Revised Huang-Yang multipolar pseudopotential

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A number of authors have recently pointed out inconsistencies of results obtained with the Huang-Yang multipolar pseudo-potential for low-energy scattering [K. Huang and K. C. Yang, Phys. Rev. A 105, 767 (1957); later revised in K. Huang, “Statistical Mechanics”, (Wiley, New York, 1963)]. The conceptual validity of their original derivation has been questioned. Here I show that these inconsistencies are rather due to an algebraic mistake made by Huang and Yang. With the corrected error, I present the revised version of the multipolar pseudo-potential.

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I. INTRODUCTION

Most many-body problems require evaluating matrix elements of interparticle interaction in the plane-wave basis. For a typical interaction with a short-range repulsive "hard" core such integrals diverge. Nevertheless, this problem can be made tractable with so-called pseudo-potential technique, which is usually attributed to Fermi [1]. In this technique, a suitably chosen pseudo-potential replaces the true interaction; the solution of the Schrödinger equation with the pseudo-potential must reproduce the long-range behavior of the wave-function derived with the original interaction. Since the most fundamental ingredient of the quantum mechanical treatment, the wavefunction, is properly recovered, any non-singular property should be well approximated in this approach.

In the Huang-Yang (HY) construction [2, 3], the pseudo-potential \( V_{ps} \) is determined as a multipolar expansion over delta-function ("lumped") contributions. For a partial wave expansion, \( \psi (r) = \sum_{l,m} \psi_{lm} (r) Y_{lm} (\hat{r}) \),

\[
V_{ps} \psi (r) = \sum_{l,m} Y_{lm} (\hat{r}) \hat{v}_l \psi_{lm} (r),
\]

where \( \mu \) is the reduced mass of the interacting pair, \( k \) is the conventional collision wavevector, and \( \eta_l \) is the phase shift for a partial wave \( l \). As to the prefactor \( f_l \), the values of the prefactor differ in the original HY paper [2] and in the Huang’s textbook [3], published later. Namely the value of the prefactor from the Huang’s textbook is used in the literature. Here, by tracing steps in the Huang derivation, I point out that still there remains an algebraic mistake in the value of the prefactor \( f_l \). The new revised value of the prefactor is

\[
f_{l}^{\text{revised}} = \frac{2l+1}{l+1} f_{l}^{\text{Huang}} = \frac{(2l+1)!!}{l^{2l}},
\]

where \( f_{l}^{\text{Huang}} \) is the original (erroneous) pre-factor from Ref.[3].

Notice that the s-wave contribution (\( l = 0 \)) to \( V_{ps} \) is not affected by the correction. Since the s waves dominate low-energy collision physics, certain inconsistencies for higher partial waves has not been noticed until very recently [4, 5], when higher order multipoles became a subject of interest. For example, for identical fermions the s-wave contribution vanishes because of the symmetry arguments, and one has to consider p-wave scattering in particular. There are other scenarios, e.g., a resonant coupling of d-waves, when the multipoles beyond \( l = 0 \) become relevant. Also the strong coupling of higher partial waves to s-waves is a prominent feature for anisotropic (e.g., dipolar) interactions.

First, Roth and Feldmeier [4] have considered mean-field correction to energies of trapped fermions. They have derived their own version of the pseudo-potential aimed at reproducing the energy shifts. By computing the same corrections with the HY pseudo-potential, these authors found that each multipolar contribution in the HY pseudo-potential must be multiplied by a factor of \( (2l+1)/(l+1) \) (just as in Eq.(2)) to bring the computed correction

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into an agreement with their independent results. These authors concluded that the HY pseudo potential "is not a proper effective interaction for a mean field description of dilute quantum gases that goes beyond s-wave interactions". Unfortunately, this statement can be interpreted as if two different versions of the pseudopotential were to be employed: one version for continuum and another version for bound-state problems.

Second, an alternative derivation of the pseudopotential has been presented by Stock et al. In this limit produced multipolar terms differing by a factor of \((2l + 1)/(l + 1)\) from the HY terms. Because of these missing factors, the authors of Ref. claimed that there is a "fundamental problem" with the HY pseudopotential based on the Huang-Yang derivation.

Here I demonstrate that there is no conceptual problem with the Huang-Yang construction. Rather there is an algebraic mistake in the derivation. I have traced the error to the erroneous application of the Gauss theorem in this version for continuum and another version for bound-state problems.

This short paper is organized as follows. In Section II by deriving phase shifts in the Born approximation with the HY pseudo-potential I present another demonstration that there is a consistency problem with the original HY expressions. In Section III I will point out the algebraic error in Huang-Yang derivation.

II. INTEGRAL EQUATION FOR THE PHASE SHIFTS AND HUANG-YANG PSEUDO-POTENTIAL

As discussed in the introduction there is some evidence from the literature that there is a difficulty with the original HY formula. Below I provide an alternative self-consistency check of the HY pseudopotential based on the integral equation for the phase shifts. I arrive at the value of the prefactor which indeed differs from the one prescribed by Huang.

The radial Lippmann-Schwinger equation for a finite-ranged spherically-symmetric potential leads to the following implicit equation for the phase shifts

\[ \tan \eta_l = -\sqrt{\frac{2\mu}{\hbar^2}} \frac{\pi}{k} \int_0^\infty kr j_l(kr) V(r) \phi_l(r) \, dr . \]  

Here \( \phi_l(r) \) is the properly normalized exact solution of the scattering problem. For the HY pseudo-potential this solution is by construction

\[ \phi_l(r) = \sqrt{\frac{2\mu}{\hbar^2}} \frac{1}{\pi k} \{ kr j_l(kr) - \tan \eta_l kr n_l(kr) \} , \]  

with \( j_l(kr) \) and \( n_l(kr) \) being the conventional spherical Bessel and Neumann functions. At small values of the argument,

\[ j_l(z) \approx \frac{1}{(2l + 1)!!} z^l, \quad n_l(z) \approx -\frac{(2l - 1)!!}{z^{l+1}} . \]

Now we substitute the solution into the Eq. with the HY pseudo-potential, Eq. The part of the solution proportional to the Neumann function vanishes upon differentiation and an intermediate result is

\[ \tan \eta_l = f_l \frac{1}{(2l + 1)!!} \frac{\tan \eta_l}{k^{2l+2}} \int_0^\infty (kr)^{l+1} \frac{\delta(r)}{r^{l+2}} \left( \frac{\partial}{\partial r} \right)^{2l+1} \left( r^{l+1} (kr)^{l+1} \right) dr . \]

This equation allows us to obtain the value of the prefactor \( f_l \). Taking into account \( (\frac{\partial}{\partial r})^{2l+1} r^{2l+2} = (2l + 1)!! r \), one arrives at the value of prefactor \( f_l = (2l + 1)!!/(2l!!) \), i.e., differing from the Huang’s prefactor by \((2l + 1)/(l + 1)\) for \( l > 0 \) multipoles. Below, I will trace the steps in Huang’s derivation and I will point out the mistake in his derivation.
III. TRACING THE ALGEBRAIC ERROR IN HUANG-YANG DERIVATION

While the original pseudopotential has been introduced in the Huang-Yang paper [2], there are certain mistakes in the final equations. These formulae have been revised later by Huang in his textbook [3]. Also additional details of the derivation are given there. Tracing the steps in the derivation, I found the error in the chain of equations (B.13) of Ref. [3]. Here Huang integrates over a small spherical volume $V_{\varepsilon}$ of infinitesimal radius $\varepsilon$

$$I_{\varepsilon} = \int_{V_{\varepsilon}} d^{3}r \frac{1}{r^{2}} \left\{ \frac{1}{r^{2}} \frac{d}{dr} \frac{d}{dr} n_{l}(kr) - \frac{l(l+1)}{r^{2}} n_{l}(kr) \right\}.$$

Noticing that $\nabla^{2}r^{l} = \frac{l(l+1)}{r} r^{l}$ and that for a spherically-symmetric function

$$\nabla^{2}f(r) = \frac{1}{r^{2}} \frac{d}{dr} \frac{d}{dr} f(r),$$

this expression is brought into a form suitable for application of the Green’s theorem (the Green’s second identity),

$$I_{\varepsilon} = \int_{V_{\varepsilon}} d^{3}r \left\{ r^{l} \nabla^{2}n_{l}(kr) - n_{l}(kr) \nabla^{2}r^{l} \right\}.$$

The second Green’s identity reads [7]

$$\int_{V} d^{3}r \left( \phi \nabla^{2}\psi - \psi \nabla^{2}\phi \right) = \oint_{S} dS \cdot \left( \phi \nabla\psi - \psi \nabla\phi \right),$$

leading to

$$I_{\varepsilon} = \oint_{S} dS \cdot \left( r^{l} \nabla n_{l}(kr) - n_{l}(kr) \nabla r^{l} \right),$$

while Huang’s formula reads

$$I_{\varepsilon}^{Huang} = \oint_{S} dS \cdot \left( r^{l} \nabla n_{l}(kr) \right).$$

The error is here. Huang is missing the second term, $-n_{l}(kr) \nabla r^{l}$. Continuing the chain of equations, we obtain

$$I_{\varepsilon} = \oint_{S} \left( r^{l} \frac{d}{dr} n_{l}(kr) - n_{l}(kr) \frac{d}{dr} r^{l} \right) dS =$$

$$= \frac{(2l-1)!!}{k^{l+1}} \oint_{S} \left( -l \frac{d}{dr} r^{l+1} + \frac{1}{r^{l+1}} \frac{d}{dr} r^{l} \right) dS =$$

$$= \frac{(2l-1)!!}{k^{l+1}} \oint_{S} \left( (l+1) \frac{1}{r^{2}} + l \frac{1}{r^{2}} \right) dS.$$

Namely the second (missed term) provides the additional contribution of $l$. Finally,

$$I_{\varepsilon} = 4\pi \frac{(2l-1)!!}{k^{l+1}} (2l+1)$$

or Eq.(B.14) of Ref. [3] should read

$$F_{l}(r) = \frac{(2l-1)!!}{k^{l+1}} (2l+1) \frac{\delta(r)}{r^{l+2}}.$$

Combining this result with the rest of the derivation we arrive at the revised Huang-Yang pseudopotential Eqs. [12].

To summarize, here a revised form of the low-energy multipolar pseudopotential by Huang and Yang [2, 3] has been presented. A mistake in the original derivation has been pointed out. The present paper reconciles the seminal Huang-Yang construction with more recent results from the literature.

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