Corrected Huang-Yang pseudopotential for partial waves

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I. TWO-BODY INTERACTION

A. Relative coordinates

The general Hamiltonian for two-body interactions is given as follows,

\[ H = -\frac{\hbar^2}{2M_1} \nabla^2_{r_1} - \frac{\hbar^2}{2M_2} \nabla^2_{r_2} + V(r_1 - r_2). \] (1)

If we define the center-of-mass coordinates \( R \) and the relative coordinates \( r \) as

\[ R = \frac{M_1 r_1 + M_2 r_2}{M_1 + M_2}, \quad r = r_1 - r_2, \] (2)

the Hamiltonian can be transformed into

\[ H = -\frac{\hbar^2}{2M} \nabla^2_{R} - \frac{\hbar^2}{2\mu} \nabla^2_{r} + V(r), \] (3)

where \( M = M_1 + M_2 \) is the total mass, and \( \mu = M_1 M_2 / (M_1 + M_2) \) is the reduced mass. In this way, we can express the wave function of the two particles as

\[ \psi(r_1, r_2) = \psi_{\text{com}}(R) \psi_{\text{rel}}(r). \] (4)

Notice that the two-body interaction term only affects \( \psi_{\text{rel}}(r) \), so we reduce the two-body problem to an effective one-body problem in relative coordinates.

B. Partial wave expansion

The two-body Schrödinger equation in the relative coordinates is given as follows,

\[ \frac{\hbar^2}{2\mu}(\nabla^2 + k^2)\psi(r) = V(r)\psi(r), \] (5)

where \( k^2 = 2\mu E/\hbar^2 \), and for simplicity we assume \( V(r) \) is a central and finite-range potential which is non-zero in the regime \( r < r_0 \). Using the partial wave expansion, we can expand the wave function \( \psi(r) \) as

\[ \psi(r) = \sum_{lm} R_{lm}(r) Y_{lm}(\theta, \phi). \] (6)
Plugging Eq. (6) into Eq. (5) outside the range of the potential \((r > r_0)\), we get the following differential equation for the radial part of the wave function,

\[
\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d R_{lm}}{dr} \right) + \left( k^2 - \frac{l(l+1)}{r^2} \right) R_{lm} = 0.
\]

The general solution of Eq. (7) is given by

\[
R_{lm}(r) = A_{lm} j_l(kr) + B_{lm} n_l(kr),
\]

where \(j_l(r)\) and \(n_l(r)\) are the spherical Bessel functions. The asymptotic behavior of \(R_{lm}(r)\) for \(kr \to \infty\) is given by

\[
R_{lm}(r) \to \frac{1}{kr} \left[ A_{lm} \sin \left( kr - \frac{l\pi}{2} \right) - B_{lm} \cos \left( kr - \frac{l\pi}{2} \right) \right] \propto \frac{1}{kr} \sin \left( kr - \frac{l\pi}{2} + \delta_l \right)
\]

where \(\delta_l\) is defined as the scattering phase shift of the \(l\)-partial wave, which depends on the finite range potential \(V(r)\). In terms of phase shift \(\delta_l\), we can rewrite \(R_{lm}(r)\) as follows,

\[
R_{lm}(r) = C_{lm} \left[ j_l(kr) - \tan \delta_l n_l(kr) \right] \quad (r > r_0).
\]

In the following discussions, we called the wave function in the regime \(r > r_0\) as \(\psi_>(r)\).

### II. HUANG-YANG PSEUDOPOTENTIAL

#### A. Derivation of pseudopotential

The idea of Huang-Yang pseudopotential is to replace the potential \(V(r)\) by a contact potential \(V_{ps}(r)\), which acts only at \(r = 0\) and gives the same wave function \(\psi_>(r)\) outside the range of the potential at the low-energy threshold \((k \to 0)\). Notice that the asymptotic behavior of \(R_{lm}(r)\) for \(kr \to 0\) is given by

\[
R_{lm}(kr) \to C_{lm} \left[ \frac{(kr)^l}{(2l+1)!!} + \tan \delta_l \frac{(2l-1)!!}{(kr)^{l+1}} \right],
\]

the Huang-Yang pseudopotential \(V_{ps}(r)\) can be constructed as

\[
V_{ps}(r)\psi_>(r) = \frac{\hbar^2}{2\mu} \nabla^2 \psi_>(kr \to 0)
\]

\[
= \frac{\hbar^2}{2\mu} \sum_{lm} C_{lm} Y_{lm}(\theta, \phi) \left( \nabla^2 - \frac{l(l+1)}{r^2} \right) \left[ \frac{(kr)^l}{(2l+1)!!} + \tan \delta_l \frac{(2l-1)!!}{(kr)^{l+1}} \right].
\]
Using the fact that
\[ \nabla^2 (r^l) = \frac{l(l+1)}{r^2} r^l, \quad (13) \]

\[
\left( \nabla^2 - \frac{l(l+1)}{r^2} \right) \frac{1}{r^{l+1}} = \frac{1}{r^l} \left[ r^l \nabla^2 \left( \frac{1}{r^{l+1}} \right) - \frac{1}{r^{l+1}} \nabla^2 (r^l) \right] \\
= \frac{1}{r^l} \nabla \cdot \left[ r^l \nabla \left( \frac{1}{r^{l+1}} \right) - \frac{1}{r^{l+1}} \nabla (r^l) \right] \\
= \frac{2l + 1}{r^l} \nabla \cdot \left( \frac{\hat{r}}{r^2} \right) \\
= \frac{2l + 1}{r^l} 4\pi \delta(r),
\quad (14)
\]
we have
\[
V_{ps}(r) \psi_>(r) = -\frac{\hbar^2}{2\mu} \sum_{lm} C_{lm} \tan \delta_l \frac{(2l + 1)!!}{k^{l+1}} \frac{\delta(r)}{r^{l+2}} Y_{lm}(\theta, \phi), \quad (15)
\]
where \( \delta(r) = 4\pi r^2 \delta(r) \). Based on Eq. (11), we can also express \( C_{lm} \) as follows,
\[
C_{lm} = \frac{1}{k^{l}(2l)!!} \left[ \left( \frac{d}{dr} \right)^{2l+1} r^{l+1} Y_{lm}(kr) \right] \bigg|_{r=0} \\
= \frac{1}{k^{l}(2l)!!} \left[ \left( \frac{\partial}{\partial r} \right)^{2l+1} r^{l+1} \int d\Omega Y_{lm}^*(\Omega) \psi_>(r) \right] \bigg|_{r=0}. \quad (16)
\]
Plugging Eq. (16) into Eq. (15), we have
\[
V_{ps}(r) \psi_>(r) = \sum_{lm} \frac{\hbar^2 a^{2l+1}_l}{2\mu} \frac{(2l + 1)!!}{(2l)!!} \frac{\delta(r)}{r^{l+2}} Y_{lm}(\theta, \phi) \left[ \left( \frac{\partial}{\partial r} \right)^{2l+1} r^{l+1} \int d\Omega Y_{lm}^*(\Omega) \psi_>(r) \right] \bigg|_{r=0}, \quad (17)
\]
where we define the scattering length for the \( l \)-partial wave as
\[
a^{2l+1}_l = - \lim_{k \to 0} \frac{\tan \delta_l}{k^{2l+1}}. \quad (18)
\]

B. Pseudopotential in momentum space

Consider the plane wave basis,
\[
\langle r | k \rangle = \frac{1}{\sqrt{V}} e^{ik \cdot r}, \quad (19)
\]
and
\[
\langle k | V_{ps} | k' \rangle = \frac{1}{V} \int d^3 r e^{-ik \cdot r} V_{ps}(r) e^{ik' \cdot r}, \quad (20)
\]
we have
\[ \langle k | V_{ps} | k' \rangle = \sum_{lm} \frac{h^2 a_l^{2l+1}}{2\mu V} \frac{2l + 1}{(2l)!} \left[ \int d^3 r \, e^{-ik\cdot r} \frac{\delta(r)}{r^{l+2}} \right] \frac{\delta(r)}{r^{l+2}} \int d\Omega Y_{l'm'}(\Omega) Y_{lm}^*(\theta, \phi) \]
\[ \times \left[ \left( \frac{\partial}{\partial r} \right)^{l+1} r^{l+1} \int d\Omega Y_{l'm'}^*(\Omega) e^{ik'\cdot r} \right] \bigg|_{r=0} \].

Using the fact that
\[ e^{ik\cdot r} = 4\pi \sum_{lm} i^l j_l(kr) Y_{lm}^*(\hat{k}) Y_{lm}(\hat{r}), \]
we have
\[ \int d^3 r \, e^{-ik\cdot r} \frac{\delta(r)}{r^{l+2}} Y_{lm}(\theta, \phi) = 4\pi \sum_{l'm'}(-i)^l Y_{l'm'}^*(\hat{k}) \int r^2 dr \, j_l(kr) \frac{\delta(r)}{r^{l+2}} \int d\Omega Y_{l'm'} Y_{lm} \]
\[ = 4\pi (-i)^l Y_{lm}(\hat{k}) \int r^2 dr \, j_l(kr) \frac{\delta(r)}{r^{l+2}} \]
\[ = 4\pi (-i)^l Y_{lm}(\hat{k}) k^l \]
\[ \frac{(2l + 1)!}{(2l + 1)!}, \]
\[ \left[ \left( \frac{\partial}{\partial r} \right)^{l+1} r^{l+1} \int d\Omega Y_{l'm'}^*(\Omega) e^{ik'\cdot r} \right] \bigg|_{r=0} = 4\pi \sum_{l'm'} i^l Y_{l'm'}^*(\hat{k}') \left[ \left( \frac{\partial}{\partial r} \right)^{l+1} r^{l+1} j_l(k'r) \int d\Omega Y_{l'm'} Y_{lm} \right] \bigg|_{r=0} \]
\[ = 4\pi i^l Y_{lm}^*(\hat{k}') \left[ \left( \frac{\partial}{\partial r} \right)^{l+1} r^{l+1} j_l(k'r) \right] \bigg|_{r=0} \]
\[ = 4\pi i^l Y_{lm}^*(\hat{k}') (k')^l (2l)!! , \]
which gives
\[ \langle k | V_{ps} | k' \rangle = \frac{8\hbar^2 \pi^2}{\mu V} \sum_{lm} \frac{a_l^{2l+1} (k')^l k^l Y_{lm}^*(\hat{k}') Y_{lm}(\hat{k})}. \]

Recall the addition theorem for spherical harmonics,
\[ P_l(\hat{k} \cdot \hat{k}') = \frac{4\pi}{2l + 1} \sum_{m} Y_{lm}(\hat{k}) Y_{lm}^*(\hat{k}'), \]
where \( P_l(x) \) is the Legendre polynomial, we have
\[ \langle k | V_{ps} | k' \rangle = \frac{2\hbar^2 \pi}{\mu V} \sum_{l} (2l + 1) a_l^{2l+1} (k')^l k^l P_l(\hat{k} \cdot \hat{k}'). \]

For s-wave \((l = 0)\), we have
\[ \langle k | V_{ps} | k' \rangle = \frac{2\hbar^2 \pi}{\mu V} a_0. \]

For p-wave \((l = 1)\), we have
\[ \langle k | V_{ps} | k' \rangle = \frac{6\hbar^2 \pi}{\mu V^3} a_1^3 (k \cdot k'). \]
III. MANY-BODY HAMILTONIAN

It’s convenient to express the many-body Hamiltonian for identical particles ($\mu = m/2$) in the second quantized form as follows,

$$H = H_0 + H_1,$$

$$H_0 = \sum_{\alpha} \int d^3r \psi_\alpha^\dagger(r) \left[ -\frac{\hbar^2}{2m} \nabla^2 \right] \psi_\alpha(r),$$

$$H_1 = \frac{1}{2} \sum_{\alpha \beta} \int d^3r_1d^3r_2 \psi_\alpha^\dagger(r_1)\psi_\beta^\dagger(r_2)V_{ps}^{\alpha\beta}(r_1 - r_2)\psi_\beta(r_2)\psi_\alpha(r_1),$$

in which $V_{ps}^{\alpha\beta}(r_1 - r_2)$ is the pseudopotential for two-body interaction, $\alpha, \beta$ denote the internal levels of the particles, and we use $a_{\alpha\beta}$ ($b_{\alpha\beta}$) to denote the s-wave scattering length (p-wave scattering volume) between particles in internal level $\alpha$ and $\beta$.

In momentum space, the field operator can be expressed as

$$\psi_\alpha(r) = \frac{1}{\sqrt{V}} \sum_k e^{i\mathbf{k}\cdot\mathbf{r}} a_{\alpha k},$$

so the interaction term can be written as

$$H_1 = \frac{1}{2V^2} \sum_{\alpha \beta} \sum_{k_1,k_2,k_3,k_4} a_{k_1\alpha}^\dagger a_{k_2\beta}^\dagger a_{k_3\beta} a_{k_4\alpha} \int d^3r_1d^3r_2 e^{-ik_1\cdot r_1} e^{-ik_2\cdot r_2} V_{ps}^{\alpha\beta}(r_1 - r_2)e^{ik_3\cdot r_2}e^{ik_4\cdot r_1}$$

$$= \frac{1}{2V^2} \sum_{\alpha \beta} \sum_{k_1,k_2,k_3,k_4} a_{k_1\alpha}^\dagger a_{k_2\beta}^\dagger a_{k_3\beta} a_{k_4\alpha} \int d^3\mathbf{R} e^{-i(k_1+2k_2-2k_3-k_4)\cdot \mathbf{R}} \int d^3\mathbf{r} e^{-i(k_1-k_2-k_3-k_4)\cdot \mathbf{r}} V_{ps}^{\alpha\beta}(r_1 - r_2)e^{i\frac{k_4-k_3}{2} \cdot \mathbf{r}}$$

$$= \frac{1}{2} \sum_{\alpha \beta} \sum_{k_1,k_2,k_3,k_4} a_{k_1\alpha}^\dagger a_{k_2\beta}^\dagger a_{k_3\beta} a_{k_4\alpha} \left( \frac{k_1 - k_2}{2} \left| \frac{k_4 - k_3}{2} \right) \delta_{k_1+k_2,k_3+k_4},\right.$$  

(32)

where $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, and $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$.

For s-wave interaction, plug in Eq. (28), we have

$$H_1 = \frac{1}{2} \sum_{\alpha \beta} \frac{4\pi \hbar^2 a_{\alpha\beta}}{mV} \sum_{k_1,k_2,k_3,k_4} a_{k_1\alpha}^\dagger a_{k_2\beta}^\dagger a_{k_3\beta} a_{k_4\alpha} \delta_{k_1+k_2,k_3+k_4}$$

$$= \frac{1}{2} \sum_{\alpha \beta} \frac{4\pi \hbar^2 a_{\alpha\beta}}{mV^2} \sum_{k_1,k_2,k_3,k_4} a_{k_1\alpha}^\dagger a_{k_2\beta}^\dagger a_{k_3\beta} a_{k_4\alpha} \int d^3\mathbf{r} e^{-i(k_1+k_2-k_3-k_4)\cdot \mathbf{r}}$$

$$= \frac{1}{2} \sum_{\alpha \beta} \frac{4\pi \hbar^2 a_{\alpha\beta}}{m} \int d^3\mathbf{r} \psi_\alpha^\dagger(\mathbf{r})\psi_\beta^\dagger(\mathbf{r})\psi_\beta(\mathbf{r})\psi_\alpha(\mathbf{r}).$$
For p-wave interaction, plug in Eq. (29), we have

\[
H_1 = \frac{1}{2} \sum_{\alpha\beta} \frac{3\pi \hbar^2 b^3_{\alpha\beta}}{mV} \sum_{k_1k_2k_3k_4} a_{k_1\alpha}^\dagger a_{k_2\beta}^\dagger a_{k_3\beta} a_{k_4\alpha} [(k_1 - k_2) \cdot (k_4 - k_3)] \delta_{k_1+k_2,k_3+k_4}
\]

\[
= \frac{1}{2} \sum_{\alpha\beta} \frac{3\pi \hbar^2 b^3_{\alpha\beta}}{mV^2} \sum_{k_1k_2k_3k_4} a_{k_1\alpha}^\dagger a_{k_2\beta}^\dagger a_{k_3\beta} a_{k_4\alpha} \int d^3r [(k_1 - k_2) \cdot (k_4 - k_3)] e^{-i(k_1+k_2-k_3-k_4) \cdot r}
\]

\[
= \frac{1}{2} \sum_{\alpha\beta} \frac{3\pi \hbar^2 b^3_{\alpha\beta}}{m} \int d^3r \left[ (\nabla \psi_\alpha^\dagger \psi_\beta^\dagger - \psi_\beta^\dagger (\nabla \psi_\alpha^\dagger)) \cdot [\psi_\beta (\nabla \psi_\alpha) - (\nabla \psi_\beta) \psi_\alpha] \right].
\]

(34)

In the derivation of s-wave and p-wave interaction above, we implicitly assume the field operators \( \psi_\alpha(r) \) and \( \psi_\alpha^\dagger(r) \) have regular spatial profile, so we do not need to include the regularization operators.

Now we use the two-component Fermi gas (internal levels \(|g\rangle, |e\rangle\)) as an example to illustrate the s-wave and p-wave interaction. Since the total wave function for two fermionic atoms is antisymmetric, the spatial wave function related to spin state \(|ge\rangle - |eg\rangle\)/\(\sqrt{2}\) is symmetric (s-wave interaction with scattering length \(a_{eg}\)), while the spatial wave functions related to spin states \(|gg\rangle, (|ge\rangle + |eg\rangle)/\sqrt{2}, |ee\rangle\) are antisymmetric (p-wave interaction with scattering volume \(b^3_{gg}, b^3_{eg}, b^3_{ee}\) respectively). So the two-body interaction term \(H_1\) takes the following form,

\[
H_1 = \frac{4\pi \hbar^2 a_{eg}}{m} \int d^3r \psi_e^\dagger(r) \psi_g^\dagger(r) \psi_g(r) \psi_e(r)
\]

\[
+ \sum_{\alpha\beta} \frac{3\pi \hbar^2 b^3_{\alpha\beta}}{2m} \int d^3r \left[ (\nabla \psi_\alpha^\dagger \psi_\beta^\dagger - \psi_\beta^\dagger (\nabla \psi_\alpha^\dagger)) \cdot [\psi_\beta (\nabla \psi_\alpha) - (\nabla \psi_\beta) \psi_\alpha] \right].
\]

(35)


