Hyperspherical Treatment of Strongly-Interacting Few-Fermion Systems in One Dimension

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Abstract. We examine a one-dimensional two-component fermionic system in a trap, assuming that all particles have the same mass and interact through a strong repulsive zero-range force. First we show how a simple system of three strongly interacting particles in a harmonic trap can be treated using the hyperspherical formalism. Next we discuss the behavior of the energy for the N-body system.

1 Introduction

Recent advances in the preparation of quasi-one-dimensional few-fermion samples in their ground states \cite{1,2} showed the need for a thorough theoretical description of such systems. This need has driven several groups to provide a numerical analysis of small systems in a harmonic trap \cite{3,4,5}. Unfortunately, a numerical analysis is not reliable for large samples with strong interaction where the effects beyond the mean field need to be included. This specific problem was addressed in Ref. \cite{6} where the recipe to calculate the spectrum close to the infinite repulsion limit (or hard core limit) was given.

In the present paper we continue investigation of strongly interacting one-dimensional systems. First we consider three harmonically trapped spinless fermions of two types using the hyperspherical formalism \cite{7}. This allows us to show that the wave function of three spinless fermions can be used to determine a leading order correction to the energy close to the infinite repulsion limit. This conclusion coincides with the result of Ref. \cite{6}. Next we offer a new detailed explanation of this result for more particles.

2 Three Particles

We first consider three harmonically trapped spinless fermionic particles two of type A (described with coordinates $y_1, y_2$) and one of type B (coordinate $x_1$). The interaction between the particles is assumed to be of zero range, which means that due to the Pauli principle particles of type A do not interact with each other but only with particle B. The Hamiltonian for such a system is written as

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial y_1^2} - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial y_2^2} + g \delta(x_1 - y_1) + g \delta(x_1 - y_2) + m \omega^2 x_1^2 + y_1^2 + y_2^2 \frac{1}{2}, \quad (1)$$

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where the mass, \( m \), is the same for all particles, \( \omega \) is the frequency of the oscillator trapping potential, and \( g \) is the strength of the interparticle repulsion. For this problem we shall use the oscillator units, i.e. all lengths are in units of the oscillator length \( \sqrt{\hbar/m\omega} \) and energies are in units of the trap oscillator energy \( \hbar \omega \). The interaction strength, \( g \), becomes dimensionless in units of \( \sqrt{\hbar/m\omega} \).

The angular functions, eigenstate \( \Phi \), where
\[
\langle \Phi | \end{equation}
\[
\text{has the solutions}
\]
\[
\frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial \rho^2} + \frac{1}{2}\left[\frac{\partial^2}{\partial \phi^2} + \frac{1}{2}\right] + \frac{g}{\sqrt{2\rho}} \left(\delta(\sqrt{3\rho} + x) + \delta(\sqrt{3\rho} - x)\right) + \frac{x^2 + y^2 + z^2}{2} = 0.
\]
(2)

First we note that the 'center-of-mass' part (\( z \)) is separable, so we focus exclusively on the \( x, y \) part. Since the wave function must be antisymmetric under the \( y \rightarrow -y \) transformation (Particles are identical fermions) and parity is conserved it is enough to consider only the \( x > 0, y > 0 \) region.

To solve the problem we adopt the hyperspherical formalism [7,8] that has been proven to be useful for three-body problems in one dimension [5,9,10,11]. In hyperspherical coordinates \( (x = r \cos(\phi), y = r \sin(\phi)) \) the Hamiltonian reads
\[
H = -\frac{1}{2} \frac{\partial^2}{\partial \phi^2} + \frac{z^2}{2} - \frac{1}{2} \frac{\partial}{\partial r} \frac{\partial}{\partial r} - \frac{1}{2} \frac{\partial^2}{\partial \phi^2} + \frac{g}{\sqrt{2\rho}} \delta(\phi - \pi/6) + \frac{g}{\sqrt{2\rho}} \delta(\phi + \pi/6) + \frac{r^2}{2}.
\]
(3)

To find the eigenstates of this Hamiltonian we write the wave function in the following form
\[
\Psi_k = \frac{\sqrt{2}}{r} \sum_{i=1}^\infty f_i(r) \Phi_i(\phi, r),
\]
where \( \phi_k(z) \) is the \( k \)th solution to the harmonic oscillator potential. The angular functions, \( \Phi_i(\phi, r) \), are chosen as the normalized solutions of the Schrödinger equation (0 < \( \phi \) < \( \pi/2 \), 0 < \( r \) < \( \infty \)) at fixed \( r \)
\[
\left(-\frac{1}{2} \frac{\partial^2}{\partial \phi^2} + \frac{g}{\sqrt{2\rho}} \delta(\phi - \pi/6)\right) \Phi_i(\phi, r) = E_i(r) \Phi_i(\phi, r),
\]
(4)

and the radial functions, \( f_i(r) \), solve the infinite system of coupled ordinary differential equations (\( E \) is now measured from the \( k \)th energy of the harmonic oscillator):
\[
\left(-\frac{1}{2} \frac{\partial^2}{\partial r^2} + \frac{E_i(r)}{r^2} + \frac{g}{\sqrt{2\rho}} \delta(\phi - \pi/6)\right) f_i(r) = \sum_j \left(Q_{ij} + P_{ij} \frac{\partial}{\partial \rho}\right) f_j(r),
\]
(5)

where \( Q_{ij} = \frac{1}{2} \langle \Phi_i | \frac{\partial^2}{\partial \rho^2} | \Phi_j \rangle \) and \( P_{ij} = \langle \Phi_i | \frac{\partial}{\partial \rho} | \Phi_j \rangle \). It is worth noting that the system trapped in the harmonic oscillator and the corresponding free system have the same set of \( \Phi_i \) and correspondingly the same couplings \( P_{ij}, Q_{ij} \). The angular equation (4) has the solutions
\[
\Phi_i = N_i(r) \begin{cases}
-\sin(\mu_i (\phi - \pi/2)); & \pi/6 < \phi < \pi/2 \\
\sin(\mu_i \pi/3) \cos(\mu_i \phi); & \text{odd parity} \quad 0 < \phi < \pi/6 \\
\sin(\mu_i \pi/3) \sin(\mu_i \phi); & \text{even parity} \quad 0 < \phi < \pi/6
\end{cases}
\]
where the normalization factor \( N_i(r) = \sqrt{4\mu_i \pi + 2\mu_i \pi \cos(\mu_i \pi/3) - 3\sin(2\mu_i \pi/3)} \); the upper sign corresponds to odd parity and the lower sign to even parity solutions. Also we defined \( \mu_i = \sqrt{2E_i} \), where \( E_i \) is chosen to reproduce the discontinuity of the derivative of the wave function which arises due to the delta function potential at \( \phi = \pi/6 \). This condition is satisfied if \( E_i \) solves the following equations for odd parity eigenstate
\[
\mu_i \cos(\mu_i \pi/2) + g \sqrt{2} \cos(\mu_i \pi/6) \sin(\mu_i \pi/3) = 0,
\]
(6)
and for even parity eigenstates

\[ \mu_1 \sin(\mu_1 \pi/2) + gr \sqrt{2} \sin(\mu_1 \pi/6) \sin(\mu_1 \pi/3) = 0. \]  

(7)

From now on we focus on the ground state solution with strong interaction, i.e. \(1/g \ll 1\); however the presented procedure is completely general and can be easily applied for excited states. The ground state has odd parity and the angular wave function for strong repulsion allows us to write a \(1/g\) expansion, \(\Phi_i(\phi, R) = a_i(\phi) + \frac{1}{g} b_i(\phi) + O(1/g^2)\), which yields \(Q_{11} \simeq 1/g^2\). Since the solutions with and without \(Q_{11}\) give an upper and lower bounds on the exact energy [12] we can use the lowest adiabatic potential alone to describe the energy up to the order \(1/g\). The lowest adiabatic potential is determined by \(\mu_1\):

\[ \mu_1(r) = \begin{cases} 3 - \frac{27}{\sqrt{2} \pi g r} & , r \gg 1/g \\ 1 + O(gr) & , r \ll 1/g \end{cases} \]

Contribution from small distances is highly suppressed due to the fermionic nature of the \(A\) particles and will not be considered below. The corresponding equation for the energy takes the form

\[ \left( -\frac{1}{2} \frac{\partial^2}{\partial r^2} + \frac{35}{8r^2} + \frac{r^2}{2} + V(r) - E \right) f(r) = 0, \]  

(8)

where \(V(r) = -\frac{81}{\sqrt{2} \pi g r^2}\) (at small distances the potential becomes regular, but this region can be neglected to linear order in \(1/g\)). We write down the solution to eq. (8) that is regular at zero using the Green’s function

\[ f(r) = R(E, r) + \int_0^r dr' g_E(r, r') V(r') f(r'), \]  

(9)

where

\[ g_E(r, r') = -\frac{\Gamma(3 - E/2) \Gamma(-2 + E/2)}{\Gamma(2 + E/2)} [R(E, r) I(E, r') - I(E, r) R(E, r')], \]  

(10)

\[ R(E, r) = e^{-r^2/2} r^2 L_{2E+2}^3/2(r^2), \quad I(E, r) = e^{-r^2/2} r^7/2 U(2 - E/2, 4, r^2), \]  

(11)

where \(\Gamma(x)\) is the Gamma function, \(U\) is the Tricomi confluent hypergeometric function, and \(L\) is the associated Laguerre polynomial. The energy, \(E\), is then determined from the condition of vanishing wave function at infinity

\[ 1 - \frac{\Gamma(3 - E/2) \Gamma(-2 + E/2)}{\Gamma(2 + E/2)} \int_0^\infty dr' I(E, r) V(r') = 0, \]  

(12)

which to linear order in \(1/g\) gives

\[ E = 4 - \frac{27}{\sqrt{2} \pi g} \int_0^\infty \frac{R^2(4, R)}{R^3} \mathrm{d}R = 4 - \frac{81}{8 \sqrt{2} \pi g}. \]  

(13)

First thing to notice is that the linear order in \(1/g\) for the energy arises from the wave function at \(1/g = 0\), which is a general conclusion as we argue in the next section. Eq. (9) allows us to access also the expansion for the solution to eq. (8). However, this expansion does not yield the exact wave function to the linear order in \(1/g\), since the non-diagonal couplings, \(P_{ij}, Q_{ij}\), are proportional to \(1/g\) and should be properly taken into account. However, these couplings can be easily written analytically which allows one to determine the corresponding contribution numerically from the set of coupled equations (5).
3 N Particles

Here we consider \( N = N_A + N_B \) spinless fermions of two types, \( N_A \) particles of type \( A \) and \( N_B \) of type \( B \), described with the sets of coordinates \( \{ y_i \} \) and \( \{ x_i \} \), respectively. Again we assume repulsive zero-range interparticle interaction and external confinement, \( V(x) \), such that the system is described by the Hamiltonian

\[
H = \sum_{i=1}^{N_B} h(x_i) + \sum_{i=1}^{N_A} h(y_i) + g \sum_{j,i \neq i} \delta(x_i - y_j), \quad \text{with} \quad h(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x). \tag{14}
\]

The Hamiltonian (14) contains delta functions, which corresponds to the Schrödinger equation

\[
\left[ \sum_{i=1}^{N_B} h(x_i) + \sum_{i=1}^{N_A} h(y_i) \right] \Psi = E \Psi, \tag{15}
\]

with the following boundary conditions when the particles meet, i.e. at \( x_i = y_j \),

\[
\left( \frac{\partial \Psi}{\partial x_i} - \frac{\partial \Psi}{\partial y_j} \right)_{x_i - y_j = 0^+} - \left( \frac{\partial \Psi}{\partial x_i} - \frac{\partial \Psi}{\partial y_j} \right)_{x_i - y_j = 0^-} = \frac{2gm}{\hbar^2} \delta(x_i = y_j). \tag{16}
\]

We focus on the strongly interacting regime where \( 1/g \ll 1 \). We write the wave function as \( \Psi = \Psi_0 + \delta \Psi \) with the energy \( E = E_0 + \delta E \) where the normalized wave function \( \Psi_0 \) is the eigenstate at \( 1/g = 0 \) of energy \( E_0 \). Note that to satisfy the boundary condition the wave function \( \Psi_0 \) should vanish whenever two particles meet, i.e. \( \Psi_0(x_i = y_j) = 0 \). We can assume that \( \langle \Psi_0 | \delta \Psi \rangle = 0 \), where \( \delta \Psi \) solves the equation

\[
\left[ \sum_{i=1}^{N_B} h(x_i) + \sum_{i=1}^{N_A} h(y_i) - \delta E - E_0 \right] \delta \Psi = \delta E \Psi_0, \tag{17}
\]

supplemented with the boundary conditions

\[
\left( \frac{\partial \Psi}{\partial x_i} - \frac{\partial \Psi}{\partial y_j} \right)_{x_i - y_j = 0^+} - \left( \frac{\partial \Psi}{\partial x_i} - \frac{\partial \Psi}{\partial y_j} \right)_{x_i - y_j = 0^-} = \frac{2gm}{\hbar^2} \delta(x_i = y_j). \tag{18}
\]

Now multiplying eq. (17) from the left with \( \Psi_0 \) and integrating over the full space except the points with \( x_i = y_j \) we get

\[
\delta E = \langle \Psi_0 | \left( \sum_{i=1}^{N_A} h(x_i) + \sum_{i=1}^{N_B} h(y_i) \right) | \delta \Psi \rangle = -\frac{g^2}{2m} \sum_{i=1}^{N_B} \sum_{j=1}^{N_A} \int dx_1 \ldots dx_{N_B} dy_1 \ldots dy_{N_A} \times \left[ \left( \frac{\partial \Psi_0}{\partial x_j} - \frac{\partial \Psi_0}{\partial y_j} \right)_{x_j - y_i = 0^+} - \left( \frac{\partial \Psi_0}{\partial x_j} - \frac{\partial \Psi_0}{\partial y_j} \right)_{x_j - y_i = 0^-} \right] \delta(x_j - y_i), \tag{19}
\]

where the second equality is found by integrating twice by parts. The boundary conditions for \( \delta \Psi \) demand that \( \delta E = -K/g + O(1/g^2) \), where

\[
K = \frac{\hbar^4}{4m^2} \sum_{i=1}^{N_B} \sum_{j=1}^{N_A} \int dx_1 \ldots dx_{N_B} dy_1 \ldots dy_{N_A} \times \left[ \left( \frac{\partial \Psi_0}{\partial x_j} - \frac{\partial \Psi_0}{\partial y_j} \right)_{x_j - y_i = 0^+} - \left( \frac{\partial \Psi_0}{\partial x_j} - \frac{\partial \Psi_0}{\partial y_j} \right)_{x_j - y_i = 0^-} \right]^2 \delta(x_j - y_i). \tag{20}
\]
This result was first derived in Ref. [6] using the Hellmann-Feynman theorem. Here we arrive at eq. (20) directly from the non-interacting Schrödinger equation with the boundary conditions at the points where particles meet. Eq. (20) becomes very useful after we realize that \( \Psi_0 \) vanishes at \( x_i = y_j \) and satisfies the free Schrödinger equation otherwise. We know that the wave function of \( N \) identical spinless fermions \( \Psi_A \), meet these requirements, which means that for each ordering of particles, i.e. \( x_1 < x_2 < \ldots < y_N \), the wave function \( \Psi_0 \) is proportional to \( \Psi_A \). For identical bosons it was pointed out in ref. [13] that the ground state wave function at each point is just an absolute value of \( \Psi_A \). For two-component fermions, to obtain \( \Psi_0 \) which is adiabatically connected to the wave function at large but finite interaction strength, the proportionality coefficients for each ordering should be chosen to extremize \( K \). For instance, for three particles in a harmonic trap it was shown [14] that for the ground state \( \psi_0(x_1 < y_1 < y_2) = \psi_A(x_1, y_1, y_2), \psi_0(y_1 < x_1 < y_2) = -2\psi_A(x_1, y_1, y_2) \), which determines \( \psi_0 \) everywhere, since parity is conserved. Now inserting this \( \psi_0 \) in eq. (20) we obtain the same energy in linear order in \( 1/g \) as in eq. (13).

4 Summary and Outlook

We demonstrate for three harmonically trapped fermions an analytical procedure to determine the eigenenergy of the system close to the hard core limit using the hyperspherical formalism. It turns out that the leading order correction to the energy can be obtained using only the known wave function of three spinless fermions. In the second part of the paper we present a new detailed derivation of the leading order correction to the energy for strongly interacting particles [6]. This correction depends solely on the wave function of spinless fermions, which can be obtained by solving a one-body problem. Let us now discuss possible extensions of this work. Here we have only considered leading order corrections to the three body problem. However since the \( 1/g \) expansions for the non-adiabatic couplings can be obtained using the presented angular wave functions we believe that the higher order corrections can be obtained numerically in a relatively simple manner. The hyperspherical approach discussed here should be of great use not only for the presented three-body case but also for more particles (bosons and/or fermions), especially in a harmonic trap [15]. Other important extensions are the systems with different masses and different interaction strengths which were successfully treated in homogeneous set-ups [9,16].

References

1. F. Serwane et al., Science 332, 336 (2011).
2. G. Zürn et al., Phys.Rev.Lett. 108, 075303 (2012).
3. S. E. Gharashi and D. Blume, Phys.Rev.Lett. 111, 045302 (2013).
4. T. Sowiński et al., Phys. Rev. A 88, 033607 (2013).
5. J. Lindgren et al., New J. Phys. 16, 063003 (2014).
6. A. G. Volosniev et al., arXiv:1306.4610.
7. J. H. Macek, J. Phys. B 1, 831 (1968).
8. E. Nielsen et al., Physics Reports 347, 373 (2001).
9. O. I. Kartavtsev et al., ZhETF 135, 419 (2009).
10. N. T. Zinzer et al., arXiv:1305.7219 (2013).
11. N. L. Harshman, Phys. Rev. A 86, 052122 (2012).
12. H. T. Coelho and J. E. Hornos, Phys. Rev. A 43, 6379 (1991).
13. M. Girardeau, J. Math. Phys. 1, 516 (1960).
14. A. G. Volosniev et al., Few-Body Systems 55, 839 (2014).
15. A. S. Dehkharghani in preparation.
16. N. P. Mehta, Phys. Rev. A 89, 052706 (2014).