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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 pseudopotential for low-energy scattering [K. Huang and K. C. Yang, Phys. Rev. **105**, 767 (1957); later revised by 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 pseudopotential.

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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 the so-called pseudopotential technique, which is attributed to Fermi [1]. In this technique, a suitably chosen pseudopotential replaces the true interaction; the solution of the Schrodinger equation with the pseudopotential 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 wave function, is properly recovered, any nonsingular property should be well-approximated in this approach.

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

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

$$\hat{v}_l\psi_{lm}(r) = -f_l\frac{\hbar^2}{2\mu}\frac{\delta(r)}{r^{l+2}}\frac{\tan\eta_l}{k^{2l+1}}\left(\frac{\partial}{\partial r}\right)^{2l+1}(r^{l+1}\psi_{lm}), \tag{1}$$

where μ is the reduced mass of the interacting pair, k is the conventional collision wave vector, and η_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 Huang's textbook [3], published later. Namely, the value of the prefactor from 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

$$f_l^{\text{revised}} = \frac{2l+1}{l+1}f_l^{\text{Huang}} = \frac{(2l+1)!!}{l!2^l}, \tag{2}$$

where f_l^{Huang} is the original (erroneous) prefactor 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 a mean-field correction to energies of trapped fermions. They have derived their own version of the pseudopotential aimed at reproducing the energy shifts. By computing the same corrections with the HY pseudopotential, these authors found that each multipolar contribution in the HY pseudopotential must be multiplied by a factor of $(2l+1)/(l+1)$ [just as in Eq. (2)] to bring the computed correction into an agreement with their independent results. These authors concluded that the HY pseudopotential "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.* [5]. Instead of delta function lumped at the origin, these authors have proposed to use a shell pseudopotential, i.e., delta function placed at the surface of the spherical shell. In the limit of zero radius of the shell each multipolar term of the HY pseudopotential is obtained. As in Ref. [4] 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. [5] claimed that there is a "fundamental problem" with 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 [3]. I have traced the error to the erroneous application of the Gauss theorem in [3]. With the corrected derivation, this additional factor of $(2l+1)/(l$

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+1) is fully recovered. There is no need to introduce the intermediate δ-shell pseudopotential as proposed in Ref. [5]. In other words, there is a reconciliation of the seminal paper by Huang and Yang with the more recent derivations.

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

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

As discussed in the Introduction there is some evidence from the literature [4,5] 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 [6]:

$$\tan \eta_l = -\sqrt{\frac{2\mu}{\hbar^2}\frac{\pi}{k}}\int_0^\infty krj_l(kr)V(r)\phi_l(r)dr. \tag{3}$$

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

$$\phi_l(r) = \sqrt{\frac{2\mu}{\hbar^2}\frac{1}{\pi k}}\{krj_l(kr) - \tan \eta_l krn_l(kr)\}, \tag{4}$$

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

$$j_l(z) \simeq \frac{1}{(2l+1)!!}z^l, \quad n_l(z) \simeq -\frac{(2l-1)!!}{z^{l+1}}.$$

Now we substitute the solution (4) into Eq. (3) with the HY pseudopotential, Eq. (1). The part of the solution proportional to the Neumann function vanishes upon differentiation and an intermediate result is

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

This equation allows us to obtain the value of the prefactor f_l. Taking into account $(\partial/\partial r)^{2l+1}r^{2l+2}=(2l+1)!r$, one arrives at the value of prefactor $f_l=(2l+1)!!/(2^l l!)$, i.e., differing from the Huang's prefactor by $(2l+1)/(l+1)$. Again, as in Refs. [4,5], we conclude that there is a self-consistency problem with the HY formula 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 formulas 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_ε of infinitesimal radius ε

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

Noticing that $\nabla^2 r^l = l[(l+1)]/r^2 r^l$ and that for a spherically symmetric function

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

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

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

The second Green's identity reads [7]

$$\int_V (\phi\nabla^2\psi - \psi\nabla^2\phi)dV = \oint_S d\mathbf{S}\cdot(\phi\,\boldsymbol{\nabla}\,\psi - \psi\,\boldsymbol{\nabla}\,\phi),$$

leading to

$$I_\varepsilon = \oint_S d\mathbf{S}\cdot[r^l\,\boldsymbol{\nabla}\,n_l(kr) - n_l(kr)\,\boldsymbol{\nabla}\,r^l],$$

while Huang's formula reads

$$I_\varepsilon^{\text{Huang}} = \oint_S d\mathbf{S}\cdot[r^l\,\boldsymbol{\nabla}\,n_l(kr)].$$

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

$$I_\varepsilon = \oint_S\left(r^l\frac{d}{dr}n_l(kr) - n_l(kr)\frac{d}{dr}r^l\right)dS = \frac{(2l-1)!!}{k^{l+1}}\oint_S\Bigg(- r^l\frac{d}{dr}\frac{1}{r^{l+1}} + \frac{1}{r^{l+1}}\frac{d}{dr}r^l\Bigg)dS = \frac{(2l-1)!!}{k^{l+1}}\oint_S\Bigg((l+1)\frac{1}{r^2} + l\frac{1}{r^2}\Bigg)dS.$$

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. (1) and (2).

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.

Note added in proof. Recent work by Idziaszek and Calarco [8] and Pricoupenko [9] reports results identical to (1) and (2)

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[1] E. Fermi, Ric Sci. 2 Ser. Pt 2 Rend **7**, 13 (1936).
[2] K. Huang and C. N. Yang, Phys. Rev. **105**, 767 (1957).
[3] K. Huang, *Statistical Mechanics* (Wiley, New York, 1963).
[4] R. Roth and H. Feldmeier, Phys. Rev. A **64**, 043603 (2001).
[5] R. Stock, A. Silberfarb, E. L. Bolda, and I. H. Deutsch, Phys. Rev. Lett. **94**, 023202 (2005).
[6] H. S. Friedrich, *Theoretical Atomic Physics*, 2nd ed. (Springer, Berlin, 2004).
[7] W. Kaplan, *Advanced Calculus*, 4th ed. (Addison-Wesley, Reading, MA, 1991).
[8] Z. Idziaszek and T. Calarco, quant-ph/0507186 (unpublished).
[9] L. Pricoupenko, cond-mat0508120 (unpublished).