Correlation induced collapse of many-body systems with zero-range potentials

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The zero-range potential is customarily employed in various mean-field calculations of many-body systems in atomic and nuclear physics within, correspondingly, Gross-Pitaevskii and Skyrme-Hartree-Fock approach. We argue, however, that a many-body system with zero-range potentials is unstable against clusterization into collapsed three-body subsystems. We show that neither the density dependence of the potential nor an additional repulsive three-body potential can prevent this unexpected correlational collapse if the potentials are of zero range. Therefore the zero-range potential can only be used in many-body calculations where all three-body correlations are explicitly excluded.

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I. INTRODUCTION

A. Many-body systems with zero-range interaction

The zero-range potential is a very useful concept for physical problems with a distinct separation of scales. If, say, the typical wavelength of a particle in a potential well is much larger than the range of the potential the latter can be approximated by a zero-range (pseudo)potential $V_0$ which acts on the particle’s wavefunction $\psi(r)$ as

$$V_0\psi(r) = t_0 \delta(r) \frac{\partial}{\partial r} r \psi(r) ,$$

where the strength of the potential $t_0$ is expressed in terms of the mass $m$ and the $s$-wave scattering length $a$ of the particle as $t_0 = -4\pi\hbar^2a/m$. For a well-behaving $\psi(r)$ the operator $\frac{\partial}{\partial r} r$ can be replaced with unity.

The zero-range potentials are widely used in different fields of physics as a practically convenient form of the effective interaction. In particular it is routinely employed in various Hartree-Fock calculations in atomic, nuclear, and astro-physics. The Hamiltonian of a many-body system is approximated by an operator

$$H = \sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} \sum_{i \neq j} t_0 \delta(\mathbf{r}_i - \mathbf{r}_j) \right) ,$$

where $\mathbf{r}_i$ is the coordinate of the $i$-th particle and $N$ is the total number of particles. If the system is exposed to an external field a corresponding term is added to the Hamiltonian.

The Hartree-Fock approximation to the wavefunction of a system of bosons leads then to the Gross-Pitaevskii energy functional

$$E_B = \int d\mathbf{r} \left( \frac{\hbar^2}{2m} \tau_B(\mathbf{r}) + \frac{1}{2} t_0 n_B^2(\mathbf{r}) \right) ,$$

where $\tau_B(\mathbf{r})$ is the kinetic energy density and $n_B(\mathbf{r})$ is the particle density of the system of bosons. For a system of fermions one obtains instead the Skyrme-Hartree-Fock energy functional which, taking symmetric nuclear matter as an example, can be written in terms of the corresponding fermionic densities $\tau_F$ and $n_F$ as

$$E_F = \int d\mathbf{r} \left( \frac{\hbar^2}{2m} \tau_F(\mathbf{r}) + \frac{3}{8} t_0 n_F^2(\mathbf{r}) \right) .$$

The ground state wavefunction of the Hamiltonian minimizes (within the Hartree-Fock approximation) the corresponding energy functional.

B. Mean-field collapse of a many-body system with attractive zero-range interaction

The kinetic energy $\tau_F$ of symmetric nuclear matter can be expressed in terms of the Fermi momentum, $k_F = (3\pi^2 n_F/2)^{1/3}$, as

$$\tau_F = \frac{2}{3\pi^2} \frac{3}{5} \frac{k_F^5}{2} = \frac{3}{5} \left( \frac{3\pi^2}{2} \right)^{2/3} n_F^{5/3} .$$

Inserting this in Eq.

Inserting this in Eq.\ref{eq:5} shows that for large $n_F$ the potential energy term, proportional to $n_F^2$, prevails over the kinetic energy term, proportional to $n_F^{5/3}$. Therefore in the case of attraction, $t_0 < 0$, the degeneracy pressure of the fermionic gas can not withstand the attraction and the system collapses: the minimum of the energy, $E_0 = -\infty$, is reached at infinitely high density $n_F = \infty$.

Since there is no degeneracy pressure in a system of bosons the collapse in this case is even more severe.

The mean field collapse, however, can be easily removed within the same approach by extending the Hamiltonian with either a repulsive three-body zero-range potential

$$W_3 = \sum_{i>j>k} t_3 \delta(\mathbf{r}_i - \mathbf{r}_j) \delta(\mathbf{r}_i - \mathbf{r}_k) ,$$

$^1$The kinetic energy $\tau_F$ depends on the Fermi momentum as $k_F = (3\pi^2 n_F/2)^{1/3}$.

$^2$The full Skyrme potential includes also momentum-dependent terms which, however, are not important for the collapse discussed here.
or a density dependent zero-range potential
\[ W_3 = \sum_{i<j} t_3 \rho^\alpha (r_i) \delta(r_i - r_j), \]  
(7)

which results in an additional term in the energy functional proportional to \( n^3 \) or \( n^{n+2} \). The energy functionals \( E \) and \( F \) acquire then a well-defined minimum at a finite saturation density \( \bar{\rho} \).

This mean-field collapse can also occur for some finite range interactions, but an appropriate density dependence can in this case also remove the collapse \( \bar{\rho} \).

C. Correlational collapse of a many body system with zero-range potentials

Curiously enough the rigorous solution of a three-body problem with zero-range potentials also exhibits a collapse known as the Thomas effect \( [17] \). However, this is a different type of collapse, where infinitely many bound states appear with exceedingly large binding energies and exceedingly small spatial extension. The many body system with Hamiltonian \( \{ E \} \) is therefore also subjected to this non-mean-field \( \text{correlational collapse} \) – clustering into collapsed three-body subsystems. Rather surprisingly this undesirable feature of the Hamiltonian \( \{ E \} \) seems to have been unnoticed so far.

The additional potential \( W_3 \) removes the \( \text{mean-field} \) collapse of the many-body system. But unless it also removes the \( \text{correlational collapse} \), the Hamiltonian \( \{ E \} \) will still have this unpleasant property of not having a finite ground state energy. The many on-going investigations would then be disturbingly close to a divergence, where even a small admixture of three-body correlations might influence the solution by a substantial and uncontrollable amount.

We shall show in this letter that neither the three-body zero-range potential \( \{ E \} \) nor the density dependent zero-range potential \( \{ F \} \) is actually able to remove the collapse of the many-body system into collapsed three-body clusters.

II. THREE-BODY SYSTEM WITH ZERO-RANGE POTENTIALS

A. Hyper-spheric coordinates

Let us first introduce the hyper-spheric coordinates \( \{ \rho, \Omega \} \) suitable for a description of a three-body system. If \( m_i \) and \( r_i \) refer to the \( i \)-th particle then the hyper-radius \( \rho \) and the hyper-angle \( \alpha_i \) are defined in terms of the Jacobi coordinates \( x_i \) and \( y_i \) as \( [15] \):

\[ x_i = \sqrt{\frac{1}{m m_j + m_k} (r_j - r_k), \]  
(8)
\[ y_i = \sqrt{\frac{1}{m m_i + m_j + m_k} (r_i - \frac{m_j r_j + m_k r_k}{m_j + m_k})}, \]  
(9)

\[ \rho \sin(\alpha_i) = x_i, \rho \cos(\alpha_i) = y_i, \]  
(10)

where \( \{ i,j,k \} \) is a cyclic permutation of \( \{ 1,2,3 \} \) and \( m \) is an arbitrary mass scale. The set of angles \( \Omega_i \) consists of the hyper-angle \( \alpha_i \) and the four angles \( x_i/y_i \) and \( y_i/y_i \). The kinetic energy operator \( T \) is defined as

\[ T = T_\rho + \frac{\hbar^2}{2 m \rho^2} \Lambda^2, \]  
\[ T_\rho = -\frac{\hbar^2}{2 m} \left( \rho^{-5/2} \frac{\partial^2}{\partial \rho^5/2} \rho^{5/2} - \frac{15}{4} \right), \]  
(11)
\[ \Lambda^2 = -\frac{1}{\sin^2(\alpha_i)} \frac{\partial^2}{\partial \alpha_i^2} \sin(2 \alpha_i) - 4 + \frac{l_{x_i}^2}{\sin^2(\alpha_i)} + \frac{l_{y_i}^2}{\cos^2(\alpha_i)}, \]  
(12)

where \( l_{x_i} \) and \( l_{y_i} \) are the angular momentum operators related to \( x_i \) and \( y_i \).

B. Hyper-spheric adiabatic expansion

Let us now consider a three-body system with the Hamiltonian \( \{ E \} \). We start with the general hyper-spheric adiabatic expansion \( \{ \Phi \} \) of the three-body wavefunction \( \Psi \):

\[ \Psi(\rho, \Omega) = \frac{1}{\rho^{1/2}} \sum_n f_n(\rho) \Phi_n(\rho, \Omega), \]  
(13)

in terms of the complete basis \( \Phi_n \) of the solutions of the hyper-angular eigenvalue equation

\[ \left( \Lambda^2 - \lambda_n(\rho) + \frac{2 m \rho^2}{\hbar^2} \sum_{i=1}^3 V_i(\rho, \Omega) \right) \Phi_n(\rho, \Omega) = 0, \]  
(14)

where \( V_i(\rho, \Omega) \) is the potential between particles \( j \) and \( k \) \( (i,j,k) \) is the cyclic permutation of \( 1,2,3 \). If we truncate the infinite sum in \( \{ \Phi \} \) we shall, according to the variational principle, obtain an upper bound on the discrete spectrum of the system. If then the truncated expansion provides a collapse the full wavefunction will collapse as well. It is then sufficient to consider only the lowest term in the expansion – the so called \( \text{hyper-spheric adiabatic approximation} \),

\[ \Psi(\rho, \Omega) = \frac{1}{\rho^{1/2}} f(\rho) \Phi(\rho, \Omega), \]  
(15)

where the angular coordinates \( \Omega \) correspond to the ”fast” subsystem while the hyper-radius \( \rho \) represents the ”slow” subsystem. Within the adiabatic approximation the lowest eigenvalue \( \lambda(\rho) \) of the ”fast” subsystem simply serves
as the effective potential for the "slow" hyper-radial subsystem,
\[ \left( -\frac{\partial^2}{\partial \rho^2} + \frac{\lambda(\rho) + 15/4}{\rho^2} - \frac{2mE}{\hbar^2} \right) f(\rho) = 0 \],
(13)
where we have neglected one term, originating from the derivatives of the angular functions \[ \frac{\phi_i}{\sin(2\alpha_i)} \], which is unimportant for the following discussion of the collapse.

For zero-range potentials the Faddeev equations provide a more convenient basis for analytic insights into the properties of the three-body system \[ \Phi \]. The Faddeev decomposition of the angular wavefunction \( \Phi \) is
\[ \Phi = \sum_{i=1}^{3} \frac{\phi_i}{\sin(2\alpha_i)} \],
(14)
where the three Faddeev components \( \phi_i \) satisfy the three coupled Faddeev equations
\[ (\Lambda^2 - \lambda(\rho) \frac{\phi_i}{\sin(2\alpha_i)} + \frac{2mE}{\hbar^2} V_i \Phi) = 0 \], \( i = 1, 2, 3 \).
(15)

The system of Faddeev equations \( i = 3 \) is equivalent to the original Schrödinger equation \( i = 1 \).

C. Adiabatic solutions for the zero-range potentials

The zero-range potentials vanish identically except at the origin and we are therefore left with the free Faddeev equations
\[ \left( -\frac{\partial^2}{\partial \rho^2} - \nu^2(\rho) \right) \phi_i(\rho, \alpha_i) = 0 \],
(16)
where \( \nu^2 = \lambda + 4 \), and where we have restricted each of the components of the wavefunction to s-waves only. The solutions, which obey the boundary condition \( \phi_i(\rho, \frac{\pi}{2}) = 0 \), are
\[ \phi_i(\rho, \alpha_i) = A_i \sin \left[ \nu \left( \alpha_i - \frac{\pi}{2} \right) \right] . \]
(17)
For three identical particles the index \( i \) can be dropped completely. For the fermionic case we imply instead that we have a system of, say, two neutrons and a proton in a state with spatially symmetric wavefunction.

The zero-range potential appears as a boundary condition at \( \alpha = 0 \)
\[ \left( \frac{1}{\alpha \Phi} \frac{\partial \alpha \Phi}{\partial \alpha} \right)_{\alpha=0} = \frac{\rho}{\sqrt{\mu a}}, \]
(18)
where \( \mu = (1/m)(m_1m_2/(m_1 + m_2)) \) is the reduced mass of the two particles in units of the mass \( m \), and \( a \) is the scattering length. The total angular wavefunction \( \Phi \) can be expressed for small angles within a given Jacobi system as
\[ \sin(2\alpha)\Phi(\alpha) = \phi(\alpha) + \frac{8}{\sqrt{3}} \alpha \phi \left( \frac{\pi}{3} \right) + O(\alpha^2) . \]
(19)

Substituting \( \phi(\alpha) \) and \( \phi(\alpha) \) into \( \Phi \) leads to the eigenvalue equation \( \Phi \) for \( \nu \)
\[ -\nu \cos(\nu \frac{\pi}{2}) + \frac{8}{\sqrt{3}} \sin(\nu \frac{\pi}{2}) \sin(\nu \frac{\pi}{2}) = \frac{\rho}{\sqrt{\mu a}} . \]
(20)

The solution \( \nu(\rho) \) of this equation defines the needed adiabatic potential \( (\nu^2 - 1/4)/\rho^2 \) for the hyper-radial equation \( \Phi \) from which one obtains the total energy and the radial wave function of the system.

III. CORRELATIONAL COLLAPSE OF MANY-BODY SYSTEM

In the small distance region, \( \rho \ll a \), the eigenvalue equation \( \Phi \) has an imaginary root \( \nu_0 = ib \), where \( b = 1.006 \), leading to an effective potential in the hyper-radial equation which in this region behaves as \( (\nu_0^2 - 1/4)/\rho^2 \equiv -C/\rho^2 \), where \( C = 1.262 \). The hyper-radial equation \( \Phi \) then becomes
\[ \left( -\frac{\partial^2}{\partial \rho^2} - \frac{C}{\rho^2} - \frac{2mE}{\hbar^2} \right) f(\rho) = 0 , \rho \ll a . \]
(21)
The (negative) energy \( E = -\hbar^2 \kappa^2/(2m) \) is negligible compared to the potential when the distance is sufficiently small, \( \rho \ll \kappa^{-1} \). The hyper-radial equation then turns into
\[ \left( -\frac{\partial^2}{\partial \rho^2} - \frac{C}{\rho^2} \right) f(\rho) = 0 , \]
(22)
which has solutions of the form \( f(\rho) \sim \rho^n \), where \( n = \frac{1}{2} \pm \frac{1}{2} \sqrt{1 - 4C} = \frac{1}{2} \pm \nu_0 \). For \( C > \frac{1}{4} \) the exponent \( n \) acquires an imaginary part \pm ib, i.e.
\[ f(\rho) \sim \sqrt{\rho} e^{\pm ib \ln(\rho)} . \]
(23)
This wavefunction has independent of energy infinitely many nodes at small distances or, correspondingly, infinitely many lower lying states at smaller distances (Thomas effect). In other words, there is actually no finite ground state – the three-body system collapses.

For the many-body system the energy minimum, minus infinity, is therefore reached at the configuration, where the many-body system is clusterized into separated three-body subsystems. The density of the many-body system in this configuration is then represented by a sum of delta-functions corresponding to collapsed three-body clusters. The Hartree-Fock ansatz for the wavefunction, however, explicitly excludes such clustered configurations. It is therefore safe to use the Hamiltonian \( H \) with additional potentials \( V \) or \( V^\prime \) as long as the model space is restricted to the Hartree-Fock product wavefunctions.
Let us now consider the extended Hamiltonian which includes the additional potential $W_3$ either as the three-body zero-range potential (6) or as the density dependent zero-range potential (7). Applied to a separated three-body cluster both potentials are non-vanishing only when all three constituents are located at the same point in space. This configuration corresponds to $\rho = 0$ or $\ln(\rho) = -\infty$. These additional potentials, therefore, will only change the boundary condition at $\rho = 0$. However, independent of the boundary condition at $\ln(\rho) = -\infty$, the infinitely many nodes of the wave function (8) remain and, therefore, the system still collapses.

The repulsive zero-range potentials (6) or (7) need three particles located at the same point to provide the stabilizing contribution to the energy of the system. Unfortunately this configuration, as we have shown, is unstable under collapse. If, however, this three-body collapse is somehow removed the four-body correlations (or higher) will not destabilize the many-body system. Indeed the repulsive potentials (6) or (7) provide a contribution to the energy, which has a higher density dependence than that from the attractive two-body potential and hence high density configurations will not be energetically favored. The removal of the three-body collapse, which allows the repulsive potentials (6) or (7) to contribute, will therefore also stabilize the four and higher order correlations.

IV. DISCUSSION

We have shown that zero-range potentials, applied to a many-body system in coordinate space, lead to a specific collapse of the system driven by three-body correlations. Neither the density dependence of the potential nor the three-body zero-range potential can remove this correlational collapse. The Hamiltonian (3), perhaps extended by the additional potential (6) or (7), can still produce meaningful results, provided the allowed variational model space is chosen consistently. Any three-body correlation must be excluded a priori from the wavefunction of the many-body system approximated by the Hamiltonian (2). Going beyond the Hartree-Fock (anti)symmetrized product wavefunction would immediately introduce dangerous effects of three-body correlations.

To remove the three-body collapse one has to regularize the zero-range potential by introducing a finite length scale $R$, which will alter the $-C/\rho^2$ behaviour of the effective potential at $\rho \sim R$. Such regularization is automatically achieved by finite-range two-body potentials. The three-body system will then have approximately $\ln(a/R)$ bound states with the ground state having a finite binding energy of the order of $\hbar^2/(2mR^2)$.

When the three-body system is regularized the correlations of higher number of particles can be safely in-

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