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,

$$H = -\frac{\hbar^2}{2M_1}\nabla^2_{\mathbf{r}_1} - \frac{\hbar^2}{2M_2}\nabla^2_{\mathbf{r}_2} + V(\mathbf{r}_1 - \mathbf{r}_2). \tag{1}$$

If we define the center-of-mass coordinates $\mathbf{R}$ and the relative coordinates $\mathbf{r}$ as

$$\mathbf{R} = \frac{M_1\mathbf{r}_1 + M_2\mathbf{r}_2}{M_1 + M_2}, \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \tag{2}$$

the Hamiltonian can be transformed into

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

where $M = M_1 + M_2$ is the total mass, and $\mu = M_1M_2/(M_1 + M_2)$ is the reduced mass. In this way, we can express the wave function of the two particles as

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \psi_{\text{com}}(\mathbf{R})\psi_{\text{rel}}(\mathbf{r}). \tag{4}$$

Notice that the two-body interaction term only affects $\psi_{\text{rel}}(\mathbf{r})$, 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,

$$\frac{\hbar^2}{2\mu}(\nabla^2 + k^2)\psi(\mathbf{r}) = V(r)\psi(\mathbf{r}), \tag{5}$$

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 $\psi(\mathbf{r})$ as

$$\psi(\mathbf{r}) = \sum_{lm} R_{lm}(r)Y_{lm}(\theta, \phi). \tag{6}$$

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,

$$\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R_{lm}}{\mathrm{d}r}\right)+\left(k^2-\frac{l(l+1)}{r^2}\right)R_{lm}=0. \tag{7}$$

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

$$R_{lm}(r)=A_{lm}j_l(kr)+B_{lm}n_l(kr), \tag{8}$$

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

$$R_{lm}(r)\to\frac{1}{kr}\left[A_{lm}\sin\left(kr-\frac{l\pi}{2}\right)-B_{lm}\cos\left(kr-\frac{l\pi}{2}\right)\right]\propto\frac{1}{kr}\sin\left(kr-\frac{l\pi}{2}+\delta_l\right) \tag{9}$$

where δ_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 δ_l, we can rewrite $R_{lm}(r)$ as follows,

$$R_{lm}(r)=C_{lm}[j_l(kr)-\tan\delta_l\, n_l(kr)] \quad (r>r_0). \tag{10}$$

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

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 $V_{ps}(\mathbf{r})$, which acts only at $\mathbf{r}=0$ and gives the same wave function $\psi_>(\mathbf{r})$ 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

$$R_{lm}(kr)\to C_{lm}\left[\frac{(kr)^l}{(2l+1)!!}+\tan\delta_l\frac{(2l-1)!!}{(kr)^{l+1}}\right], \tag{11}$$

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

$$\begin{aligned}V_{ps}(\mathbf{r})\psi_>(\mathbf{r}) &= \frac{\hbar^2}{2\mu}\nabla^2\psi_>(kr\to 0)\\ &= \frac{\hbar^2}{2\mu}\sum_{lm}C_{lm}Y_{lm}(\theta,\phi)\left(\nabla^2-\frac{l(l+1)}{r^2}\right)\left[\frac{(kr)^l}{(2l+1)!!}+\tan\delta_l\frac{(2l-1)!!}{(kr)^{l+1}}\right].\end{aligned} \tag{12}$$

Using the fact that

$$\nabla^2(r^l) = \frac{l(l+1)}{r^2} r^l, \tag{13}$$

$$\begin{aligned}
\left(\nabla^2 - \frac{l(l+1)}{r^2}\right)\frac{1}{r^{l+1}} &= \frac{1}{r^l}\left[r^l \nabla^2\left(\frac{1}{r^{l+1}}\right) - \frac{1}{r^{l+1}}\nabla^2(r^l)\right] \\
&= \frac{1}{r^l}\nabla\cdot\left[r^l \nabla\left(\frac{1}{r^{l+1}}\right) - \frac{1}{r^{l+1}}\nabla(r^l)\right] \\
&= -\frac{2l+1}{r^l}\nabla\cdot\left(\frac{\hat{r}}{r^2}\right) \\
&= -\frac{2l+1}{r^l} 4\pi\delta(\mathbf{r}),
\end{aligned} \tag{14}$$

we have

$$V_{ps}(\mathbf{r})\psi_>(\mathbf{r}) = -\frac{\hbar^2}{2\mu}\sum_{lm} C_{lm}\tan\delta_l \frac{(2l+1)!!}{k^{l+1}}\frac{\delta(r)}{r^{l+2}} Y_{lm}(\theta,\phi), \tag{15}$$

where $\delta(r) = 4\pi r^2 \delta(\mathbf{r})$. Based on Eq. (11), we can also express C_{lm} as follows,

$$\begin{aligned}
C_{lm} &= \frac{1}{k^l (2l)!!}\left[\left(\frac{\mathrm{d}}{\mathrm{d}r}\right)^{2l+1} r^{l+1} R_{lm}(kr)\right]\Bigg|_{r=0} \\
&= \frac{1}{k^l (2l)!!}\left[\left(\frac{\partial}{\partial r}\right)^{2l+1} r^{l+1}\int \mathrm{d}\Omega Y^*_{lm}(\Omega)\psi_>(\mathbf{r})\right]\Bigg|_{r=0}.
\end{aligned} \tag{16}$$

Plugging Eq. (16) into Eq. (15), we have

$$V_{ps}(\mathbf{r})\psi_>(\mathbf{r}) = \sum_{lm}\frac{\hbar^2 a_l^{2l+1}}{2\mu}\frac{(2l+1)!!}{(2l)!!}\frac{\delta(r)}{r^{l+2}} Y_{lm}(\theta,\phi)\left[\left(\frac{\partial}{\partial r}\right)^{2l+1} r^{l+1}\int \mathrm{d}\Omega Y^*_{lm}(\Omega)\psi_>(\mathbf{r})\right]\Bigg|_{r=0}, \tag{17}$$

where we define the scattering length for the l-partial wave as

$$a_l^{2l+1} = -\lim_{k\to 0}\frac{\tan\delta_l}{k^{2l+1}}. \tag{18}$$

B. Pseudopotential in momentum space

Consider the plane wave basis,

$$\langle \mathbf{r}|\mathbf{k}\rangle = \frac{1}{\sqrt{V}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}, \tag{19}$$

and

$$\langle \mathbf{k}|V_{ps}|\mathbf{k}'\rangle = \frac{1}{V}\int \mathrm{d}^3\mathbf{r}\, \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}} V_{ps}(\mathbf{r})\mathrm{e}^{i\mathbf{k}'\cdot\mathbf{r}}, \tag{20}$$

we have

$$\langle \mathbf{k}|V_{ps}|\mathbf{k}'\rangle = \sum_{lm} \frac{\hbar^2 a_l^{2l+1}}{2\mu V} \frac{(2l+1)!!}{(2l)!!} \left[\int \mathrm{d}^3\mathbf{r}\, \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}} \frac{\delta(r)}{r^{l+2}} Y_{lm}(\theta,\phi) \right] \times \left[\left(\frac{\partial}{\partial r}\right)^{2l+1} r^{l+1} \int \mathrm{d}\Omega Y^*_{lm}(\Omega) \mathrm{e}^{i\mathbf{k}'\cdot\mathbf{r}} \right]\Bigg|_{r=0}. \tag{21}$$

Using the fact that

$$\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{lm} i^l j_l(kr) Y^*_{lm}(\hat{k}) Y_{lm}(\hat{r}), \tag{22}$$

we have

$$\begin{aligned} \int \mathrm{d}^3\mathbf{r}\, \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}} \frac{\delta(r)}{r^{l+2}} Y_{lm}(\theta,\phi) &= 4\pi \sum_{l'm'} (-i)^{l'} Y_{l'm'}(\hat{k}) \int r^2 \mathrm{d}r\, j_{l'}(kr) \frac{\delta(r)}{r^{l+2}} \cdot \int \mathrm{d}\Omega\, Y^*_{l'm'} Y_{lm} \\ &= 4\pi (-i)^l Y_{lm}(\hat{k}) \int r^2 \mathrm{d}r\, j_l(kr) \frac{\delta(r)}{r^{l+2}} \\ &= \frac{4\pi(-i)^l Y_{lm}(\hat{k}) k^l}{(2l+1)!!}, \end{aligned} \tag{23}$$

$$\begin{aligned} \left[\left(\frac{\partial}{\partial r}\right)^{2l+1} r^{l+1} \int \mathrm{d}\Omega Y^*_{lm}(\Omega) \mathrm{e}^{i\mathbf{k}'\cdot\mathbf{r}} \right]\Bigg|_{r=0} &= 4\pi \sum_{l'm'} i^{l'} Y^*_{l'm'}(\hat{k}') \left[\left(\frac{\partial}{\partial r}\right)^{2l+1} r^{l+1} j_{l'}(k'r) \int \mathrm{d}\Omega Y^*_{lm} Y_{l'm'} \right]\Bigg|_{r=0} \\ &= 4\pi\, i^l Y^*_{lm}(\hat{k}') \left[\left(\frac{\partial}{\partial r}\right)^{2l+1} r^{l+1} j_l(k'r) \right]\Bigg|_{r=0} \\ &= 4\pi\, i^l Y^*_{lm}(\hat{k}') (k')^l (2l)!!, \end{aligned} \tag{24}$$

which gives

$$\langle \mathbf{k}|V_{ps}|\mathbf{k}'\rangle = \frac{8\hbar^2\pi^2}{\mu V} \sum_{lm} a_l^{2l+1} (k')^l k^l Y^*_{lm}(\hat{k}') Y_{lm}(\hat{k}). \tag{25}$$

Recall the addition theorem for spherical harmonics,

$$P_l(\hat{k}\cdot\hat{k}') = \frac{4\pi}{2l+1} \sum_m Y_{lm}(\hat{k}) Y^*_{lm}(\hat{k}'), \tag{26}$$

where $P_l(x)$ is the Legendre polynomial, we have

$$\langle \mathbf{k}|V_{ps}|\mathbf{k}'\rangle = \frac{2\hbar^2\pi}{\mu V} \sum_l (2l+1) a_l^{2l+1} (k')^l k^l P_l(\hat{k}\cdot\hat{k}'). \tag{27}$$

For s-wave ($l=0$), we have

$$\langle \mathbf{k}|V_{ps}|\mathbf{k}'\rangle = \frac{2\hbar^2\pi}{\mu V} a_0. \tag{28}$$

For p-wave ($l=1$), we have

$$\langle \mathbf{k}|V_{ps}|\mathbf{k}'\rangle = \frac{6\hbar^2\pi}{\mu V} a_1^3 (\mathbf{k}\cdot\mathbf{k}'). \tag{29}$$

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,

$$
\begin{aligned}
H &= H_0 + H_1, \\
H_0 &= \sum_\alpha \int \mathrm{d}^3\mathbf{r}\, \psi_\alpha^\dagger(\mathbf{r}) \Big[-\frac{\hbar^2}{2m}\nabla^2 \Big] \psi_\alpha(\mathbf{r}), \\
H_1 &= \frac{1}{2}\sum_{\alpha\beta} \int \mathrm{d}^3\mathbf{r}_1 \mathrm{d}^3\mathbf{r}_2\, \psi_\alpha^\dagger(\mathbf{r}_1)\psi_\beta^\dagger(\mathbf{r}_2) V_{ps}^{\alpha\beta}(\mathbf{r}_1-\mathbf{r}_2)\psi_\beta(\mathbf{r}_2)\psi_\alpha(\mathbf{r}_1),
\end{aligned}
\tag{30}
$$

in which $V_{ps}^{\alpha\beta}(\mathbf{r}_1 - \mathbf{r}_2)$ is the pseudopotential for two-body interaction, α, β denote the internal levels of the particles, and we use $a_{\alpha\beta}$ ($b_{\alpha\beta}^3$) to denote the s-wave scattering length (p-wave scattering volume) between particles in internal level α and β.

In momentum space, the field operator can be expressed as

$$
\psi_\alpha(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}\alpha},
\tag{31}
$$

so the interaction term can be written as

$$
\begin{aligned}
H_1 &= \frac{1}{2V^2}\sum_{\alpha\beta}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} a_{\mathbf{k}_1\alpha}^\dagger a_{\mathbf{k}_2\beta}^\dagger a_{\mathbf{k}_3\beta} a_{\mathbf{k}_4\alpha} \int \mathrm{d}^3\mathbf{r}_1\mathrm{d}^3\mathbf{r}_2\, \mathrm{e}^{-i\mathbf{k}_1\cdot\mathbf{r}_1}\mathrm{e}^{-i\mathbf{k}_2\cdot\mathbf{r}_2} V_{ps}^{\alpha\beta}(\mathbf{r}_1-\mathbf{r}_2)\mathrm{e}^{i\mathbf{k}_3\cdot\mathbf{r}_2}\mathrm{e}^{i\mathbf{k}_4\cdot\mathbf{r}_1} \\
&= \frac{1}{2V^2}\sum_{\alpha\beta}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} a_{\mathbf{k}_1\alpha}^\dagger a_{\mathbf{k}_2\beta}^\dagger a_{\mathbf{k}_3\beta} a_{\mathbf{k}_4\alpha} \int \mathrm{d}^3\mathbf{R}\, \mathrm{e}^{-i(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)\cdot\mathbf{R}} \int \mathrm{d}^3\mathbf{r}\, \mathrm{e}^{-i\frac{\mathbf{k}_1-\mathbf{k}_2}{2}\cdot\mathbf{r}} V_{ps}^{\alpha\beta}(\mathbf{r}_1-\mathbf{r}_2)\mathrm{e}^{i\frac{\mathbf{k}_4-\mathbf{k}_3}{2}\cdot\mathbf{r}} \\
&= \frac{1}{2}\sum_{\alpha\beta}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} a_{\mathbf{k}_1\alpha}^\dagger a_{\mathbf{k}_2\beta}^\dagger a_{\mathbf{k}_3\beta} a_{\mathbf{k}_4\alpha} \Big\langle \frac{\mathbf{k}_1-\mathbf{k}_2}{2} \Big| V_{ps}^{\alpha\beta} \Big| \frac{\mathbf{k}_4-\mathbf{k}_3}{2} \Big\rangle \delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4},
\end{aligned}
\tag{32}
$$

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

$$
\begin{aligned}
H_1 &= \frac{1}{2}\sum_{\alpha\beta}\frac{4\pi\hbar^2 a_{\alpha\beta}}{mV}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} a_{\mathbf{k}_1\alpha}^\dagger a_{\mathbf{k}_2\beta}^\dagger a_{\mathbf{k}_3\beta} a_{\mathbf{k}_4\alpha}\, \delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4} \\
&= \frac{1}{2}\sum_{\alpha\beta}\frac{4\pi\hbar^2 a_{\alpha\beta}}{mV^2}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} a_{\mathbf{k}_1\alpha}^\dagger a_{\mathbf{k}_2\beta}^\dagger a_{\mathbf{k}_3\beta} a_{\mathbf{k}_4\alpha} \int \mathrm{d}^3\mathbf{r}\, \mathrm{e}^{-i(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)\cdot\mathbf{r}} \\
&= \frac{1}{2}\sum_{\alpha\beta}\frac{4\pi\hbar^2 a_{\alpha\beta}}{m}\int \mathrm{d}^3\mathbf{r}\, \psi_\alpha^\dagger(\mathbf{r})\psi_\beta^\dagger(\mathbf{r})\psi_\beta(\mathbf{r})\psi_\alpha(\mathbf{r}).
\end{aligned}
\tag{33}
$$

For p-wave interaction, plug in Eq. (29), we have

$$
\begin{aligned}
H_1 &= \frac{1}{2}\sum_{\alpha\beta}\frac{3\pi\hbar^2 b_{\alpha\beta}^3}{mV}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} a_{\mathbf{k}_1\alpha}^\dagger a_{\mathbf{k}_2\beta}^\dagger a_{\mathbf{k}_3\beta} a_{\mathbf{k}_4\alpha}[(\mathbf{k}_1-\mathbf{k}_2)\cdot(\mathbf{k}_4-\mathbf{k}_3)]\,\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4} \\
&= \frac{1}{2}\sum_{\alpha\beta}\frac{3\pi\hbar^2 b_{\alpha\beta}^3}{mV^2}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} a_{\mathbf{k}_1\alpha}^\dagger a_{\mathbf{k}_2\beta}^\dagger a_{\mathbf{k}_3\beta} a_{\mathbf{k}_4\alpha}\int \mathrm{d}^3\mathbf{r}\,[(\mathbf{k}_1-\mathbf{k}_2)\cdot(\mathbf{k}_4-\mathbf{k}_3)]\mathrm{e}^{-i(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)\cdot\mathbf{r}} \\
&= \frac{1}{2}\sum_{\alpha\beta}\frac{3\pi\hbar^2 b_{\alpha\beta}^3}{m}\int \mathrm{d}^3\mathbf{r}\,[(\nabla\psi_\alpha^\dagger)\psi_\beta^\dagger-\psi_\alpha^\dagger(\nabla\psi_\beta^\dagger)]\cdot[\psi_\beta(\nabla\psi_\alpha)-(\nabla\psi_\beta)\psi_\alpha].
\end{aligned}
\tag{34}
$$

In the derivation of s-wave and p-wave interaction above, we implicitly assume the field operators $\psi_\alpha(\mathbf{r})$ and $\psi_\alpha^\dagger(\mathbf{r})$ 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 $b_{gg}^3, b_{eg}^3, b_{ee}^3$ respectively). So the two-body interaction term H_1 takes the following form,

$$
\begin{aligned}
H_1 = &\frac{4\pi\hbar^2 a_{eg}}{m}\int \mathrm{d}^3\mathbf{r}\,\psi_e^\dagger(\mathbf{r})\psi_g^\dagger(\mathbf{r})\psi_g(\mathbf{r})\psi_e(\mathbf{r}) \\
&+\sum_{\alpha\beta}\frac{3\pi\hbar^2 b_{\alpha\beta}^3}{2m}\int \mathrm{d}^3\mathbf{r}\,[(\nabla\psi_\alpha^\dagger)\psi_\beta^\dagger-\psi_\alpha^\dagger(\nabla\psi_\beta^\dagger)]\cdot[\psi_\beta(\nabla\psi_\alpha)-(\nabla\psi_\beta)\psi_\alpha].
\end{aligned}
\tag{35}
$$

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[1] K. Huang and C. N. Yang, Phys. Rev. 105, 767 (1957).

[2] A. Derevianko, Phys. Rev. A 67, 033607 (2003).

[3] A. Derevianko, Phys. Rev. A 72, 044701 (2005).

[4] Z. Idziaszek and T. Calarco, Phys. Rev. Lett. 96, 013201 (2006).

[5] Z. Idziaszek, Phys. Rev. A 79, 062701 (2009).