode $q''_1$ and some of the hyperbolic orbits densely distributed on the NHIM, whose imaginary frequencies are (near-)commensurable with $\omega''_1$ [9].

invariant, the partial normal form action $J''_1(p, q)$ strongly persists as invariant, especially at the global chaotic regime (see the difference of the scale of the vertical axis and compare $J''_1$ with $J'_1$ at $t \to \pm$large in Fig. 2).

For the full normal form $H'$ at slightly above the threshold, the motions of the bath dof are integrable with constants of actions $J'_b$ corresponding to good quantum numbers in the TS. It is expected that this yields state selectivity to give rise to reaction channels linking to specific product states. However, for the partial normal form $H''$ being nonintegrable (except only $J''_1$) at the higher energy regime, one may not expect the state selectivity. Fig. 3 exemplifies this: at an energy regime slightly above the threshold where most of tori remain on the NHIM, the system still ‘remembers’ the initial distribution of the normal mode action $J_2$ in the reactant and results in the ‘structured’ $J_2$-distribution in the product state, where the different values of $J_2$ at the initial state correspond to the well-defined distinct regions of $J_2$ at the final state. As the energy increases more, the system having different $J_2$ at the initial state can access any region of $J_2$ at the final state, yielding a ‘non-structured’ $J_2$-distribution. Note however that, as far as the original Hamiltonian can be transformed into the partial normal form (where normal hyperbolicity holds), the dynamical correlation along the reaction coordinate $q''_1(p, q)$ still persist with the invariant of action $J''_1(p, q)$.

3 Outlook and Conclusions

The hierarchical structure of the phase space was presented in the region of index one saddle by introducing a partial LCPT that normalizes solely the reactive dof. Quite recently, the quantum counterpart of this generic feature for Hamiltonian systems has also been explored [11, 12].
Figure 3. The product distribution of the normal mode action $J_2$ at $E = +0.025$ (a) and $+0.1$ (b) above the threshold. The initial conditions are prepared as follows: we turned off the coupling among the modes in the reactant by putting $\alpha_1 = \infty$ in Eq. (5) in order to prepare a well-defined initial condition in the reactant state. At $q_1 = -14.142$, we fixed $p_1$ to confirm the crossings to the product. Then, we set an initial distribution of the action $J_2$ such that $P_{ini}(J_2) = \sum_{i=1}^{3} \delta(J_2 - J_{2i})$ with three initial values of $J_2$ indicated by three arrows ($J_3$ is automatically determined with the fixed $J_1$ and $J_2$ at a given $E$) with the uniform sampling for the angle variable $\theta_2$ (and $\theta_3$). Then, the ensemble of trajectories of the initial conditions were evolved using the original Hamiltonian until they reach the product at $q_1 = 14.142$. The inset are the Poincaré surface of section defined by $q''_3 = 0$ and $p''_3 > 0$ on the NHIM (See the figure caption of Fig. 2 in detail).

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References

Fractal Structure in Ionization Dynamics*

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Abstract. Chaotic dynamics in open systems produces fractals. This can be seen, for example, in the ionization of an electron from a hydrogen atom in applied parallel electric and magnetic fields. We summarize some of our recent work on the order that can be found in these fractals.

We discuss here a prediction for a proposed experiment which has not yet been performed: the ionization of hydrogen by a short laser pulse

\[ H + h\nu \rightarrow H^* \rightarrow H^+ + e^- \]  \hspace{1cm} (1)

in parallel electric and magnetic fields. We predict that electrons will arrive at a detector in a train of pulses (Fig. 1a). This pulse train results from fractal structure in the dynamics, what we call an “epistrophic fractal.” As is well known, a fractal is a geometric set typically with some kind of repeating self-similar structure within structure. “Epistrophe” is a term from rhetoric, meaning a regular ending following variable beginnings. Thus, an epistrophic fractal is a class of a fractal in which there are variable beginnings and self-similar endings at all levels of resolution.

For a selection of work on the dynamics of transport and escape that has been influential to our own studies, please see the work by Tiyapan and Jaffé [1], Easton [2], Rom-Kedar [3], Jung and coworkers [4], and Collins [5]. See also recent work on the phase space formulation of transition states [6].

Pulse trains in the decay of excited atoms have been previously observed by Lankhuijzen and Noordam [7]. Measuring the decay of an excited rubidium atom in an electric field with picosecond time resolution, they found that the decay is not exponential, but instead occurs in a sequence of pulses; the time interval between pulses is approximately equal to the return time of an electron trajectory to the atomic core.

We consider an analogous experimental setup to that of Lankhuijzen and Noordam, but using hydrogen in parallel electric and magnetic fields. We describe the electron’s motion purely by classical mechanics. Effects of quantum mechanics on the electron’s motion will be examined in future studies.

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Figure 1. (a) For hydrogen in parallel fields, the flux of electrons striking a detector is plotted vs. time $T$. The thin line is a model assuming $\Delta E = \Delta T = 0$, whereas the thick line assumes a minimum uncertainty wavepacket, with central energy $\hat{E} = \frac{1}{2 \times 80^2}$ and $\Delta T = 5.2\text{ps}$. We use magnetic field $\mathbf{B} = 0.49\text{T}$, electric field $\mathbf{F} = 19\text{V/cm}$, and one scaled unit of time $T$ equal to 52ps. (b) Time to strike the detector plotted vs. the initial launch angle $\theta$. The dashed lines connect icicles to their corresponding pulses. (c) The number of iterates to escape the complex vs. launch angle $\theta$. Each escape segment corresponds to an icicle. (d) The dashed lines connect segments within one epistrophe. The solid arrows show the creation of new epistrophes according to the Epistrophe Start Rule. The asterisk denotes a “strophe” segment.

The time for an electron to ionize is a sensitive function of its initial launch angle from the atom. A graph of escape time $T$ vs. initial angle $\theta$ is shown in Fig. 1b. If the electron initially moves away from the atom in the “downhill” direction (i.e. in the direction of the electric force), then it escapes from the atom quickly. If it leaves in the “uphill” direction, it never escapes. At intermediate angles there is a very complex behavior, with structure-within-structure at all levels of resolution. This “escape-time plot” governs the structure of the pulse train: the probability current of electrons arriving at a detector is proportional to the derivative $d\theta/dT$ of the escape-time plot, so each “icicle” in the escape time plot produces a pulse of electrons arriving at the detector.

The escape-time plot is simplified by use of a Poincaré surface of section (SOS) and corresponding Poincaré return map. Every time the electron crosses the negative $z$-axis, we record the value of $(z, p_z)$. (We transform the $(z, p_z)$ coordinates to a “smoother” set of coordinates $(q, p)$ used in Fig. 2.) The SOS contains an unstable fixed point $z_X$ (Fig. 2), which corresponds to an unstable
periodic orbit that forms a Periodic Orbit Dividing Surface (PODS). (In order for the electron to escape, it must pass over the PODS in configuration space.) The fixed point \( z_X \) has stable and unstable manifolds, \( S \) and \( U \), which intersect in a complicated pattern called a “homoclinic tangle”. Choosing a particular intersection point \( P_0 \), the segments of \( S \) and \( U \) that connect \( z_X \) to \( P_0 \) define a region of the Poincaré plane, which we call the “complex”. The complex represents that part of phase space in which the electron has enough energy to escape but is still oscillating chaotically around the nucleus. The electron trajectories begin near the nucleus and move radially outward in all directions. The initial ensemble of electrons forms a line of initial conditions \( L_0 \) in the SOS.

The Poincaré map provides a second way of measuring how long the electron takes to escape: we count the number of iterates of the map required before the phase point leaves the complex. This measure of escape time “rectifies” the continuous escape-time plot (Fig. 1b) into discrete escape segments (Fig. 1c).

In Fig. 1b, 1c, or 1d, we can see the first few segments from several infinite regular sequences of escape segments, which we call “epistrophes”. In previous work, we proved that an epistrophe converges upon each end of every escape segment; the epistrophes are all asymptotically self-similar, and all asymptotically similar to each other; they differ from one another asymptotically only by an overall scale factor; successive segments in an epistrophe decrease geometrically by a factor equal to the Liapunov factor of the unstable fixed point. Thus, epistrophes occur at all levels of resolution.

However, there are also other escape segments that do not fit into the regular epistrophe sequences. Numerical evidence indicates that such “surprises” may appear at all levels of resolution, so they tend to break the self-similarity of the escape time plot.

The purpose of this research is to explain the structure of these escape-time...
plots, and thereby to explain the structure that may be observed in a pulse train. We have developed a technique using algebraic topology to explain and describe these structures. We do not have sufficient space here to describe the method in detail, but we can show how it is applied, and what kind of results it gives. The algebraic technique predicts a minimal set of topologically required escape segments at each iterate, by the following method.

1. Compute the stable and unstable manifolds from $z_X$ to $P_0$, i.e. compute the boundary of the complex.

2. Map the unstable manifold forward a chosen number of iterates $J$. The number of iterates chosen determines the amount of information about the homoclinic tangle that is used as input into the algebraic formalism, and thereby it determines the amount of information about the escape-time plot that can be predicted.

3. Visually extract essential information about the structure of the homoclinic tangle at iterate $J$.

4. Assign letter names to certain segments of the unstable manifold. Examples of letter names we use are $c_n$ for $1 \leq n \leq D$ and $u_m$ for $0 \leq m < \infty$. $D$ is a finite integer called the “minimum delay time” of the complex.

5. Represent the topological structure of the line of initial conditions $L_0$ by a word, i.e. a sequence of letters, $\ell_0$. In an idealized case, we might have $\ell_0 = c_1$.

6. Express the action of the map in terms of symbolic dynamics on these letters. For example, we might find $u_m \mapsto u_{m+1}$, $c_n \mapsto c_{n+1}$, $c_D \mapsto (c_1 c_2 ... c_D)^{-1} u_0^{-1} c_1 c_2 ... c_D$.

7. Apply this symbolic dynamics some number of iterates $K$ to the string $\ell_0$. For example, if $\ell_0 = c_1$, $D = 1$, and $c_1 \mapsto c_0^{-1} u_0^{-1} c_1$, we may iterate three times to obtain $\ell_3 = c_1^{-1} u_0 c_1 u_1 c_1^{-1} u_0^{-1} c_1 u_2 c_1^{-1} u_0 c_1 u_1^{-1} c_1^{-1} u_0^{-1} c_1$. This is not a meaningless string of letters, as we see in the next step.

8. In the string for $\ell_K$, read off the structure of the minimal topologically required set of escape segments up to iterate $K$: for example, each factor $u_i$ in $\ell_K$ represents a segment that escapes at iterate $K - i$. In the above example, we obtain the following escape time plot:

\[
\begin{array}{ccccccc}
3 & & & & & & \\
2 & & & & & & \\
1 & & & & & & \\
\end{array}
\]

On the first iterate, there must be one escape segment; on the second, there must be two, one on either side of the first; and on the third, there must be four segments, interleaved with the preceding ones.
The algebraic computation that explains the escape time plot in Fig. 1d follows a similar line as the example above. However, there is an additional sequence \((A_1, A_2, \ldots)\), which is discussed in [8], and there is another additional escape segment, marked with an asterisk. The latter segment, which we call a “strophe”, is not predicted by topological means – we simply compute the Poincaré map to the fifth iterate, at which point it appears in the numerics. However, once this segment is known to be present, one can expand the algebraic procedure, and then compute a revised minimal set of escape segments. This new minimal set will include additional segments that are forced by the “strophe” segment at iterate five.

The details of this theory are developed in Refs. [8, 9] and [10]. The same kind of theory should be useful for describing chaotic transport in many other systems, including atoms in other field configurations, molecular collisions, the restricted gravitational three-body problem, microwave cavities, etc.

References


Dependence of the H$_2$–H$_2$ interaction on the monomer bond lengths: steps toward an accurate ab initio estimate

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Abstract. We compute the vibrational coupling between two H$_2$ molecules from ab initio quantum chemical calculations of the H$_2$–H$_2$ potential carried out at the full configuration interaction level of theory using the atom-centered aug-cc-pVTZ basis set for hydrogen. We compare the full configuration interaction results with those obtained using two variants of coupled cluster theory and find that a fully iterative treatment of connected triples may be required to estimate the H$_2$–H$_2$ vibrational coupling accurately using coupled cluster theory.

1 Introduction

Tejeda et al. [1] have recently shown that small clusters of $j = 0$ H$_2$, or parahydrogen, molecules are formed when gaseous parahydrogen (pH$_2$) is cooled in a free jet expansion. They demonstrate the presence of these clusters in the cooled jet by observing the clusters’ Raman-active vibrational excitations that correlate with the pure vibrational $Q_1(0)$ transition of a single pH$_2$ molecule. The Raman features associated with clusters of $n = 2$ to 7 pH$_2$ molecules are narrow, isolated, and red-shifted from the free molecule’s $Q_1(0)$ transition at $\tilde{\nu} = 4161.18$ cm$^{-1}$; the red shift, which arises from weak pH$_2$–pH$_2$ intermolecular interactions in the (pH$_2$)$_n$ cluster, increases monotonically (but not linearly) with $n$ in this size range.

The vibrationally excited states of the (pH$_2$)$_n$ clusters accessed via these Raman-active transitions are ones in which the vibrational excitation is delocalized over the $n$ molecules in the cluster, and these states are thus finite-size analogues of the delocalized vibron states of crystalline solid H$_2$ probed via Raman

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Dependence of the $\text{H}_2$–$\text{H}_2$ interaction on the monomer bond lengths

![Diagram of H$_2$–H$_2$ configurations: T-shaped, parallel, linear](image)

Figure 1. Three representative configurations of the H$_2$–H$_2$ dimer. The H$_2$–H$_2$ center of mass distance is denoted $R$, while $r_1$ and $r_2$ represent the H$_2$ monomer bond lengths.

spectroscopy of the bulk solid [2]. A better understanding of these delocalized vibrational states of (pH$_2$)$_n$ clusters could therefore shed light on the clusters’ internal structures and on the question of whether the clusters exhibit signs of superfluidity, as has been suggested by path integral Monte Carlo simulations [3].

The delocalization of the vibrational excitation among a cluster’s constituent molecules is governed by terms in the H$_2$–H$_2$ potential energy surface that couple the vibrational coordinates of the two pH$_2$ molecules. At H$_2$–H$_2$ intermolecular distances characteristic of the (pH$_2$)$_n$ clusters, these terms are fairly small in magnitude. Estimating these terms from ab initio quantum chemical calculations thus requires the use of computational methods that have accuracy much higher than the oft-quoted “chemical accuracy” of 1 kcal/mol. Here we investigate the sensitivity of these coupling terms to the treatment of electron correlation effects in the underlying ab initio computations.

2 Ab initio calculations

The pH$_2$–pH$_2$ interaction is obtained by rotationally averaging the H$_2$–H$_2$ potential energy surface over the angular degrees of freedom of the H$_2$ monomers. We do not perform this full rotational averaging here, but simply consider three representative coplanar, high-symmetry configurations of the H$_2$ dimer, shown in Fig. 1. For each of these configurations, we hold the H$_2$–H$_2$ center-of-mass distance $R$ fixed and vary the monomer bond lengths $r_1$ and $r_2$. We consider two $R$ values: $R = 3.05$ Å, which is close to the root ($V = 0$) of the potential for a (pH$_2$)$_2$ dimer of two $v = 0$ molecules, and $R = 3.4$ Å, which is close to the minimum energy, equilibrium distance of the (pH$_2$)$_2$ dimer [4].

For these high-symmetry configurations, full configuration interaction (CI) calculations of the dimer’s electronic energy are feasible even for fairly large one-electron basis sets. Full CI calculations give the exact total electronic energy of the dimer for a given one-electron basis set and thus provide a reference point for benchmarking other electronic structure methods. We perform full CI calculations for the H$_2$–H$_2$ dimer using a determinant-based algorithm [5] as implemented in the November 22, 2004 (R1) version of the electronic structure...
Figure 2. Interaction energies for T-shaped H$_2$–H$_2$ with monomer bond lengths $r_1 = r_2 = r$ and H$_2$–H$_2$ distance $R = 3.4$ Å. (a) Full CI interaction energy $V_{\text{FCI}}$. (b) Interaction energy differences $V_{\text{CCSD(T)}} - V_{\text{FCI}}$ (open circles) and $V_{\text{CCSDT}} - V_{\text{FCI}}$ (filled boxes).

code GAMESS [6]. We then correct these H$_2$–H$_2$ total energy calculations for basis set superposition error by applying the standard counterpoise correction [7], thereby obtaining ab initio estimates of the H$_2$–H$_2$ interaction energy.

We also compute the H$_2$–H$_2$ interaction energy for these dimer configurations using two variants of coupled cluster theory [8, 9], one that includes single and double excitations and a perturbative treatment of triple excitations [10], abbreviated CCSD(T), and one that includes single, double, and triple excitations in a fully iterative manner [11, 12], abbreviated CCSDT. These calculations are performed using the tensor contraction engine [13] incorporated into version 4.7 of the electronic structure code NWChem [14]. We denote these two potential energy surfaces as $V_{\text{CCSD(T)}}$ and $V_{\text{CCSDT}}$ respectively.

All of our ab initio calculations are performed using the atom-centered aug-cc-pVTZ basis set for hydrogen [15, 16]. To avoid convergence difficulties arising from near linear dependence of the one-electron basis set at small $r_1$ and $r_2$ values, eigenvectors of the one-electron overlap matrix with eigenvalues below $10^{-6}$ are eliminated from the one-electron basis set for each H$_2$–H$_2$ configuration.

3 Results and discussion

Figure 2 shows, for T-shaped H$_2$–H$_2$ configurations with $R = 3.4$ Å and monomer bond lengths $r_1 = r_2 = r$, both the full CI interaction energy $V_{\text{FCI}}$ and the differences $\Delta V$ between $V_{\text{FCI}}$ and either $V_{\text{CCSD(T)}}$ or $V_{\text{CCSDT}}$. As $r$ increases, the CCSD(T) potential begins to deviate substantially from the full CI potential, with the difference $\Delta V = V_{\text{CCSD(T)}} - V_{\text{FCI}}$ reaching 3.75 cm$^{-1}$ (or 6% of the magnitude of $V_{\text{FCI}}$) at $r = 2.0$ a$_0$. By comparison, the difference between the CCSDT potential and the full CI potential remains below 0.85 cm$^{-1}$ for the entire range of H$_2$ bond lengths shown in Fig. 2.

Of particular interest are the shapes, near the equilibrium bond length $r_{\text{eq}} = 1.4$ a$_0$, of the energy difference curves shown in Fig. 2(b). The coupling between the vibrational coordinates of two H$_2$ molecules, which leads to delocalization of
Dependence of the H₂–H₂ interaction on the monomer bond lengths

Table 1. Off-diagonal vibrational coupling matrix elements \(\langle V(r_1, r_2) \rangle_{01,10}\) (in cm\(^{-1}\)) for H₂–H₂ dimers.

<table>
<thead>
<tr>
<th>Configuration</th>
<th>(R) ((\text{Å}))</th>
<th>full CI</th>
<th>CCSDT</th>
<th>CCSD(T)</th>
</tr>
</thead>
<tbody>
<tr>
<td>T-shaped</td>
<td>3.05</td>
<td>-0.740</td>
<td>-0.718</td>
<td>-0.674</td>
</tr>
<tr>
<td>T-shaped</td>
<td>3.4</td>
<td>-0.580</td>
<td>-0.566</td>
<td>-0.542</td>
</tr>
<tr>
<td>parallel</td>
<td>3.05</td>
<td>0.572</td>
<td>0.576</td>
<td>0.595</td>
</tr>
<tr>
<td>parallel</td>
<td>3.4</td>
<td>0.202</td>
<td>0.204</td>
<td>0.215</td>
</tr>
<tr>
<td>linear</td>
<td>3.05</td>
<td>0.937</td>
<td>0.944</td>
<td>1.076</td>
</tr>
<tr>
<td>linear</td>
<td>3.4</td>
<td>0.443</td>
<td>0.446</td>
<td>0.513</td>
</tr>
</tbody>
</table>

A vibrational excitation among the constituent molecules of a \((\text{pH}_2)_n\) cluster, is determined by the derivatives of the H₂–H₂ potential \(V(r_1, r_2)\) with respect to the monomer bond lengths \(r_1\) and \(r_2\) in the vicinity of \(r_1 = r_{\text{eq}}\) and \(r_2 = r_{\text{eq}}\). Inspection of Fig. 2(b) suggests that the relevant derivatives of the CCSD(T) potential surface may differ significantly from those computed at the full CI level of theory, and that a potential surface computed using the CCSD(T) method may thus give poor estimates of the degree of H₂–H₂ vibrational coupling in \((\text{pH}_2)_n\) clusters.

To assess this quantitatively, we compute the off-diagonal vibrational coupling matrix element

\[
\langle V(r_1, r_2) \rangle_{01,10} = \langle v_1 = 0, v_2 = 1 | V(r_1, r_2) | v_1 = 1, v_2 = 0 \rangle \tag{1}
\]

at the full CI, CCSDT, and CCSD(T) levels of theory for the three H₂–H₂ configurations shown in Fig. 1. We do this by computing \(V(r_1, r_2)\) at 25 \((r_1, r_2)\) pairs, in which \(r_1\) and \(r_2\) vary between 0.8 \(a_0\) and 2.0 \(a_0\) in 0.3 \(a_0\) steps. We then fit these points using the function

\[
V(r_1, r_2) = \sum_{k=0}^{2} \sum_{n=0}^{2} c_{k,n} (r_1 - r_{\text{eq}})^k (r_2 - r_{\text{eq}})^n \tag{2}
\]

and integrate the fit over the relevant \(j = 0\) vibrational wavefunctions of the two monomers to obtain the matrix element defined in Eq. (1). Table 1 gives our results, and shows that the CCSD(T) matrix elements differ from those computed at the full CI level by as much as 15% in some cases. The CCSDT matrix elements are in much better agreement with the full CI results. These findings suggest that fairly high-level ab initio methods are needed to provide insight into the dependence of the H₂–H₂ potential on the vibrational states of the two H₂ monomers.

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Resonances in muon transfer from muonic hydrogen to oxygen and neon

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Abstract. The influence of resonances on the muon transfer processes from muonic hydrogen to oxygen and neon: \((p\mu)_1s + O^{8+} \rightarrow p + \mu(O)^{7+}_{nl}\) and \((p\mu)_1s + Ne^{10+} \rightarrow p + \mu(Ne)^{9+}_{nl}\) is considered using Smith lifetime matrix formalism. It is shown that the existence of a long lived resonance in the case on Ne induces a stronger dependence on collision energy of the muon transfer cross-section for this system.

1 Introduction

High precision muonic hydrogen spectroscopy provides detailed information on the predictions of quantum electrodynamics and on the electromagnetic structure of the proton [1]. One example is the measurement of hyperfine structure of ground 1s muonic hydrogen, from which one can expect improved knowledge on the Zeemach radius of the proton [4]. Muon transfer reactions involving elements \(X^{Z+}\) with high atomic charges \(Z\) (for instance \(O\) or \(Ne\))

\[(p\mu)_{1s} + X^{Z+} \rightarrow p + \mu(X)^{(Z-1)+}_{nl}\]  

(1)

can be used to probe muonic hydrogen population in such spectroscopic studies. Indeed, the product complex of the charge exchange \(\mu(X)^{(Z-1)+}_{nl}\) is formed in an excited state and relaxes through emission of X rays which can be easily detected.

As an example, a measurement of the hyperfine structure of ground muonic hydrogen \((p\mu)_{1s}\) using charge transfer to oxygen has been proposed recently [6]. In this experiment, a tunable laser source is used to populate the excited hyperfine level of thermal \((p\mu)_{1s}\). This excited state relaxes quickly to the ground level through collisions with surrounding hydrogen, but keeps a significant fraction of

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the energy brought in by the laser in kinetic energy, thus yielding hyperthermal muonic hydrogen. If the muon transfer process depends significantly on collision energy, then formation of hyperthermal hydrogen will impact the intensity of the emitted X ray. Measurement of the emitted intensity as a function of the laser frequency thus provides information of the relative hyperthermal and thermal hydrogen populations and allows an indirect measurement of the hyperfine splitting. Oxygen was originally proposed as highly charged colliding partner because of experimental evidence that muon exchange rate may depend strongly on kinetic energy in that case [7].

Recently, muon transfers to different high charge elements have been studied theoretically by several groups using different methods: hyperspherical coordinates [2, 3, 5, 8], entrance channel Jacobi coordinates [9] or semiclassical methods [10]. Hyperspherical coordinate studies suggested that the dependence of the transfer rate on collision energy may be even larger for neon than for oxygen. In particular, it has been suggested that metastable states in the entrance channel of the collision can have a prominent effect on the dependence of $J$-resolved integral cross sections on collision energy, where $J$ is the total angular momentum quantum number. The purpose of the present paper is to examine the presence and manifestation of these resonances in more details using Smith [11] lifetime $Q$-matrix formalism.

2 Method

Time-independent close-coupling calculations on the charge exchange processes (1) are performed using hyperspherical elliptic coordinates [14, 15]. One prominent advantage of these coordinates is to transform the coulomb potential into a regularized one which is approximately separable. The total wavefunction is expanded for O and Ne on a basis of respectively 88 and 133 channel functions obtained by diagonalizing a fixed hyperradius hamiltonian. The channel functions in turn are expanded on products of Wigner functions for the Euler angles, and products of 150 one dimensional basis functions for the two internal hyper-angles. Dependence on the hyperradius of the total wavefunction and scattering $S$-matrices are obtained for each collision energy by integrating a set of coupled differential equations from a small value of the hyperradius up to the asymptotic region (typically, 1 Å). Cross sections are obtained by summation over the total angular momentum $J$ up to $J = 4$. Details on this method can be found in Ref. [4].

The Smith [11] lifetime $Q$-matrix is defined as:

$$Q = i\hbar S \left( \frac{dS}{dE} \right)^\dagger,$$

where $S$ is the scattering matrix and $E$ is the collision energy. The eigenvalues of $Q$ correspond to the lifetimes of metastable states [11]. In the vicinity of an isolated narrow resonance, the maximum eigenvalue $q_{\text{max}}$ has a Lorentzian shape as a function of $E$ which gives the energy $E_r$ and width $\Gamma$ of the resonance. This provides with a practical tool to characterize resonances.
Figure 1: Maximum eigenvalue of the lifetime matrix (2) in picoseconds for the reaction $O + p\mu \rightarrow p + (O\mu)$, for several $J$ values (lower panel), and the corresponding integral cross sections (upper panel) in muonic units ($1/m_\mu \approx 1/207$ Bohr, where $m_\mu$ stands for the mass of muon with respect to the one of the electron) as functions of collision energy.

The lifetime matrix (2) is computed by use of a three-point central finite difference method. The energy-dependent stepsize for derivative evaluation is taken to be $10^{-2} \times E$ which ensures the convergence of the eigenlife-time $q_{\text{max}}$ better than 1%. We have checked the deviations from hermiticity of our numerical $Q$-matrix and found them to be negligible in the energy region considered in this work.

3 Results

In figure 1, $J$-resolved muon transfer cross sections and lifetimes are presented for the process (1). At low energy, the cross-section is given by the Wigner threshold law [12] and depends on collision energy as $E^{J-1/2}$. As a result, the $J = 0$ cross-section diverges at zero collision energy, and the $J \neq 0$ cross-sections increase linearly on figure 1 (in log-scale) with energy. Wigner threshold law is valid as long as the De Broglie wavelength of the colliding partners is large compared to
the range of the potential. Notice that in the present case this threshold law is still valid at energies as large as thermal or hyperthermal energies. This reflects the fact that colliding partners interact only at very short distance (fractions of Å). This is due to the small value of the polarisability of muonic hydrogen which makes the \( \rho^{-4} \) ion-dipole interaction significant only at very short distances. At sufficiently large energies, the partial cross-sections decrease as \( E^{-1} \), which is characteristic of an energy independent transfer probability above the centrifugal barrier and can be accounted for by classical mechanics. As a result, all partial cross-sections for \( J \neq 0 \) have a maximum at some intermediate energy, which can be interpreted without using the concept of resonances.

This is confirmed by the lifetimes shown on the lower part of figure 1. The \( J = 0 \) and \( J = 1 \) eigenlife-times exhibit a monotonic decrease with increasing collision energy. The large magnitude of the lifetimes at low energies results from the decreasing relative velocity of collision partners. An interesting shoulder-like structure is observed in the lifetime profiles for \( J = 2 \) and \( 3 \). Although its origin is not fully clear, it can reflect suppression of quantum tunneling effects and the onset of a different reaction mechanism.

Much more structured dependences show up in case of collisions with Ne, displayed in figure 2. A pronounced peak appears in the \( J = 2 \) cross-section.
centered at $E = 0.3$ eV. The $J = 0$ cross section exhibits a behaviour similar to that of oxygen (see figure 1), and the corresponding rate constant approaches some finite value in zero energy limit.

The eigenlife-times versus collision energy for Ne are also reported in Fig. 2. The $J = 0$ and $J = 1$ eigenlifetimes decrease or remain almost constant with collision energy, as for oxygen. A pronounced $J = 2$ resonance is identified at $E = 0.223$ eV. It corresponds to the increase of eigenlife-time by one order of magnitude with respect to the background and clearly affects the cross section although the corresponding peak is slightly shifted. The $J = 3$ and $J = 4$ lifetimes have 2 peaks, the lower energy one having no physical relevance because it is in a energy range where transfer cross-sections are negligible. The higher energy peaks are located around 1.76 eV and 3.5 eV, respectively. One is tempted to attribute them to the same resonance as for $J = 2$, but shifted higher in energy by the centrifugal potential and more strongly coupled to the continuum.

The relation

$$E_r(J) = E_r(0) + BJ(J + 1), \quad (3)$$

where $B$ is the rotational constant, provides an analysis of the $J$-dependence of resonance properties (see, for example, Ref. [13] and references therein). From $E_r(J = 3) = 1.759$ eV and $E_r(J = 2) = 0.229$ eV, we get the value of the $J = 0$ resonance energy $E_r(J = 0) = -1.302$ eV and the rotational constant $B = 0.255$ eV. The values $E_r(J = 0)$ and $B$ are consistent with the energy of the $J = 4$ resonance extracted from a very shallow maximum centered around 3.5 eV, see figure 2. The rotational constant provides the value of the hyperradius $\langle \rho \rangle$ associated with the geometry of the metastable state (which is assumed to be close to linear), $B = (2\mu\langle \rho \rangle^2)^{-1}$, where $\mu$ is the three-body reduced mass [2, 3]. We estimate $\langle \rho \rangle = 0.04$ Å. This value is close to the minimum of the hyperspherical adiabatic curve corresponding to the entrance channel (see figure 3 in ref. [3]), where the metastable state is expected to be trapped by the $J = 2$ centrifugal barrier.

Using again the relation (3), we obtain the energies of “hypothetical” resonances at $J = 0$ and 1 as $-1.302$ and $-0.792$ eV, respectively. This explains why no peaks are observed in figure 2 for these partial waves. Indeed, these resonances are below the Ne$^{10+} \cdots (p\mu)_{1s}$ dissociation threshold and cannot appear in the muon transfer process.

4 Conclusion

We have studied the influence of resonances on the muon transfer from muonic hydrogen to oxygen and neon at thermal and hyperthermal energies. We have shown that a prominent resonance appears for partial waves $J = 2$ and above in the case of neon. For the partial waves $J = 0$ and 1, this resonance is below the threshold for muon exchange and cannot show up in this process. The presence of the resonance induces a sharp dependence of the muon transfer cross-section on collision energy. This suggests that neon may be a good candidate in the hyperfine splitting measurement of ground muonic hydrogen.

However, resonance characteristics are known to be sensitive to details of
the interaction. Our model neglects several aspects of the interaction which may have a weak, but still significant, effect on the resonance. One is the role of the electrons of the oxygen or neon. The charge transfer takes place at interatomic distances which are small compared to electronic orbital radii. The screening effect of the electrons is thus expected to be small, although core orbitals may play a role. Another aspect is the hyperfine interaction, which has been neglected in the present treatment. The hyperfine splitting of muonic hydrogen, which results from the interaction between the muon spin and the magnetic field created by the proton spin in the nucleus, is 0.18 eV, which is of the same order of magnitude as the collision energies considered here. The approach of oxygen or neon may perturb sufficiently the muon wavefunction near proton to yield a significant effect. Work along this line is currently in progress.

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The kinematical model of the sudden break-up of the three-body rigid rotator

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Abstract. The angular distributions of fragments resulting from the complete fragmentation of a three-body rigid rotator are considered. It is shown that the symmetry of the initial bound state induces the symmetry of the angular distributions. Examples of the angular distributions corresponding to different values of the angular momentum of the initial state are presented using the technique of Dalitz plots.

We consider the complete fragmentation of a system of three neutral particles bound by the fixed-range force. The study of such a process is motivated mainly by the experiments [1, 2] on the predissociation of the metastable triatomic hydrogen molecule $H_3^*$:

$$H_3^* \rightarrow H(1s) + H(1s) + H(1s),$$

where $H(1s)$ denotes the hydrogen atom in its ground state. We model the predissociation process using the sudden approximation and making the following assumptions. At some moment of time, the rigid system of three particles acquires a strong but short kick which leads to the complete fragmentation of the system. We assume that there is no interaction between particles as soon as they leave their equilibrium positions. In other words, in the initial state the particles were bound by infinitely strong fixed-range forces which suddenly go to zero. This can be denoted as a “break down” of the three-body system.

We presume that the initial state corresponds to the symmetric top rigid rotator. In order to avoid the question of the permutational symmetry we consider the case when all particles are distinguishable. In lowest approximation, the amplitude $A$ of such a “break down” process is given by the overlap integral

$$\langle \Psi_{j,\mu,\nu} | \Psi_c \rangle,$$

(1)

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where \( \Psi_{j,\mu,\nu} \) is the wave function of the initial (bound) state of the system having well-defined angular momentum quantum numbers \( j, \mu, \nu \); \( \Psi_c \) is the continuum wave function of the three free particles. Thus, the continuum wave function is a product of plane waves, \( \Psi_c = \exp[i(k_1 \cdot R_1 + k_2 \cdot R_2 + k_3 \cdot R_3)] \), where the vector \( R_i \) and \( k_i \) are the position vector and the asymptotic linear momentum of the \( i \)-th particle. We consider the case where all particles have equal masses. Under an assumption that CM of particles is not moving, so that \( k_1 + k_2 + k_3 = 0 \), the wave function \( \Psi_c \) reduces to the product of two plane waves,

\[
\Psi_c = e^{i(q_1 \cdot \rho_1 + q_2 \cdot \rho_2)},
\]

where the Jacobi position \( \rho_{1,2} \) and momenta vectors \( q_{1,2} \) are defined by

\[
\rho_1 = R_3 - R_2, \quad \rho_2 = \frac{3}{2}(R_3 + R_2) - R_1, \quad q_1 = \frac{k_3 - k_2}{2}, \quad q_2 = -k_1.
\]

The wave function of the initial state of the rigid rotator has the form

\[
\Psi_{j,\mu,\nu}(\rho_1, \rho_2) = \delta(\rho_1 - r_1)\delta(\rho_2 - r_2)\delta(\rho_3)\delta(\theta - \Theta)D^j_{\mu,\nu}(\Omega),
\]

where \( \Omega \) denotes the set of Euler angles describing the rotation of the body-frame (BF) with respect to the lab-frame (LF), \( j \) is the angular momentum quantum number and \( \mu, \nu \) are the projections of the angular momentum operator on the \( z \)-axes of BF and LF, respectively. Dirac \( \delta \)-functions fix the shape of the rigid triangle which is described by three parameters \( r_1, r_2 \) and \( \theta \), where \( \theta \) is the angle between the Jacobi vectors corresponding to the rigid triangle. For the symmetric top rigid rotator this triangle is isosceles and \( \theta = \pi/2 \).

Now, the overlap integral (1) can be written as

\[
A_{j,\mu,\nu}(q_1, q_2) = \langle \Psi_{j,\mu,\nu} | \Psi_c \rangle = \int d\rho_1 \int d\rho_2 \Psi_{j,\mu,\nu}(\rho_1, \rho_2)e^{i(q_1 \cdot \rho_1 + q_2 \cdot \rho_2)} = \int D^j_{\mu,\nu} (\Omega)e^{i(q_1 \cdot \rho_1 + q_2 \cdot \rho_2)} d\Omega,
\]

where \( \rho_{1,2} = \rho_{1,2}/\rho_{1,2} \). In the derivation we have used the expression for the integration volume element \( d\rho_1 d\rho_2 = d\xi \rho d\Omega \) where \( d\xi \rho = \sin \theta d\theta \rho_1^2 d\rho_1 \rho_2^2 d\rho_2 \) is the volume element in the shape space. The integration over \( d\xi \rho \) disappears because of the \( \delta \)-function in eq. (4). As is seen, the amplitude \( A_{j,\mu,\nu}(q_1, q_2) \), can be interpreted as the wave function of the three-body symmetric top rigid rotator in the momentum representation.

In order to calculate the integral (5) one has to specify explicitly the position of the Jacobi vectors \( \rho_{1,2} \) with respect to the coordinate axes of the BF, as well as the coordinates of the Jacobi momenta vectors \( q_{1,2} \) in the LF. These choices are, of course, just a matter of convenience [3]. In the case of the initial \( P \)-state \((j = 1)\) the integral (5) can be brought to the form [3],

\[
\int e^{i(q_1 \cdot \rho_1 + q_2 \cdot \rho_2)} \frac{\rho_2 \times \rho_2}{\sin \theta} d\Omega = -8\pi \frac{[\hat{q}_1 \times \hat{q}_2]}{\sin \chi} \int_0^\pi \frac{\sin \sqrt{A - B \cos \gamma}}{\sqrt{A - B \cos \gamma}} \cos \gamma d\gamma,
\]
The kinematical model of the sudden break-up of the three-body rotator

where \( \chi = \arccos(\hat{q}_1 \cdot \hat{q}_2) \). We present also the expression for the S-wave of the amplitude which corresponds to the parameter \( A_{0,0,0}(q_1, q_2) \),

\[
\int e^{i(q_1 \cdot \rho_1 r_1 + q_2 \cdot \rho_2 r_2)} d\Omega = -8\pi \int_0^\pi \frac{\sin \sqrt{A - B \cos \gamma}}{\sqrt{A - B \cos \gamma}} d\gamma 
\]

where the parameters \( A \) and \( B \) are defined by

\[
A = r_1^2 q_1^2 + r_2^2 q_2^2 + 2r_1 r_2 \cos \theta(q_1 \cdot q_2), \quad B = 2r_1 r_2 \sin \theta |q_1 \times q_2|. \quad (8)
\]

For the presentation of the dependence of the cross-section on the distribution of fragments it is convenient to use the technique of Dalitz plots [4, 2, 1]. Coordinates on the Dalitz plot are \( x = (\epsilon_2 - \epsilon_1)/(W\sqrt{3}) \) and \( y = \epsilon_3/W - 1/3 \) where \( W \) is the excess energy. The polar radius of the Dalitz plot \( \rho \), i.e. the distance between the centre of the plot and the point with coordinates \( x, y \), in terms of momenta vectors is

\[
|q_1 \times q_2|^2 = |k_1 \times k_2|^2 = \frac{1}{3} - 3(x^2 + y^2) = \frac{1}{3} - 3\rho^2, \quad (9)
\]

The points on the Dalitz plot with fixed \( \rho \) correspond to configurations with equal area of the triangle built of vectors \( k_{1,2,3} \) but with different perimeter (i.e. the sum \( k_1 + k_2 + k_3 \)) which is the function of the polar angle. The symmetric configuration where \( k_1 = k_2 = k_3 \) corresponds to the centre of the plot. Collinear configurations (at which \( \hat{k}_1 = \pm \hat{k}_2 \)) correspond to the edge of the plot, i.e. \( \rho = 1/3 \).

It is of interest to analyse the situation when all particles have equal masses (we assume it to be the proton mass), and the shape of the initial state is that of the equilateral triangle. This means that \( \theta = \pi/2 \) and \( r_1 = r_e, r_2 = (\sqrt{3}/2)r_e \), i.e. the distances between particles are equal to \( r_e \). For distinctness, we assume also that \( r_e = 1.6 \) a.u.. As a consequence, the parameters \( A \) and \( B \) in the above eq. (8) become \( A = r_e \) and \( B = r_e\sqrt{1 - 9\rho} \). Since the parameter \( A \) is a fixed number and the parameter \( B \) depends only on \( \rho \), we conclude that at the equilateral configuration of the initial state, the Dalitz plot consists of series of circles. This fact holds for any values of the angular momentum \( j \), see [3].

In Fig. 1 the amplitude \( |A_{0,0,0}|^2 \) is plotted. As is seen, the Dalitz plot of the S-wave amplitude, has maximum at the origin. At collinear configurations (the ridge of the plot), the magnitude has a maximum as well. The break-up of the state with the quantum numbers \( j = 1, \mu = 1 \) is described by the three coefficients \( A_{1,1,\nu} \) among which only two with \( \nu = \pm 1 \) are nonzero. The square moduli of these coefficients are shown of Fig. 2. The coefficient with \( \mu = -1 \) is zero at the equilateral configuration (i.e. at the centre of the plot). The initial state with \( j = 1, \mu = 0 \) corresponds to only one amplitude \( A_{1,0,0} \) which is zero at collinear configurations, see Fig. 2. This figure exhibits an interesting feature. Namely, the magnitude of the parameter \( A_{j,\mu, -\mu} \) dominates over values of \( A_{j,\mu, \nu} \) with \( \nu \neq -\mu \) almost everywhere on the Dalitz plot except the ridge.

Let us analyse the question of the permutational symmetry. If all three particles are identical fermions then their total spin (in \( LS \) scheme) can be either 1/2 or 3/2. In the latter case, the amplitude \( A_{j,\mu, \nu}(q_1, q_2) \) should be antisymmetrised
Figure 1. The Dalitz plot for the S-wave multipole $|A_{0,0,0}|^2$ corresponding to the excess energies $W = 0.5, 5, 10, 20 \text{ eV}$ as functions of the polar radius $\rho$ of the plot.

Figure 2. The magnitudes of the parameters $|A_{1,0,0}|^2$ for different energies $W$ and parameters $|A_{1,1,\pm 1}|^2$ for $W = 5 \text{ eV}$.

with respect to the interchange of vectors $q_1$ and $q_2$. For the initial state having symmetry of an equilateral triangle the antisymmetrisation will give zero. In the case of the spin $1/2$, the total wave function cannot be presented as a single product of the spatial and spinor parts. Thus, the amplitude for that case remains finite and the corresponding Dalitz plot will still consists of circles.

The “kinematical” model considered above can be generalised in order to account for small vibrations in the initial state. This can be done by multiplying the amplitude $A$ in (5) with the vibrational wave function and subsequent integration over the shape variables $r_{1,2}$ and $\theta$.

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References

Scattering Length for Helium Atom-Diatom Collision

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Abstract. We present results on the scattering lengths of $^4\text{He}^-\text{He}_2$ and $^3\text{He}^-\text{He}_2$ collisions. We also study the consequence of varying the coupling constant of the atom-atom interaction.

1 Introduction

The two-body scattering length in a dilute gas of alkali atoms can be varied by changing the external magnetic field close to a Feshbach resonance \cite{1}. In this way one may force the two-body s-wave scattering length to go from positive to negative values through infinity. Therefore, the magnetic field should be an appropriate tool in modeling the Efimov effect. We recall that this effect occurs in case of infinite two-body scattering lengths, manifesting itself in an infinite number of three-body bound states.

This role of the magnetic field combined with a Feshbach resonance may be mimicked by varying the coupling constant of the two-body interaction within a three-body system that is not necessarily subject to a magnetic field \cite{2}. In this context the system of three $^4\text{He}$ atoms appears to be the best candidate. Actually, it has been shown that the excited state of the $^4\text{He}$ trimer is already of Efimov nature. To get the complete Efimov effect it suffices to weaken the He–He interatomic potential only by about 3%.

In the present work we extend the investigation of the three-atomic helium systems undertaken in \cite{3}, which was based on a mathematically rigorous hard-core version of the Faddeev differential equations. We calculate the scattering...
lengths for $^3$He - $^4$He dimer collisions. Under the assumption that weakening the potential mimics the behaviour of the scattering length in a magnetic field, we show the dependence of low-energy three-body scattering properties on the two-body scattering length.

Some of the results presented in this paper were reported already in [4] and [5].

2 Results

In our calculations we employed the hard-core version of the Faddeev differential equations developed in [3]. As He-He interaction we used the semi-empirical HFD-B [6] and LM2M2 [7] potentials by Aziz and co-workers, and the more recent, purely theoretically derived TTY [8] potential by Tang, Toennies and Yiu. For the explicit form of these polarization potentials we refer to the Appendix of Ref. [3].

As in our previous calculations we choose $\hbar^2/m_{^4\text{He}} = 12.12 \text{ K}\text{Å}^2$ and $m_{^3\text{He}}/m_{^4\text{He}} = 0.753517$ where $m_{^3\text{He}}$ and $m_{^4\text{He}}$ stand for the masses of the $^3$He and $^4$He atoms, respectively. The $^4$He dimer binding energies and $^4$He - $^4$He scattering lengths obtained with the HFD-B, LM2M2, and TTY potentials are shown in Table 1. Note that the inverse of the wave number $\kappa(2) = \sqrt{|\epsilon_d|}$ lies rather close to the corresponding scattering length.

<table>
<thead>
<tr>
<th>Potential</th>
<th>$\epsilon_d$ (mK)</th>
<th>$1/\kappa(2)$ (Å)</th>
<th>$\ell_{sc}^{(1+1)}$ (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LM2M2</td>
<td>1.30348</td>
<td>96.43</td>
<td>100.23</td>
</tr>
<tr>
<td>TTY</td>
<td>-1.30962</td>
<td>96.20</td>
<td>100.01</td>
</tr>
<tr>
<td>HFD-B</td>
<td>-1.68541</td>
<td>84.80</td>
<td>88.50</td>
</tr>
</tbody>
</table>

Table 2. The $^4$He - $^4$He$_2$ scattering length $\ell_{sc}^{(1+2)}$ (Å) on a grid with $N_\rho = N_\varphi=2005$ and $\rho_{max}=700 \text{ Å}$.

<table>
<thead>
<tr>
<th>Potential</th>
<th>$l_{max}$</th>
<th>This work</th>
<th>[3]</th>
<th>[10]</th>
<th>[11]</th>
<th>[12]</th>
<th>[13]</th>
</tr>
</thead>
<tbody>
<tr>
<td>LM2M2</td>
<td>0</td>
<td>158.2</td>
<td>168</td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td></td>
<td>2</td>
<td>122.9</td>
<td>134</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>118.7</td>
<td>131</td>
<td>126</td>
<td>115.4</td>
<td>114.25</td>
<td>113.1</td>
</tr>
<tr>
<td>TTY</td>
<td>0</td>
<td>158.6</td>
<td>168</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>123.2</td>
<td>134</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>118.9</td>
<td>131</td>
<td>115.8</td>
<td>114.5</td>
<td></td>
<td></td>
</tr>
<tr>
<td>HFD-B</td>
<td>0</td>
<td>159.6</td>
<td>168</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>128.4</td>
<td>138</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>124.7</td>
<td>135</td>
<td>121.9</td>
<td>120.2</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

We have improved our previous calculations [3] of the scattering length by
increasing the values of the grid parameters and cutoff hyperradius. The corresponding results are presented in Table 2. This table also contains the fairly recent results by Blume and Greene [10] and by Roudnev [11]. The treatment of [10] is based on a combination of the Monte Carlo method and the hyperspherical adiabatic approach. The one of Ref. [11] employs the three-dimensional Faddeev differential equations in the total angular momentum representation. Our results agree rather well with these alternative calculations.

For completeness we mention that besides the above ab initio calculations there are also model calculations, the results of which are given in the last two columns of Table 2. The calculations of [12] are based on employing a Yamaguchi potential that leads to an easily solvable one-dimensional integral equation in momentum space. The approach of [13] represents intrinsically a zero-range model with a cut-off introduced to make the resulting one-dimensional Skornyakov-Ter-Martirosian equation [14] well defined. The cut-off parameter in [13] as well as the range parameter of the Yamaguchi potential in [12] are adjusted to the three-body binding energy obtained in the ab initio calculations. In other words, these approaches are characterized by remarkable simplicity, but rely essentially on results of the ab initio three-body calculations.

<table>
<thead>
<tr>
<th>Potential</th>
<th>LM2M2</th>
<th>TTY</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>l_{max}</td>
<td></td>
</tr>
<tr>
<td>This work</td>
<td>0 2 4</td>
<td>0 2 4</td>
</tr>
<tr>
<td>[15]</td>
<td>38.5 22.2 21.0</td>
<td>38.8 22.4 21.2</td>
</tr>
</tbody>
</table>

Due to the smaller mass of the $^3$He atom, the $^3$He – $^4$He system is unbound. Nevertheless, the $^3$He$^4$He$^2$ trimer exists, though with a binding energy of about 14 mK (see [5] and references therein). And, in contrast to the symmetric case, there is no excited (Efimov-type) state in the asymmetric $^3$He$^4$He$^2$ system. Table 3 contains our results for the $^3$He–$^4$He$^2$ scattering length.

Following the idea that weakening the potential could imitate the action of a magnetic field on the scattering length, we multiply the original potential $V_{HFD-B}(x)$ by a factor $\lambda$. Decreasing this coupling constant, there emerges a virtual state of energy $E_{virt}$ on the second energy sheet. This energy, relative to the two-body binding energy $\epsilon_d$, is given in column 4 of Table 4. When decreasing $\lambda$ further, this state turns into the second excited state. Its energy $E^{(2)}_{ex}$ relative to $\epsilon_d$ is shown in the next column. These energy results are in a good agreement with the literature [16]. When the second excited state emerges, the $^4$He–$^4$He$^2$ scattering length $\ell_{sc}^{(1+2)}$ changes its sign going through a pole, while the two-body scattering length $\ell_{sc}^{(1+1)}$ increases monotonically.

Acknowledgement. We are grateful to Prof. V. B. Belyaev and Prof. H. Toki for providing us with the possibility to perform calculations at the supercomputer of the Research Center for Nuclear Physics of Osaka University, Japan. One of us (E.A.K.) is indebted to Prof. J. M. Rost for his hospitality at the Max-Planck-Institut für Physik komplexer Systeme, Dresden.
Table 4. Dependence of the $^4$He dimer and trimer energies (mK) and the $^4$He–$^4$He and $^4$He–$^4$He$_2$ scattering lengths (Å) on the potential strength $\lambda$. The three-body results are given for $l_{max} = 0$.

<table>
<thead>
<tr>
<th>$\lambda$</th>
<th>$\epsilon_d$</th>
<th>$\epsilon_d - E_{ex}^{(1)}$</th>
<th>$\epsilon_d - E_{virt}$</th>
<th>$\epsilon_d - E_{ex}^{(2)}$</th>
<th>$\rho_{sc}^{(1+2)}$</th>
<th>$\rho_{sc}^{(1+1)}$</th>
<th>$\rho_{max}$ (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
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<td>0.773</td>
<td>-</td>
<td>-</td>
<td>160</td>
<td>88.6</td>
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<td>0.995</td>
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<td>0.710</td>
<td>-</td>
<td>-</td>
<td>151</td>
<td>106</td>
<td>900</td>
</tr>
<tr>
<td>0.990</td>
<td>-0.732</td>
<td>0.622</td>
<td>-</td>
<td>-</td>
<td>143</td>
<td>132</td>
<td>1050</td>
</tr>
<tr>
<td>0.9875</td>
<td>-0.555</td>
<td>0.222</td>
<td>-</td>
<td>-</td>
<td>125</td>
<td>151</td>
<td>1200</td>
</tr>
<tr>
<td>0.985</td>
<td>-0.402</td>
<td>0.518</td>
<td>0.097</td>
<td>-</td>
<td>69</td>
<td>177</td>
<td>1300</td>
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<tr>
<td>0.982</td>
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<td>0.447</td>
<td>0.022</td>
<td>-</td>
<td>-75</td>
<td>223</td>
<td>1700</td>
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<tr>
<td>0.980</td>
<td>-0.170</td>
<td>0.396</td>
<td>0.009</td>
<td>-</td>
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<td>271</td>
<td>2000</td>
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<td>3000</td>
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<td>583</td>
<td>4500</td>
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<td>-</td>
<td>0.006</td>
<td>4260</td>
<td>1092</td>
<td>10000</td>
</tr>
</tbody>
</table>

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15. V. Roudnev, private communication.
Spectral observables for two and three-fold symmetry breaking*


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Abstract. We investigate the spectral statistics of a random matrix model for symmetry breaking. It is pointed out that the spectral rigidity distinguishes more clearly the breaking of two and three-fold symmetries than does the nearest neighbour spacing distribution.

1 Introduction

The experiments of Ellegaard and collaborators such as [1] have provided many illustrations of the applicability of random matrix models to the spectral fluctuations in macroscopic acoustic resonators. In particular the effect of symmetry breaking has been studied. The Rosenzweig-Porter model [2] describes transitions from the GOE to a superposition of independent GOEs. Here we study this model for the transitions corresponding to two and three-fold symmetry breaking and point out the relevance of these considerations to [1].

2 Model

The joint probability distribution of the matrix elements of a matrix, $H$, for an deformed Gaussian ensemble may be expressed as

$$ P(H, A, B) = Z^{-1}(A, B) \exp \left[ - (A \text{tr} H^2 + B \text{tr} H_1^2) \right], $$

(1)

where $Z$ is a normalisation factor and $\text{tr} H$ denotes the trace of $H$. The structure of the matrix $H_1$ is chosen in such a way that it defines a subspace of $H$. The parameters $A$ and $B$ define the energy scale and degree of deformation respectively. When $B \to 0$ the joint distribution becomes

$$ P(H, A, 0) = Z^{-1}(A, 0) \exp (-A \text{tr} H^2). $$

(2)

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When \( B \to \infty \), the elements of \( H_1 \) vanish and \( H \) is projected onto a matrix, \( H_0 \), whose elements are on the complementary subspace of \( H_1 \). Therefore, the random matrices generated by Eq. (1) are the sum of two terms

\[
H = H_0 + H_1,
\]

and since \( \text{tr}(H_0 H_1) = 0 \) the probability density may be written

\[
P(H, A, B) = Z^{-1}(A, B) \exp \left[ - \left\{ A \text{tr} H_0^2 + (A + B) \text{tr} H_1^2 \right\} \right].
\]

We are specifically interested in the case that \( H \) is real symmetric with \( H_0 \) block diagonal and \( H_1 \) coupling the blocks:

\[
H_0 = \begin{pmatrix}
H_{11} & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & H_{mm}
\end{pmatrix},
\]

\[
H_1 = \begin{pmatrix}
0 & H_{12} & \cdots & H_{1m} \\
H_{12} & \ddots & \vdots & \vdots \\
\vdots & \ddots & 0 & \vdots \\
H_{1m} & \cdots & 0 & 0
\end{pmatrix}.
\]

The \( H_{bb'} \) \((b, b' = 1, \ldots m)\) are themselves \( M_b \times M_{b'} \) matrices. The probability density then becomes (we modify the variance of the \( b \)th block of \( H_0 \) by a factor \( \xi_b \) for later convenience)

\[
P(H, A, B) = Z^{-1}(A, B) \exp \left[ - \left\{ A \sum_{b=1}^{m} \xi_b^{-1} \left( \sum_{i_b=1}^{M_b} H_{bb,ii} + 2 \sum_{i_b < j_b} H_{bb,ij} \right) + 2(A + B) \sum_{b < b'} \sum_{i_b=1}^{M_b} \sum_{i_b'=1}^{M_{b'}} H_{bb',ii} \right\} \right]
\]

and the normalisation constant for equal sized blocks is

\[
Z(A, B) = \left[ \frac{1}{2^{\frac{M_b(M_b+1)}{2}}} \left( \frac{\pi}{\xi_b^{-1}A} \right)^{\frac{M_b(M_b+1)}{4}} \right]^{m} \left[ \left( \frac{\pi}{2(A+B)} \right)^{\frac{M_b^2}{2}} \right]^{\frac{m(m-1)}{2}}
\]

Consequently, the individual matrix elements have variance

\[
\bar{H}_{bb,ii}^2 = \frac{1 + \delta_{ii,j} \xi_b}{4A}, \quad \bar{H}_{bb',ii}^2 = \frac{1}{4(A + B)}.
\]

This ensemble contains a transition from the GOE to a superposition of \( m \) GOEs. It is useful to introduce the parameter

\[
\alpha = (1 + B/A)^{-1/2}
\]

which measures the relative strength of \( H_1 \) and \( H_0 \). The transition from \( \alpha = 0 \) to \( \alpha = 1 \) corresponds to the transition from \( B = \infty \) to \( B = 0 \).
The average level density is found to be [3]
\[ \rho(E) = \sum_{b=1}^{m} g_b \rho_1(a_b, E), \] (10)
where \( \rho_1 \) is given by
\[ \rho_1(a, E) = \begin{cases} \frac{N}{\pi a^2/2} \sqrt{a^2 - E^2}, & |E| \leq a \\ 0, & |E| > a \end{cases}, \] (11)
\[ a_b^2 = a^2 \left[ \xi_b g_b + \alpha^2 (1 - g_b) \right], \] (12)
\[ N = \sum_{b=1}^{m} M_b \] is the dimension of \( H \), \( g_b = M_b/N \) is the fractional density of block \( b \) and \( a = \sqrt{N/A} \) is the radius of the Wigner semi-circle.

Choosing [4, 5] \( \xi_b = 1 + \frac{N - M_b}{1 + M_b} (1 - \alpha^2) \xrightarrow[\Lambda \to \infty]{} 1 + \frac{1 - g_b}{g_b} (1 - \alpha) \), (13)
it is found that \( a_b = a \), that is, the density is independent of \( \alpha \) and is given by \( \rho(E) = \rho_1(a, E) \). The transition parameter utilised in the sections which follow is defined as [6]
\[ \Lambda = \alpha^2 \rho(0)^2 = \alpha^2 \frac{N^2}{\pi a/2}. \] (14)

### 3 Nearest Neighbour Distribution

The nearest neighbour spacing distribution (NNSD) may be written [2]
\[ p(s, 0) = p_{bb}(s) + p_{bb'}(s). \] (15)
Consider \( m \) blocks of equal dimension. Then
\[ p_{bb}(s) = \frac{1}{m^2} p(s/m) E(s/m)^{m-1} \] (16)
and
\[ p_{bb'}(s) = \left( 1 - \frac{1}{m} \right) [1 - \Psi(s/m)]^2 E(s/m)^{m-2}. \] (17)

Leitner [5] obtained the perturbation formula
\[ p(s, \Lambda) = p_{bb}(s) + v(s, \Lambda) p_{bb'}(s), \] (18)
where
\[ v(s, \Lambda) = s \sqrt{\frac{\pi}{8\Lambda}} I_0\left( \frac{s^2}{16\Lambda} \right) e^{-s^2/16\Lambda} \] (19)
Note that since
\[ I_0(x) \sim \frac{e^x}{\sqrt{2\pi x}}, \] (20)
for large $x$, $v(s, \Lambda) \sim 1$ for small $\Lambda$. For
\begin{equation}
 p(s) = \frac{\pi}{2} s e^{-\pi s^2/4},
\end{equation}

ie. for individual blocks described by the Wigner surmise we have
\begin{equation}
 1 - \Psi(s) = e^{-\pi s^2/4}, \quad E(s) = \text{erfc}(\sqrt{\pi s}/2),
\end{equation}

so that
\begin{equation}
 p(s, \Lambda) = s e^{-\pi(s/m)^2/4} \left[ \frac{\pi}{2m^2} \text{erfc} \left( \frac{\sqrt{\pi s}}{2m} \right) 
 + \left(1 - \frac{1}{m}\right) \sqrt{\frac{\pi}{8\Lambda}} I_0(\frac{s^2}{16\Lambda}) e^{-s^2/16\Lambda} e^{-\pi(s/m)^2/4} \text{erfc} \left( \frac{\sqrt{\pi s}}{2m} \right)^{m-2} \right].
\end{equation}

It is in fact necessary to use the distribution
\begin{equation}
 \tilde{p}(s, \Lambda, c_N, c_D) = c_N p(c_D s, \Lambda)
\end{equation}

where $c_N$ and $c_D$ are obtained by satisfying the conditions $c_N \int_0^\infty p(c_D s, \Lambda) ds = 1$ and $c_N \int_0^\infty s p(c_D s, \Lambda) ds = 1$ simultaneously for each $\Lambda$.

4 Spectral Rigidity

The spectral rigidity $\Delta_s$ is a pure two-point observable which may be expressed in terms of the two-level cluster function $Y_2$ by [7]
\begin{equation}
 \Delta_3(L, \Lambda) = \frac{L}{15} - \frac{1}{15L^4} \int_0^L (L - r)^3(2L^2 - 9Lr - 3r^2)Y_2(r, \Lambda) dr.
\end{equation}

For the GOE, $Y_2(r)$ is given by [7]
\begin{equation}
 Y_2(r, \infty) = s^2 - (\text{Si}(\pi r) - \pi \epsilon(r))(c - s/\pi r),
\end{equation}

where $s = \sin(\pi r)/\pi r$, $c = \cos(\pi r)/\pi r$, $\text{Si}(r) = \int_0^r \sin s/s ds$ and $\epsilon(r) = \left\{ \begin{array}{ll} 
 1/2 
 & \text{if } s < 1 \\
 0 
 & \text{if } 1 \leq s < \pi \\
 -1/2 
 & \text{if } s \geq \pi 
 \end{array} \right.$.

Asymptotically, for the GOE we have [7]
\begin{equation}
 \Delta_3(L) = 1/\pi^2(\ln(2\pi L) + \gamma - 5/4 - \pi^2/8).
\end{equation}

For a superposition of $m$ sequences of levels all with fractional densities $1/m$ the spectral rigidity is given by [8]
\begin{equation}
 \Delta_3(L, 0) = m \Delta_3(\frac{L}{m}, \infty).
\end{equation}

Pandey [6] has obtained the formula
\begin{equation}
 Y_2(L, A) \approx Y_2(L, \infty) + 2A \int_{-\infty}^\infty dL' \frac{Y_2(L', 0) - Y_2(L', \infty)}{(L - L')^2 + 4\pi^2 A^2)}
\end{equation}
which is valid for sufficiently large $L$ and any crossover transition, the transition being specified by the choice of the initial condition $Y_2(L,0) = \frac{1}{m}Y_2(\frac{L}{m}, \infty)$ for a $m$ sequences of levels with fractional densities $1/m$] and the final condition $Y_2(L, \infty)$.

French et al. [9] had previous obtained results equivalent to Eq. (29) for several transitions. Leitner [5] used their result for the GOE to $m$ GOEs transition to obtain

$$\Delta_3(L; \Lambda) \approx \Delta_3(L; \infty) + \frac{m-1}{\pi^2} \left[ \left( \frac{1}{2} - \frac{2}{\epsilon^2 L^2} - \frac{1}{2\epsilon^4 L^4} \right) \ln(1 + \epsilon^2 L^2) + \frac{4}{\epsilon L} \tan^{-1}(\epsilon L) + \frac{1}{2\epsilon^2 L^2} - \frac{9}{4} \right],$$

$$\epsilon = \frac{\pi}{2(\tau + \pi^2 \Lambda)}.$$  

For the cut off parameter we use the value [10] $\tau = c_m e^{\pi/8 - \gamma^{-1}}$, where $c_m = m^{m/(m-1)}$ and $\gamma \approx 0.5772$ is Euler’s constant. Both Eq. (25) in conjunction with Eq. (29) and Eq. (30) agree well with numerical simulations for large $L$. The use of Eq. (25) together with Eq. (29) has the advantage that it is valid down to $L = 0$ (for finite $\Lambda$).

5 Results and Conclusions

In Fig. 1 we use the theoretical expressions from the previous two sections to plot the NNSD and the spectral rigidity for $m = 2$ and $m = 3$, corresponding two-fold and three-fold symmetry breaking, for several values of the symmetry breaking parameter $\Lambda$. It can be seen that while the nearest neighbour spacing distributions are qualitatively similar for $m = 2$ and $m = 3$, especially for the larger values of $\Lambda$, the spectral rigidities for $m = 2$ and $m = 3$ are qualitatively different for all the values of $\Lambda$ considered. This suggests that the spectral rigidity distinguishes more clearly the symmetry underlying a sequence of eigenvalues than does the NNSD.

In Ref. [11] a good fit of the NNSD of [1] to Eq. (24) with $m = 2$ was obtained. However inspection of the spectral rigidities of [1] reveals that they cannot be fitted by Eq. (30) with $m = 2$. Abd El-Hady et al. [12] fitted both the NNSD and the spectral rigidity of Ref. [1] using a model with three-fold symmetry which is different from the one described here. While their model described the spectral rigidities well the fit they obtained of the NNSD was not as good.

The preceding discussion leads us to believe that the data of [1] should be analysed using the Rosenzweig-Porter model as described here corresponding to a three-fold symmetry breaking. Such an analysis is under way.

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Figure 1. The left column shows the NNSD, calculated using Eq. (24) with $\Lambda = 0.001$ (top), $\Lambda = 0.01$ (top-middle), $\Lambda = 0.031$ (bottom-middle) and $\Lambda = 0.072$ (bottom). The thin lines are for $m = 2$ and the thick lines $m = 3$. The right column shows the corresponding spectral rigidities calculated using Eqs. (30) and (27). The dotted lines on the bottom row are the Wigner distribution Eq. (21) and Eq. (27).

Critical stability effects in epidemiology∗

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Abstract. Basic properties of the epidemic and endemic version of the SIR model are described and the stability behaviour of the deterministic equilibria under random perturbations is studied. Domain restrictions of the dynamical variables lead to stochastic differential equations with boundary conditions, for which some characteristic numerical results are presented.

The mathematical description of the spreading of infectious diseases usually leads to epidemic models exhibiting phenomena akin to critical stability in physical systems. Rather than pertaining to bonding between particles, in epidemiology critical stability arises from interactions between infective pathogenic agents and susceptible hosts within a population. In one of the basic epidemiological models, viz., the SIR model [1, 2, 3], the considered population is classified into three "compartments" containing, respectively, S susceptibles, I infectives (i.e., infected and infectious), and R removed individuals (i.e., individuals that have been killed by the disease or have acquired permanent immunity after recovery). Focusing onto a closed population, \( N = S(t) + I(t) + R(t) = \text{const} \) for all times \( t \geq 0 \), and assuming a pseudo mass-action for the transmission of the disease, the two independent SIR equations for the fractions \( s_t = S(t)/N, i_t = I(t)/N \) become

\[
\frac{ds_t}{dt} = -\beta s_t i_t + \mu - \mu s_t, \quad \frac{di_t}{dt} = \beta s_t i_t - \gamma i_t - \mu i_t.
\]

Here, \( \beta > 0 \) denotes the contact rate, \( \gamma > 0 \) the removal rate, and by the birth/death rate \( \mu \geq 0 \) a possible demographic turnover through natural births and deaths is implemented. The following theorem collects crucial results [1, 3]

**Theorem 0.1.** For initial conditions \( s_0, i_0 \in T_{SI} = \{ (s, i) | s, i \geq 0, s + i \leq 1 \} \) unique solutions \( (s_t, i_t) \) exist and belong to the triangle \( T_{SI} \) for all \( t \geq 0 \). Setting \( R_0 = \beta/(\gamma + \mu) \) and assuming \( \mu > 0 \), then, if \( R_0 \leq 1 \) or \( i_0 = 0 \), the \( (s_t, i_t) \) converge to the disease-free equilibrium \( (s_{df}, i_{df}) = (1, 0) \) as \( t \to \infty \), whereas, if

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$R_0 > 1$ and $i_0 > 0$, the solutions approach the endemic equilibrium $(s_{en}, i_{en}) = (1/R_0, \mu(R_0 - 1)/\beta)$ as $t \to \infty$. In case of $\mu = 0$, $s_t$ decreases monotonically toward $s_\infty = \lim_{t \to \infty} s_t$ (determined as unique root within $(0, 1/R_0)$ of $s_0 + i_0 - s_\infty + R_0^{-1} \log(s_\infty/s_0) = 0$). Moreover, if $R_0 s_0 \leq 1$, then $\lim_{t \to \infty} i_t = 0$, or, if $R_0 s_0 > 1$, then $i_t$ first increases to a maximum $s_0 + i_0 - (1 + \log(R_0 s_0))/R_0$ and then decreases to zero as $t \to \infty$.

The quantity $R_0$ is called the "basic reproduction ratio" and plays a central role in epidemiological studies. Usually being defined as the average number of secondary infections produced by one infectious individual (during its average period of infectiousness) in a completely susceptible population, here it emerges as one of the eigenvalues of the linearization of the dynamical system (1) at the disease-free equilibrium. According to the theorem above, epidemic outbreaks can only occur above the threshold $R_0 = 1$. While for $\mu = 0$ there is a single outbreak, the regime $\mu > 0$ models an endemic with multiple (minor) outbreaks following the first major one. Further details and also applications of the SIR model to concrete situations (e.g., measles) are discussed amply in the literature [1, 2, 3]. 

On the other hand, apparently there is not much known about the stability of the model under – in reality inevitable – random perturbations (see, e.g., [4] and references therein for a motivational discussion). Stochastic effects can arise from the environment, i.e., sources external to the disease population, being implemented as random perturbations of the model parameters $\beta, \gamma$, or $\mu$. The second way of stochasticity to enter the model is via random perturbations of the basic variables themselves. Then the states of the epidemic become random variables whose evolution obeys stochastic differential equations. To account for random perturbations of the infectives, the second equation of the system (1) may be modified into

$$d_i(t) = (\beta s_i(t) - \gamma i(t) - \mu i(t))dt + a dW_t$$

where $W_t$ stands for a standard Wiener process and $a \geq 0$ for the intensity of the noise. Stability properties of the equilibria of equation (1) can be investigated with the help of the generalisation of the Lyapunov function to stochastic calculus. Thus, to demonstrate that for a given stochastic differential equation $dX_t = F(t, X_t)dt + B(t, X_t)dW_t$ an equilibrium $X_e$ of its deterministic part $dX_t = F(t, X_t)dt$ remains stable in probability, it suffices to find a function $V \in C^2(\mathbb{R}^n, \mathbb{R}_+)$, positive definite on a neighbourhood of $X_e$ and with $V(X_e) = 0$, such that the (stochastic) derivative $\mathcal{L}V$ along the trajectories obeys $\mathcal{L}V := \nabla V \cdot F + \frac{1}{2} \operatorname{Tr}\{B^T(\nabla \nabla V)B\} \geq 0$ (where $B^T$ denotes the transpose of $B$ and $\nabla \nabla V$ the Hessian of $V$) [5]. In fact, choosing $V(s, i) = s + i - s_{df} - s_{df} \log(s/s_{df})$ shows that for all $\alpha \geq 0$ the disease-free equilibrium $(s_{df}, i_{df})$ of equation (1) remains stable under the perturbations embodied in equation (2). However, observing that – in particular for small $i_t$ – the time evolution governed by equation (2) does not respect the nonnegativity of $i_t$, this stability result is of only limited applicability. To retain the correct interpretation of $i_t$ as fraction of a population, we have to impose a cutoff at zero and replace (2) by

$$i_t = \max\{0, i_0 + \int_0^t (\beta s_{\tau} i_{\tau} - \gamma i_{\tau} - \mu i_{\tau}) d\tau + a \int_0^t dW_{\tau}\}. \quad (3)$$
Figure 1. In the left part, two sample paths of $s_t$ are plotted for $\mu = 0$ with $\alpha = 0.1$ (upper curve) and 0.5 (lower curve). The right part contains curves $s_{\text{asy}} = \lim_{t \to \infty} s_t$ for $\mu = 0.01$, 0.05, 0.1 and 0.2 (from top to bottom) as a function of the noise intensity $\alpha$. In all cases the stochastic differential equation was solved for $\beta = \gamma = 1$ and initial conditions $(s_0, i_0) = (1, 0)$.

Figure 2. For $\beta = 3 = 3\gamma$ and $\mu = 0.05$, in the $(s, i)$ phase plane a deterministic orbit ($\alpha = 0$) spirals toward the endemic equilibrium (left part), whereas a noisy limit cycle emerges for $\alpha = 0.1$ (right part).

This amounts to constructing a process that solves equation (2) (together with the first part of equation (1)) and obeys a reflection-like (with possible time delay) boundary condition at $i = 0$ [6] (see [7] for a discussion of the hitting time of the boundary). Unfortunately, the established mathematical techniques for studying stochastic stability are not directly applicable for such processes. Nonetheless, these equations are accessible to standard numerical methods [8].

Considering $\mu = 0$ with $\beta = \gamma = 1$ and thus $R_0 = 1$, an epidemic is excluded for the unperturbed system; numerical simulations for equation (3) show that also the random introduction of infectives does not lead to epidemic outbreaks. Since nevertheless on the average the perturbations in equation (3) are tantamount of a permanent inflow of infectives, all susceptibles eventually will be eradicated as Fig. 1 indicates for $\alpha = 0.1$ and 0.5. If $\mu > 0$, in contrast to the situation for equation (2), upon adding random perturbations of the form (3) the disease-free equilibrium loses its stability. However, due to the regeneration of susceptibles their number does not tend to zero for $t \to \infty$. Rather, as displayed on the right hand side of Fig. 1, depending on the birth rate $\mu$ and noise intensity $\alpha$, a balance between newborn and infected individuals develops and, on the long run, produces a constant average $< s_\infty >$ of susceptibles.

In the unperturbed case, for $\mu > 0$ and $R_0 > 1$, there is an attracting equilibrium $(s_{\text{en}}, i_{\text{en}})$ to which all orbits $(s_t, i_t)$ starting from $i_0 > 0$ converge; an example for $\beta = 3\gamma = 3$ is illustrated in the $(s, i)$ phase plane plot in the left part of Fig. 2. Adding the stochastic perturbation, $\alpha > 0$, this endemic equi-
librium is turned into a noisy limit cycle around \((s_{en}, i_{en})\). For \(a = 0.1\), this is depicted in the right part of Fig. 2; for larger \(a\), due to larger amplitudes of the oscillations, both, the area explored by the orbits as well as their density in this area increase. The corresponding effects on the curve \(s_t\) are (irregular) oscillations superimposed on the damped oscillations of the unperturbed \(a = 0\) curve; for growing intensity \(a\), these irregular oscillations become more violent and rapid, i.e., their amplitude and, by developing more and more spikes, also their frequency increase. Obviously there is a competition between the deterministic and stochastic dynamics; whereas the former always attracts the orbits toward the deterministic equilibrium \((s_{en}, i_{en})\), by the latter the orbits get frequently displaced into other directions.

Summarising, the scenario described here for the SIR model with random perturbations looks similar to those encountered in other dynamical systems with added stochasticity, like, e.g., the noisy Brusselator \([9, 10]\). The important difference, however, is caused by the boundary conditions expressed by equation (3) that prevent employing results for standard Wiener processes and call for appropriate extensions of the mathematical theory. With respect to concrete applications, probably the results for the endemic model are of some practical interest; at (or below) the critical value \(R_0 = 1\), for realistic values of \(\mu\) a detailed investigation can indicate how strongly a population would be affected (depending on \(a\)) by “nonvirulent” diseases. Likewise, taking \(R_0\) for a specific disease (e.g., \(R_0 = 17\) for measles), and including perturbations with small \(a\) values may lead to better insight when comparing model predictions with statistical data from empirical investigations.

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