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An in-depth study of spin- and momentum-dependent interaction potentials between two spin-1/2 fermions mediated by light spin-0 particles

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Abstract

We present a calculation by including the relativistic and off-shell contributions to the interaction potentials between two spin-1/2 fermions mediated by the exchange of light spin-0 particles, in both momentum and coordinate spaces. Our calculation is based on the four-point Green's function rather than the scattering amplitude. Among the sixteen potential components, eight that vanish in the non-relativistic limit are shown to acquire nonzero relativistic and off-shell corrections. In addition to providing relativistic and off-shell corrections to the operator basis commonly used in the literature, we introduce an alternative operator basis that facilitates the derivation of interaction potentials in the coordinate space. Furthermore, we calculate both the long-range and short-range components of the potentials, which can be useful for future experimental analyses at both macroscopic and atomic scales.

Keywords: axion, potential, relativistic correction

1. Introduction

In recent years, tabletop-scale laboratory experiments have emerged as a promising approach for exploring new physics phenomena beyond the Standard Model (BSM). These experiments are typically sensitive to long-range forces mediated by light BSM particles, such as axions, dilatons, and dark photons, etc [1]. Notably, precision measurements at atomic and macroscopic scales have begun to probe exotic spin- and velocity-dependent interaction potentials with high sensitivity [1–17]. Such studies provide valuable complementary constraints on BSM dynamics, in contrast to large-scale collider experiments..

The interaction potential of the two-body system offers not only a systematical theoretical frame to analyze various laboratory experiments, but also sets a convenient connection between the experimental constraints and the BSM theories. As the underlying objects of the laboratory measurements at both the atomic and macroscopic scales are basically electrons and nucleons, the interaction potentials arising from the light BSM particle exchanges between two spin-1/2 fermions have been the central focus since the pioneering work in [18], which calculated the long-range static spin-dependent potentials from the axion exchange. This formalism was extended in [2], which provides the complete sixteen components of the long-range spin-dependent potentials of the two fermions with the contributions from the spin-0 and spin-1 particles. In the former reference [2], a hybrid representation in the momentum and coordinate spaces is employed to describe the spin- and velocity-dependent interaction potentials. Namely the relative velocity $\boldsymbol{v}$ between the two fermions is treated more like a classical vector, instead of an operator as adopted in quantum theory. The hybrid representation of [2] is sufficient for the description of the macroscopic experiments, while for the atomic-scale phenomenon it is necessary to treat both coordinate $\boldsymbol{r}$ and momentum (or velocity) $\boldsymbol{p}$ as operators. Accordingly, the hybrid representation formalism is further developed in [7] with the emphasis on the application at the atomic scale. The two main improvements are made for this purpose [7]: on one hand the momentum $\boldsymbol{p}$ was promoted as an operator and the potentials are consistently derived in the coordinate space; on the other hand the short-distance effects, characterized by the $\delta(\boldsymbol{r})$ terms, are explicitly worked out and kept in the potentials. Although the latter terms accompanied by $\delta(\boldsymbol{r})$ are not very relevant in the macroscopic phenomenon, they could be crucial for the experiments at the atomic scale.

In this work, we introduce two main improvements over previous studies. First, we derive the relativistic and off-shell corrections to the two-fermion potentials mediated by spin-0 particles, using the Green's function rather than the scattering amplitude. While several potential components that vanish in the non-relativistic (NR) limit remain zero in the relativistic case, three terms pick up non-vanishing contributions from the relativistic corrections and seven terms receive contributions due to the off-shell effects. Second, different from the operator basis used in [2], we propose an alternative operator basis that is particularly useful for deriving potentials in a coordinate space. The short-distance effects, characterized by $\delta(\boldsymbol{r})$, are explicitly retained in our potentials. As a result, our potentials are applicable to both atomic-scale and macroscopic-scale experimental analyses.

This paper is structured as follows. The relativistic and off-shell corrections to the interaction potentials between two fermions mediated by the exchange of spin-0 particles in the momentum space are derived in detail in section 2. Both the results for the operator bases of [2] and ours are analyzed. In section 3, we take into account the newly calculated relativistic and off-shell effects to proceed the discussions in the coordinate space. A brief summary and conclusions are given in section 4.

2. Quasi-potential between two spin-1/2 fermions in momentum space

2.1. Potential in the hybrid representation [2]

We consider an elastic scattering process $1+2\to 3+4$ of two spin-1/2 fermions with four-momentum $p_{i=1,2,3,4}$, where particles 1 and 3 correspond to the same species, and particles 2 and 4 correspond to another same species, i.e., $m_1=m_3=m_a$ and $m_2=m_4=m_b$. In the special case when all the four particles are identical, one would have $m_a=m_b$. The potential of this process in momentum space, evaluated in the center-of-mass (CM) frame, is expressed as [2]

$$\overline{V}(\boldsymbol{q},\boldsymbol{P})=\mathcal{P}(\boldsymbol{q}^2)\sum_{i=1}^{16}\mathcal{O}_i^{\mathrm{I}}(\boldsymbol{q},\boldsymbol{P})f_i(\boldsymbol{q}^2,\boldsymbol{P}^2), \tag{1}$$

where $\boldsymbol{q}$ and $\boldsymbol{P}$ represent the spatial components of the four-momentum

$$q=p_3-p_1,\qquad P=\frac{1}{2}(p_1+p_3), \tag{2}$$

respectively. The function $\mathcal{P}(\boldsymbol{q}^2)$ denotes the denominator of the propagator for the exchanged boson

$$\mathcal{P}(\boldsymbol{q}^2)=-\frac{1}{\boldsymbol{q}^2+m_0^2}, \tag{3}$$

with m_0 the mass of the exchanged light spin-0 particle. The operators $\mathcal{O}_i^{\mathrm{I}}$ are given in equations (2.2) and (2.3) of [2], and for the sake of completeness we list their explicit expressions

$$\begin{aligned}
&\mathcal{O}_1^{\mathrm{I}}=1,\quad \mathcal{O}_2^{\mathrm{I}}=\boldsymbol{\sigma}^a\cdot\boldsymbol{\sigma}^b,\\
&\mathcal{O}_3^{\mathrm{I}}=\tfrac{1}{m_1^2}(\boldsymbol{\sigma}^a\cdot\boldsymbol{q})(\boldsymbol{\sigma}^b\cdot\boldsymbol{q}),\\
&\mathcal{O}_{4,5}^{\mathrm{I}}=\tfrac{\mathrm{i}}{2m_1^2}(\boldsymbol{\sigma}^a\pm\boldsymbol{\sigma}^b)\cdot(\boldsymbol{P}\times\boldsymbol{q}),\\
&\mathcal{O}_{6,7}^{\mathrm{I}}=\tfrac{\mathrm{i}}{2m_1^2}[(\boldsymbol{\sigma}^a\cdot\boldsymbol{P})(\boldsymbol{\sigma}^b\cdot\boldsymbol{q})\pm(\boldsymbol{\sigma}^a\cdot\boldsymbol{q})(\boldsymbol{\sigma}^b\cdot\boldsymbol{P})],\\
&\mathcal{O}_8^{\mathrm{I}}=\tfrac{1}{m_1^2}(\boldsymbol{\sigma}^a\cdot\boldsymbol{P})(\boldsymbol{\sigma}^b\cdot\boldsymbol{P}),
\end{aligned} \tag{4}$$

and

$$\begin{aligned}
\mathcal{O}_{9,10}^{\mathrm{I}}&=\tfrac{\mathrm{i}}{2m_1}(\boldsymbol{\sigma}^a\pm\boldsymbol{\sigma}^b)\cdot\boldsymbol{q},\\
\mathcal{O}_{11}^{\mathrm{I}}&=\tfrac{\mathrm{i}}{m_1}(\boldsymbol{\sigma}^a\times\boldsymbol{\sigma}^b)\cdot\boldsymbol{q},\\
\mathcal{O}_{12,13}^{\mathrm{I}}&=\tfrac{1}{2m_1}(\boldsymbol{\sigma}^a\pm\boldsymbol{\sigma}^b)\cdot\boldsymbol{P},\\
\mathcal{O}_{14}^{\mathrm{I}}&=\tfrac{1}{m_1}(\boldsymbol{\sigma}^a\times\boldsymbol{\sigma}^b)\cdot\boldsymbol{P},\\
\mathcal{O}_{15}^{\mathrm{I}}&=\tfrac{1}{2m_1^3}\{[\boldsymbol{\sigma}^a\cdot(\boldsymbol{P}\times\boldsymbol{q})](\boldsymbol{\sigma}^b\cdot\boldsymbol{q})\\
&\quad+(\boldsymbol{\sigma}^a\cdot\boldsymbol{q})[\boldsymbol{\sigma}^b\cdot(\boldsymbol{P}\times\boldsymbol{q})]\},\\
\mathcal{O}_{16}^{\mathrm{I}}&=\tfrac{\mathrm{i}}{2m_1^3}\{[\boldsymbol{\sigma}^a\cdot(\boldsymbol{P}\times\boldsymbol{q})](\boldsymbol{\sigma}^b\cdot\boldsymbol{P})\\
&\quad+(\boldsymbol{\sigma}^a\cdot\boldsymbol{P})[\boldsymbol{\sigma}^b\cdot(\boldsymbol{P}\times\boldsymbol{q})]\}.
\end{aligned} \tag{5}$$

Here, $\boldsymbol{\sigma}^{a/b}$ stands for the spin operator of the particle a / b. The operators of $\mathcal{O}_{1,\cdots,8}^{\mathrm{I}}$ are invariant under the parity transformation. In contrast, the operators of $\mathcal{O}_{9,\cdots,16}^{\mathrm{I}}$ change their signs under parity transformation. The operators of $\mathcal{O}_{1,2,3,9,10,11}^{\mathrm{I}}$, which are independent of $\boldsymbol{P}$, describe the static interaction potentials. While, the remaining operators that depend on $\boldsymbol{P}$, can describe the interaction potentials with non-vanishing relative velocity between the two fermions. The functions $f_i(\boldsymbol{q}^2,\boldsymbol{P}^2)$ in equation (1) are determined from the two-body elastic scattering amplitude. It should be noted that the labels of the momenta used here differ slightly from those in [2], and there is a sign difference between the functions f_i presented above and the functions f_i^{eN} in the former reference.

In [2], the potential is derived from the on-shell condition, leading to the following relations

$$p_i^0=E_i\equiv\sqrt{\boldsymbol{p}_i^2+m_i^2}\,. \tag{6}$$

Combining these on-shell relations with the four-momentum conservation condition $p_1+p_2=p_3+p_4$ and the three-momentum relations in the CM frame, i.e., $\boldsymbol{p}_1+\boldsymbol{p}_2=\boldsymbol{p}_3+\boldsymbol{p}_3=\boldsymbol{0}$, one gets the following equalities in the

CM frame

$$E_1 = E_3, \qquad E_2 = E_4, \qquad \boldsymbol{q}\cdot\boldsymbol{P} = 0\,. \tag{7}$$

As a result, only two independent variables, $\boldsymbol{P}^2$ and $\boldsymbol{q}^2$, remain in the potential. However, the relations in equation (7) do not hold any more for off-shell particles. Since the objective electrons or nucleons in the laboratory measurements are not totally free, the on-shell condition can only be considered as an approximation and we will explore the off-shell effects by releasing the on-shell relations in equation (7) later in this work.

For the exchange of a spin-0 boson ϕ between two types of fermions ψ_a and ψ_b, we consider the following general interaction Lagrangian [2, 18]

$$\mathcal{L}_\phi = -\phi\bar{\psi}_a(g_S^a + i\gamma_5 g_P^a)\psi_a - \phi\bar{\psi}_b(g_S^b + \mathrm{i}\gamma_5 g_P^b)\psi_b\,, \tag{8}$$

where $g_S^{a/b}$ and $g_P^{a/b}$ stand for the scalar and pseudoscalar types of couplings between the spin-0 boson ϕ and the fermion $\psi_{a/b}$, respectively.

For the electron-nucleon system, i.e., by taking $m_a = m_e$ and $m_b = m_N$, the following results are presented in equation (6.2) of [2]

$$\begin{aligned}
f_1^{eN}(0,0) &= -g_S^e g_S^N,\\
f_3^{eN}(0,0) &= -\frac{m_e}{4m_N} g_P^e g_P^N,\\
f_{4,5}^{eN}(0,0) &= -\frac{1}{4}\left(1 \pm \frac{m_e^2}{m_N^2}\right) g_S^e g_S^N,\\
f_{9,10}^{eN}(0,0) &= \frac{1}{2}\left(g_P^e g_S^N \mp g_S^e g_P^N \frac{m_e}{m_N}\right),\\
f_{15}^{eN}(0,0) &= \frac{m_e}{4m_N}\left(g_S^e g_P^N - g_P^e g_S^N \frac{m_e}{m_N}\right).
\end{aligned} \tag{9}$$

These formulas are obtained by taking the NR limit and the on-shell condition. Next, we generalize these results by including the relativistic and off-shell corrections.

2.2. Derivation of potential from Bethe–Salpeter equation

In principle, the quasi-potential in the Schrödinger-like equation is determined by the interaction kernel in the four-dimensional Bethe–Salpeter (BS) equation. Within this framework, the total four-momentum conservation holds, while the momenta of the incoming and outgoing particles may be defined as off-shell, indicating that $p_i^0 \neq E_i$. This can lead to $\boldsymbol{q}\cdot\boldsymbol{P} \neq 0$, comparing with the on-shell case in equation (7). Therefore one would expect that the interaction potentials should also contain additional terms with $\boldsymbol{q}\cdot\boldsymbol{P}$, which are however absent in [2] due to the assumption of on-shell condition.

In the CM frame, the exact quasi-potential for an elastic two-fermion scattering process $1 + 2 \to 3 + 4$, is derived as [19]

$$\begin{aligned}
&\chi_{\bar{i}}^\dagger(\lambda_3)\chi_{\bar{j}}^\dagger(\lambda_4)\overline{V}_{\bar{i}i,\bar{j}j}(\boldsymbol{q},\boldsymbol{P})\chi_i(\lambda_1)\chi_j(\lambda_2)\\
&\quad\equiv \mathrm{i}\widetilde{K}_{\lambda_3\lambda_1,\lambda_4\lambda_2}(\boldsymbol{q},\boldsymbol{P},\sqrt{s}),
\end{aligned} \tag{10}$$

where χ represents the Pauli spinor, λ_i denote the helicities and $s \equiv (p_1 + p_2)^2 = (E_1 + E_2)^2$. The expression for $\widetilde{K}_{\lambda_3\lambda_1,\lambda_4\lambda_2}(\boldsymbol{q},\boldsymbol{P},\sqrt{s})$ is given by

$$\begin{aligned}
\widetilde{K}_{\lambda_3\lambda_1,\lambda_4\lambda_2}(\boldsymbol{q},\boldsymbol{P},\sqrt{s}) \equiv\; & \frac{\bar{u}_{\bar{\alpha}}(\boldsymbol{p}_3, m_3, \lambda_3)\bar{u}_{\bar{\beta}}(\boldsymbol{p}_4, m_4, \lambda_4)}{\sqrt{4E_3E_4}}\\
&\times \bar{K}_{\bar{\alpha}\alpha,\bar{\beta}\beta}(\boldsymbol{q},\boldsymbol{P},\sqrt{s})\\
&\times \frac{u_\alpha(\boldsymbol{p}_1, m_1, \lambda_1)u_\beta(\boldsymbol{p}_2, m_2, \lambda_2)}{\sqrt{4E_1E_2}}\,,
\end{aligned}$$

where $u(\boldsymbol{p}_i, m_i, \lambda_i)$ is the Dirac spinor normalized as

$$\bar{u}(\boldsymbol{p}_i, m_i, \lambda_i)u(\boldsymbol{p}_i, m_i, \lambda_i) = 2m_i. \tag{11}$$

Additionally, $\bar{K}(\boldsymbol{q},\boldsymbol{P},\sqrt{s})$ is defined as

$$\begin{aligned}
\bar{K}(\boldsymbol{q},\boldsymbol{P},\sqrt{s}) &\equiv \bar{K}(q, P, p_1 + p_2)|_{p_1^0 = p_3^0 = \tau\sqrt{s}},\\
\bar{K} &\equiv [I - K_{\mathrm{BS}}(G_0 - \bar{G}_0)]^{-1}K_{\mathrm{BS}},
\end{aligned} \tag{12}$$

where $\tau \equiv \frac{m_1}{m_1 + m_2}$, I is the identity matrix, K_{BS} is the interaction kernel in the conventional four-dimensional BS equation, and

$$\begin{aligned}
G_0(p_1, p_2) &\equiv S_{full}^{(a)}(p_1, m_a)S_{full}^{(b)}(p_2, m_b),\\
\bar{G}_0(p_1, p_2, q) &\equiv 2\pi\,\mathrm{i}\,\delta(q^0)\left[\frac{\Lambda_+^{(a)}(\boldsymbol{p}_1)\Lambda_+^{(b)}(-\boldsymbol{p}_1)}{\sqrt{s} - E_1 - E_3} - \frac{\Lambda_-^{(a)}(\boldsymbol{p}_1)\Lambda_-^{(b)}(-\boldsymbol{p}_2)}{\sqrt{s} + E_1 + E_3}\right]\\
&\approx 2\pi\,\mathrm{i}\,\delta(q^0)\frac{\Lambda_+^{(a)}(\boldsymbol{p}_1)\Lambda_+^{(b)}(-\boldsymbol{p}_1)}{\sqrt{s} - E_1 - E_3}.
\end{aligned} \tag{13}$$

Here, $S_{full}^{(a,b)}$ are the full propagators of the particles 1 and 2 with masses m_a and m_b [20], respectively, and $\Lambda_\pm^{(a,b)}(\boldsymbol{k})$ are

$$\begin{aligned}
\Lambda_\pm^{(a,b)}(\boldsymbol{k}) &\equiv [E_{a,b}(\boldsymbol{k})\gamma^0 \mp (\boldsymbol{k}\cdot\vec{\gamma} - m_{a,b})]/2E_{a,b}(\boldsymbol{k}),\\
E_{a,b}(\boldsymbol{k}) &\equiv \sqrt{\boldsymbol{k}^2 + m_{a,b}^2}.
\end{aligned} \tag{14}$$

In the aforementioned CM frame, since both $\sqrt{s}$ and $p_{1,3}^0$ are fixed, three independent variables remain, which will be taken as $\boldsymbol{q}^2$, $\boldsymbol{P}^2$ and $\boldsymbol{q}\cdot\boldsymbol{P}$. The general potential in the momentum space can be then expressed as

$$\overline{V}(\boldsymbol{q},\boldsymbol{P}) = \mathcal{P}(\boldsymbol{q}^2)\sum_{i=1}^{16}\mathcal{O}_i^{\mathrm{I}}(\boldsymbol{q},\boldsymbol{P})f_i(\boldsymbol{q}^2,\boldsymbol{P}^2,\boldsymbol{q}\cdot\boldsymbol{P}). \tag{15}$$

At leading order (LO) in the couplings $g_{S,P}^{a,b}$, one has

$$\begin{aligned}
&\bar{K}_{\bar{\alpha}\alpha,\bar{\beta}\beta}(q, P, p_1 + p_2)|_{p_1^0 = p_3^0 = \tau\sqrt{s}}\\
&\approx K_{\mathrm{BS}}(q, P, p_1 + p_2)|_{p_1^0 = p_3^0 = \tau\sqrt{s}}\\
&= \mathrm{i}(g_S^a + \mathrm{i}g_P^a\gamma_5)_{\bar{\alpha}\alpha}(g_S^b + \mathrm{i}g_P^b\gamma_5)_{\bar{\beta}\beta}\mathcal{P}(\boldsymbol{q}^2)\,.
\end{aligned} \tag{16}$$

By utilizing these relations, the coefficients of the quasi-potential at LO in the couplings, accounting for the relativistic effects and the off-shell terms, can be written as follows:

$$
\begin{aligned}
f_1^{\rm full} &= -\tfrac{1}{16} g_S^a g_S^b F Y_1 Y_2,\\
f_2^{\rm full} &= g_S^a g_S^b F[\boldsymbol{P}^2\boldsymbol{q}^2 - (\boldsymbol{q}\cdot\boldsymbol{P})^2],\\
f_3^{\rm full} &= -g_S^a g_S^b F m_a^2 \boldsymbol{P}^2 - \tfrac{1}{4} g_P^a g_P^b F m_a^2 (X_1 + X_3)\\
&\quad \times (X_2 + X_4),\\
f_4^{\rm full} &= -\tfrac{1}{4} g_S^a g_S^b F m_a^2 (Y_1 + Y_2),\\
f_5^{\rm full} &= g_S^a g_S^b F m_a^2 (X_1X_3 - X_2X_4),\\
f_6^{\rm full} &= -2{\rm i} g_S^a g_S^b F m_a^2 (\boldsymbol{q}\cdot\boldsymbol{P}) + {\rm i} g_P^a g_P^b m_a^2 F\\
&\quad \times (E_1X_2 + E_2 m_a - E_3X_4 - E_4 m_a),\\
f_7^{\rm full} &= {\rm i} g_P^a g_P^b F m_a^2 (E_1X_4 - E_2X_3\\
&\quad - E_3 m_b + E_4 m_a),\\
f_8^{\rm full} &= -g_S^a g_S^b F m_a^2 \boldsymbol{q}^2 - g_P^a g_P^b F m_a^2 (E_1 - E_3)\\
&\quad \times (E_2 - E_4),
\end{aligned} \tag{17}
$$

and

$$
\begin{aligned}
f_9^{\rm full} &= -\tfrac{1}{8} g_S^a g_P^b F m_a (X_2 + X_4) Y_1\\
&\quad + \tfrac{1}{8} g_P^a g_S^b F m_a (X_1 + X_3) Y_2,\\
f_{10}^{\rm full} &= \tfrac{1}{8} g_S^a g_P^b F m_a (X_2 + X_4) Y_1\\
&\quad + \tfrac{1}{8} g_P^a g_S^b F m_a (X_1 + X_3) Y_2,\\
f_{11}^{\rm full} &= -\tfrac{1}{8} g_S^a g_P^b F m_a (E_2 - E_4) Y_1\\
&\quad + \tfrac{1}{8} g_P^a g_S^b F m_a (E_1 - E_3) Y_2,\\
f_{12}^{\rm full} &= \tfrac{1}{4}{\rm i} g_S^a g_P^b F m_a (E_2 - E_4) Y_1\\
&\quad + \tfrac{1}{4}{\rm i} g_P^a g_S^b F m_a (E_1 - E_3) Y_2,\\
f_{13}^{\rm full} &= \tfrac{1}{2} g_S^a g_P^b F m_a Z_1 + \tfrac{1}{2} g_P^a g_S^b F m_a Z_2,\\
f_{14}^{\rm full} &= -\tfrac{1}{4} g_S^a g_P^b F m_a Z_3 - \tfrac{1}{4} g_P^a g_S^b F m_a Z_4,\\
f_{15}^{\rm full} &= \tfrac{1}{2} g_S^a g_P^b F m_a^3 (X_2 + X_4)\\
&\quad - \tfrac{1}{2} g_P^a g_S^b F m_a^3 (X_1 + X_3),\\
f_{16}^{\rm full} &= -{\rm i} g_S^a g_P^b F m_a^3 (E_2 - E_4)\\
&\quad + {\rm i} g_P^a g_S^b F m_a^3 (E_1 - E_3),
\end{aligned} \tag{18}
$$

with

$$
\begin{aligned}
X_i &\equiv E_i + m_i,\\
F &\equiv \frac{1}{4\sqrt{X_1X_2X_3X_4E_1E_2E_3E_4}},\\
Y_1 &\equiv -4\boldsymbol{P}^2 + \boldsymbol{q}^2 + 4X_1X_3,\\
Y_2 &\equiv -4\boldsymbol{P}^2 + \boldsymbol{q}^2 + 4X_2X_4,\\
Z_1 &\equiv 2\boldsymbol{P}^2(E_2 - E_4) + \boldsymbol{q}\cdot\boldsymbol{P}(X_2 + X_4),\\
Z_2 &\equiv 2\boldsymbol{P}^2(E_1 - E_3) + \boldsymbol{q}\cdot\boldsymbol{P}(X_1 + X_3),\\
Z_3 &\equiv 2(E_2 - E_4)\boldsymbol{q}\cdot\boldsymbol{P} + \boldsymbol{q}^2(X_2 + X_4),\\
Z_4 &\equiv 2(E_1 - E_3)\boldsymbol{q}\cdot\boldsymbol{P} + \boldsymbol{q}^2(X_1 + X_3).
\end{aligned} \tag{19}
$$

We would like to note that the denominator of F is related to the factors we introduced in $\widetilde{K}_{\lambda_3\lambda_1,\lambda_4\lambda_2}(\boldsymbol{q}, \boldsymbol{P}, \sqrt{s})$ and is free of kinematic singularities in the regions we discuss.

To make an easy comparison with the results in the non-relativistic (NR) limit presented in [2], we expand the above coefficients in terms of the small momenta $\boldsymbol{P}$ and $\boldsymbol{q}$, while not imposing the on-shell conditions. Then the contributions can be separated into the on-shell (containing the constant, $\boldsymbol{q}^2$ and $\boldsymbol{P}^2$ factors) and off-shell (containing the $\boldsymbol{q}\cdot\boldsymbol{P}$ factor) parts

$$
\overline{V}(\boldsymbol{q}, \boldsymbol{P}) \to \overline{V}^{\rm I,NR} = \mathcal{P}(\boldsymbol{q}^2)\sum_{i=1}^{16}\mathcal{O}_i^{\rm I}(\boldsymbol{q}, \boldsymbol{P}) \times [f_{i,\rm on}^{\rm NR}(\boldsymbol{q}^2, \boldsymbol{P}^2) + f_{i,\rm off}^{\rm NR}(\boldsymbol{q}\cdot\boldsymbol{P})], \tag{20}
$$

where the nonzero on-shell terms read

$$
\begin{aligned}
f_{1,\rm on}^{\rm NR} &= -g_S^a g_S^b\left(1 - \frac{\boldsymbol{P}^2}{2m_a^2} - \frac{\boldsymbol{P}^2}{2m_b^2}\right),\\
f_{2,\rm on}^{\rm NR} &= g_S^a g_S^b \frac{\boldsymbol{P}^2\boldsymbol{q}^2}{16m_a^2m_b^2},\\
f_{3,\rm on}^{\rm NR} &= -g_S^a g_S^b \frac{\boldsymbol{P}^2}{16m_b^2} - g_P^a g_P^b\left(\frac{m_a}{4m_b} - \frac{m_a\boldsymbol{P}^2}{8m_b^3} - \frac{m_a\boldsymbol{q}^2}{32m_b^3}\right.\\
&\quad \left. - \frac{\boldsymbol{P}^2}{8m_am_b} - \frac{\boldsymbol{q}^2}{32m_am_b}\right),\\
f_{4,\rm on}^{\rm NR} &= -g_S^a g_S^b\left(\frac{1}{4} + \frac{m_a^2}{4m_b^2} - \frac{3m_a^2\boldsymbol{P}^2}{16m_b^4} - \frac{3m_a^2\boldsymbol{q}^2}{64m_b^4} - \frac{\boldsymbol{P}^2}{4m_b^2}\right.\\
&\quad \left. - \frac{3\boldsymbol{P}^2}{16m_a^2} - \frac{3\boldsymbol{q}^2}{64m_a^2}\right),\\
f_{5,\rm on}^{\rm NR} &= -g_S^a g_S^b\left(\frac{1}{4} - \frac{m_a^2}{4m_b^2} + \frac{3m_a^2\boldsymbol{P}^2}{16m_b^4} + \frac{3m_a^2\boldsymbol{q}^2}{64m_b^4}\right.\\
&\quad \left. - \frac{3\boldsymbol{P}^2}{16m_a^2} - \frac{3\boldsymbol{q}^2}{64m_a^2}\right),\\
f_{8,\rm on}^{\rm NR} &= -g_S^a g_S^b \frac{\boldsymbol{q}^2}{16m_b^2},\\
f_{9,\rm on}^{\rm NR} &= -g_S^a g_P^b\left(\frac{m_a}{2m_b} - \frac{m_a\boldsymbol{P}^2}{4m_b^3} - \frac{m_a\boldsymbol{q}^2}{16m_b^3} - \frac{\boldsymbol{P}^2}{4m_am_b}\right)\\
&\quad + g_P^a g_S^b\left(\frac{1}{2} - \frac{\boldsymbol{P}^2}{4m_a^2} - \frac{\boldsymbol{P}^2}{4m_b^2} - \frac{\boldsymbol{q}^2}{16m_a^2}\right),\\
f_{10,\rm on}^{\rm NR} &= g_S^a g_P^b\left(\frac{m_a}{2m_b} - \frac{m_a\boldsymbol{P}^2}{4m_b^3} - \frac{m_a\boldsymbol{q}^2}{16m_b^3} - \frac{\boldsymbol{P}^2}{4m_am_b}\right)\\
&\quad + g_P^a g_S^b\left(\frac{1}{2} - \frac{\boldsymbol{P}^2}{4m_a^2} - \frac{\boldsymbol{P}^2}{4m_b^2} - \frac{\boldsymbol{q}^2}{16m_a^2}\right),\\
f_{14,\rm on}^{\rm NR} &= -g_S^a g_P^b \frac{\boldsymbol{q}^2}{16m_am_b} - g_P^a g_S^b \frac{\boldsymbol{q}^2}{16m_b^2},\\
f_{15,\rm on}^{\rm NR} &= g_S^a g_P^b \frac{m_a}{8m_b} - g_P^a g_S^b \frac{m_a^2}{8m_b^2},
\end{aligned} \tag{21}
$$

and the nonzero off-shell terms are

$$
\begin{aligned}
f_{1,\rm off}^{\rm NR} &= g_S^a g_S^b\left(-\frac{5(\boldsymbol{q}\cdot\boldsymbol{P})^2}{32m_a^4} - \frac{5(\boldsymbol{q}\cdot\boldsymbol{P})^2}{32m_b^4}\right),\\
f_{2,\rm off}^{\rm NR} &= -g_S^a g_S^b \frac{(\boldsymbol{q}\cdot\boldsymbol{P})^2}{16m_a^2m_b^2},\\
f_{6,\rm off}^{\rm NR} &= -g_S^a g_S^b \frac{{\rm i}\boldsymbol{q}\cdot\boldsymbol{P}}{8m_b^2} + g_P^a g_P^b\left(-\frac{{\rm i}\boldsymbol{q}\cdot\boldsymbol{P}}{8m_am_b} - \frac{{\rm i}m_a\boldsymbol{q}\cdot\boldsymbol{P}}{8m_b^3}\right),\\
f_{7,\rm off}^{\rm NR} &= g_P^a g_P^b\left(\frac{{\rm i}m_a\boldsymbol{q}\cdot\boldsymbol{P}}{8m_b^3} - \frac{{\rm i}\boldsymbol{q}\cdot\boldsymbol{P}}{8m_am_b}\right),\\
f_{11,\rm off}^{\rm NR} &= g_S^a g_P^b \frac{m_a\boldsymbol{q}\cdot\boldsymbol{P}}{8m_b^3} - g_P^a g_S^b \frac{\boldsymbol{q}\cdot\boldsymbol{P}}{8m_a^2},\\
f_{12,\rm off}^{\rm NR} &= -g_S^a g_P^b \frac{{\rm i}m_a\boldsymbol{q}\cdot\boldsymbol{P}}{4m_b^3} - g_P^a g_S^b \frac{{\rm i}\boldsymbol{q}\cdot\boldsymbol{P}}{4m_a^2},\\
f_{13,\rm off}^{\rm NR} &= g_S^a g_P^b \frac{\boldsymbol{q}\cdot\boldsymbol{P}}{8m_am_b} + g_P^a g_S^b \frac{\boldsymbol{q}\cdot\boldsymbol{P}}{8m_a^2},
\end{aligned} \tag{22}
$$

with all other terms equal to zero. In the above expressions, most of the terms are expanded up to the next-leading order (NLO) with respect to the small momenta, except for $f^{\rm NR}_{2,\rm on}$, $f^{\rm NR}_{1,\rm off}$ and $f^{\rm NR}_{2,\rm off}$, which are expanded up to the next-to-next-leading-order (NNLO), because these latter three terms vanish at LO and NLO.

By neglecting the terms $\boldsymbol{P}^2$, $\boldsymbol{q}^2$ and $\boldsymbol{q}\cdot\boldsymbol{P}$, the above results in equations (21) and (22) reduce exactly to the formulas presented in [2], except for a global factor $\frac{1}{2}$ difference in f_{15}. The new contributions arising from the terms with $\boldsymbol{P}^2$ and $\boldsymbol{q}^2$ account for the NLO or NNLO relativistic contributions, in the meanwhile off-shell effects are also taken into account by the $\boldsymbol{q}\cdot\boldsymbol{P}$ terms.

We would like to clarify that the above discussion on the quasi-potential is based on the Lorentz covariant BS equation, analyzed order by order. At the LO of couplings, the only approximation used is the neglect of the positive part contributions in equation (13). In the literature, quasi-potentials are typically deduced by simply matching the physical scattering amplitudes in quantum field theory and quantum mechanics. It is important to note that these two methods are not exactly equivalent. Generally, they yield the same results at LO. However, at higher orders of three-momenta (and with specific orders of the coupling), one of the main differences between the two methods lies in how they handle the terms involving $\boldsymbol{q}\cdot\boldsymbol{P}$. These terms are exactly zero in the latter method, while they can be determined in a unique form by the former method. In this work, these off-shell terms are considered our accompanying results, and for completeness, we have conveniently retained them.

In the non-relativistic limit only the coefficients of the operators $\mathcal{O}^{\rm I}_{1,3,4,5,9,10,15}$, i.e., $f_{1,3,4,5,9,10,15}$, receive nonzero contributions from the interaction Lagrangian in equation (8) [2]. It is worthy noting that after imposing the on-shell condition the operators of $\mathcal{O}^{\rm I}_{8,14}$ acquire finite contributions at NLO in the non-relativistic expansion, and $\mathcal{O}^{\rm I}_{2}$ starts to receive finite contribution at NNLO. When retaining the off-shell effects, the operators of $\mathcal{O}^{\rm I}_{6,7,11,12,13}$, which vanish in the on-shell case, receive nonzero contributions that are proportional to $\boldsymbol{q}\cdot\boldsymbol{P}$. Therefore the physical systems that have nonzero matrix elements with $\mathcal{O}^{\rm I}_{6,7,11,12,13}$ could be sensitive to the off-shell effects.

For physical systems such as hydrogen atom, practical calculations for the matrix elements of these terms indicate that these terms may contribute nonzero values at higher orders. For example, when only considering the orbital part, one has

$$\left\langle n10\left|\frac{\boldsymbol{q}\cdot\boldsymbol{P}}{\mu^2(\boldsymbol{q}^2+m_0^2)}\right|n10\right\rangle=0,$$
$$\left\langle 210\left|\frac{\boldsymbol{q}\cdot\boldsymbol{P}}{\mu^2(\boldsymbol{q}^2+m_0^2)}\right|310\right\rangle=\frac{2\alpha_e^3\mu}{1875\pi}\ \text{when}\ m_0=0,\tag{23}$$

where n, l, 0 refer to the quantum numbers of the wave functions of hydrogen atom under Coulomb potential, and α_e denotes the fine-structure constant.

2.3. Potential in another form suitable for both momentum and coordinate spaces

As pointed out in [7], it is not straightforward to match the potential form of [2] into the coordinate space when promoting the momentum as an operator. It is noted that for atomic systems there is a simple recipe to overcome this issue by choosing proper kinematical variables. E.g., typically one could take $\boldsymbol{q}$ and $\boldsymbol{p}_1$ (the three-momentum of particle 1) [21], instead of $\boldsymbol{q}$ and $\boldsymbol{P}$, to conveniently relate the potentials in the momentum and coordinate spaces. Therefore we propose a different form to express the potential in momentum space as

$$\overline{V}(\boldsymbol{q},\boldsymbol{P})=\mathcal{P}(\boldsymbol{q}^2)\sum_{i=1}^{16}\mathcal{O}^{\rm II}_i(\boldsymbol{q},\boldsymbol{p}_1)g_i(\boldsymbol{q},\boldsymbol{p}_1),\tag{24}$$

where the three-momenta $\boldsymbol{p}_1$ and $\boldsymbol{q}$ are utilized. Here we introduce the superscript II for the operators $\mathcal{O}^{\rm II}_i$, in order to distinguish the operator basis of [2], labeled as $\mathcal{O}^{\rm I}_i$ in this work. The operator basis $\mathcal{O}^{\rm II}_i$ can be separated into three types, spin-independent, one-spine-dependent, and two-spine-dependent. The spin-independent and one-spin-dependent operators are chosen as

$$\begin{aligned}
\mathcal{O}^{\rm II}_1&\equiv 1,\\
\mathcal{O}^{\rm II}_2&\equiv \frac{\rm i}{\mu^2}\boldsymbol{\sigma}^a\cdot\boldsymbol{Q},\\
\mathcal{O}^{\rm II}_3&\equiv \frac{\rm i}{\mu^2}\boldsymbol{\sigma}^b\cdot\boldsymbol{Q},\\
\mathcal{O}^{\rm II}_4&\equiv \frac{\rm i}{\mu}\boldsymbol{\sigma}^a\cdot\boldsymbol{q},\\
\mathcal{O}^{\rm II}_5&\equiv \frac{\rm i}{\mu}\boldsymbol{\sigma}^b\cdot\boldsymbol{q},\\
\mathcal{O}^{\rm II}_6&\equiv \frac{\rm i}{\mu}\boldsymbol{\sigma}^a\cdot\boldsymbol{p}_1,\\
\mathcal{O}^{\rm II}_7&\equiv \frac{\rm i}{\mu}\boldsymbol{\sigma}^b\cdot\boldsymbol{p}_1,
\end{aligned}\tag{25}$$

and the two-spin-dependent operators are chosen as

$$\begin{aligned}
\mathcal{O}^{\rm II}_8&\equiv \boldsymbol{\sigma}^a\cdot\boldsymbol{\sigma}^b,\\
\mathcal{O}^{\rm II}_9&\equiv \frac{1}{\mu^2}\boldsymbol{\sigma}^a\cdot\boldsymbol{q}\boldsymbol{\sigma}^b\cdot\boldsymbol{q},\\
\mathcal{O}^{\rm II}_{10}&\equiv \frac{1}{\mu^2}\boldsymbol{\sigma}^a\cdot\boldsymbol{p}_1\boldsymbol{\sigma}^b\cdot\boldsymbol{q},\\
\mathcal{O}^{\rm II}_{11}&\equiv \frac{1}{\mu^2}\boldsymbol{\sigma}^a\cdot\boldsymbol{q}\boldsymbol{\sigma}^b\cdot\boldsymbol{p}_1,\\
\mathcal{O}^{\rm II}_{12}&\equiv \frac{1}{\mu^2}\boldsymbol{\sigma}^a\cdot\boldsymbol{p}_1\boldsymbol{\sigma}^b\cdot\boldsymbol{p}_1,\\
\mathcal{O}^{\rm II}_{13}&\equiv \frac{1}{\mu^3}\boldsymbol{\sigma}^a\cdot\boldsymbol{Q}\boldsymbol{\sigma}^b\cdot\boldsymbol{q},\\
\mathcal{O}^{\rm II}_{14}&\equiv \frac{1}{\mu^3}\boldsymbol{\sigma}^a\cdot\boldsymbol{Q}\boldsymbol{\sigma}^b\cdot\boldsymbol{p}_1,\\
\mathcal{O}^{\rm II}_{15}&\equiv \frac{1}{\mu}(\boldsymbol{\sigma}^a\times\boldsymbol{\sigma}^b)\cdot\boldsymbol{q},\\
\mathcal{O}^{\rm II}_{16}&\equiv \frac{1}{\mu}(\boldsymbol{\sigma}^a\times\boldsymbol{\sigma}^b)\cdot\boldsymbol{p}_1,
\end{aligned}\tag{26}$$

with $\mu\equiv\frac{m_a m_b}{m_a+m_b}$ and $\boldsymbol{Q}\equiv\boldsymbol{q}\times\boldsymbol{p}_1$. In principle, one could also construct additional forms for the operators, such as

$$\begin{aligned}
\mathcal{O}^{\rm II}_{17}&\equiv \frac{1}{\mu^3}\boldsymbol{\sigma}^a\cdot\boldsymbol{q}\boldsymbol{\sigma}^b\cdot\boldsymbol{Q},\\
\mathcal{O}^{\rm II}_{18}&\equiv \frac{1}{\mu^3}\boldsymbol{\sigma}^a\cdot\boldsymbol{p}_1\boldsymbol{\sigma}^b\cdot\boldsymbol{Q},
\end{aligned}\tag{27}$$

which are however not independent from the above sixteen terms due to the following relations

$$\mathcal{O}_{17}^{\rm II}=\mathcal{O}_{13}^{\rm II}+\frac{1}{\mu^2}\boldsymbol{q}\cdot\boldsymbol{p}_1\,\mathcal{O}_{15}^{\rm II}-\frac{1}{\mu^2}\boldsymbol{q}^2\mathcal{O}_{16}^{\rm II},$$
$$\mathcal{O}_{18}^{\rm II}=\mathcal{O}_{14}^{\rm II}+\frac{1}{\mu^2}\boldsymbol{p}_1^2\,\mathcal{O}_{15}^{\rm II}-\frac{1}{\mu^2}\boldsymbol{q}\cdot\boldsymbol{p}_1\,\mathcal{O}_{16}^{\rm II}. \quad (28)$$

Unlike the organization rule of the operators in equations (4) and (5) as adopted in [2], we take a different strategy to classify the operators into two groups in equations (25) and (26). Except for the identity operator $\mathcal{O}_1^{\rm II}$, the other operators in equation (25) contain one spin, which can be used to describe the system with one polarized object. For the operators in equation (26), they all involve two spins, which can be used to describe the physical system with two polarized objects. The operators of $\mathcal{O}_{1,2,3,8,9,10,11,12}^{\rm II}$ are parity-conserving ones. In contrast, the operators of $\mathcal{O}_{4,5,6,7,13,14,15,16}^{\rm II}$ parity-odd.

Similar to the calculation in the last subsection, the coefficients g_i of the quasi-potential (24) at the LO of couplings and with the full relativistic and off-shell effects, can be expressed as

$$\begin{aligned}
g_1^{\rm full}&=-g_S^a g_S^b F(X_1X_3-\boldsymbol{p}_1^2-\boldsymbol{q}\cdot\boldsymbol{p}_1)\\
&\quad\times(X_2X_4-\boldsymbol{p}_1^2-\boldsymbol{q}\cdot\boldsymbol{p}_1),\\
g_2^{\rm full}&=g_S^a g_S^b F\mu^2(X_2X_4-\boldsymbol{p}_1^2-\boldsymbol{q}\cdot\boldsymbol{p}_1),\\
g_3^{\rm full}&=g_S^a g_S^b F\mu^2(X_1X_3-\boldsymbol{p}_1^2-\boldsymbol{q}\cdot\boldsymbol{p}_1),\\
g_4^{\rm full}&=g_P^a g_S^b F\mu X_1(X_2X_4-\boldsymbol{p}_1^2-\boldsymbol{q}\cdot\boldsymbol{p}_1),\\
g_5^{\rm full}&=-g_S^a g_P^b F\mu X_2(X_1X_3-\boldsymbol{p}_1^2-\boldsymbol{q}\cdot\boldsymbol{p}_1),\\
g_6^{\rm full}&=g_P^a g_S^b F\mu(E_1-E_3)(X_2X_4-\boldsymbol{p}_1^2-\boldsymbol{q}\cdot\boldsymbol{p}_1),\\
g_7^{\rm full}&=-g_S^a g_P^b F\mu(E_2-E_4)(X_1X_3-\boldsymbol{p}_1^2-\boldsymbol{q}\cdot\boldsymbol{p}_1),\\
g_8^{\rm full}&=g_S^a g_S^b F[\boldsymbol{p}_1^2\boldsymbol{q}^2-(\boldsymbol{q}\cdot\boldsymbol{p}_1)^2],
\end{aligned} \quad (29)$$

and

$$\begin{aligned}
g_9^{\rm full}&=-g_P^a g_P^b F\mu^2X_1X_2\\
&\quad-g_S^a g_S^b F\mu^2\boldsymbol{p}_1^2,\\
g_{10}^{\rm full}&=g_S^a g_S^b F\mu^2\boldsymbol{q}\cdot\boldsymbol{p}_1\\
&\quad-g_P^a g_P^b F\mu^2X_2(E_1-E_3),\\
g_{11}^{\rm full}&=g_S^a g_S^b F\mu^2\boldsymbol{q}\cdot\boldsymbol{p}_1\\
&\quad-g_P^a g_P^b F\mu^2X_1(E_2-E_4),\\
g_{12}^{\rm full}&=-g_S^a g_S^b F\mu^2\boldsymbol{q}^2\\
&\quad-g_P^a g_P^b F\mu^2(E_1-E_3)(E_2-E_4),\\
g_{13}^{\rm full}&=-g_S^a g_P^b F\mu^3X_2+g_P^a g_S^b F\mu^3X_1,\\
g_{14}^{\rm full}&=-g_S^a g_P^b F\mu^3(E_2-E_4)\\
&\quad+g_P^a g_S^b F\mu^3(E_1-E_3),\\
g_{15}^{\rm full}&=g_P^a g_S^b F\mu[(E_1-E_3)\boldsymbol{p}_1^2\\
&\quad+X_1\boldsymbol{q}\cdot\boldsymbol{p}_1],\\
g_{16}^{\rm full}&=-g_P^a g_S^b F\mu\\
&\quad\times[(E_1-E_3)\boldsymbol{q}\cdot\boldsymbol{p}_1+X_1\boldsymbol{q}^2].
\end{aligned} \quad (30)$$

After expanding these coefficients in terms of the small three-momenta $\boldsymbol{p}_1$ and $\boldsymbol{q}$, we obtain

$$V(\boldsymbol{q},\boldsymbol{p}_1)\to V^{\rm II,NR}=\mathcal{P}(\boldsymbol{q}^2)\sum_{i=1}^{16}\mathcal{O}_i^{\rm II}(\boldsymbol{q},\boldsymbol{p}_1)g_i^{\rm NR}(\boldsymbol{q},\boldsymbol{p}_1), \quad (31)$$

where the coefficients of the NR potential are given by

$$\begin{aligned}
g_1^{\rm NR}&=-g_S^a g_S^b\left(1-\frac{4\boldsymbol{p}_1^2+\boldsymbol{q}^2+4\boldsymbol{q}\cdot\boldsymbol{p}_1}{8m_a^2}-\frac{4\boldsymbol{p}_1^2+\boldsymbol{q}^2+4\boldsymbol{q}\cdot\boldsymbol{p}_1}{8m_b^2}\right),\\
g_2^{\rm NR}&=g_S^a g_S^b\mu^2\left(\frac{1}{4m_a^2}-\frac{4\boldsymbol{p}_1^2+\boldsymbol{q}^2+4\boldsymbol{q}\cdot\boldsymbol{p}_1}{32m_a^2m_b^2}-\frac{6\boldsymbol{p}_1^2+3\boldsymbol{q}^2+6\boldsymbol{q}\cdot\boldsymbol{p}_1}{32m_a^4}\right),\\
g_3^{\rm NR}&=g_S^a g_S^b\mu^2\left(\frac{1}{4m_b^2}-\frac{4\boldsymbol{p}_1^2+\boldsymbol{q}^2+4\boldsymbol{q}\cdot\boldsymbol{p}_1}{32m_a^2m_b^2}-\frac{6\boldsymbol{p}_1^2+3\boldsymbol{q}^2+6\boldsymbol{q}\cdot\boldsymbol{p}_1}{32m_b^4}\right),\\
g_4^{\rm NR}&=g_P^a g_S^b\mu\left(\frac{1}{2m_a}-\frac{4\boldsymbol{p}_1^2+\boldsymbol{q}^2+4\boldsymbol{q}\cdot\boldsymbol{p}_1}{16m_am_b^2}-\frac{4\boldsymbol{p}_1^2+3\boldsymbol{q}^2+6\boldsymbol{q}\cdot\boldsymbol{p}_1}{16m_a^3}\right),\\
g_5^{\rm NR}&=-g_S^a g_P^b\mu\left(\frac{1}{2m_b}-\frac{4\boldsymbol{p}_1^2+\boldsymbol{q}^2+4\boldsymbol{q}\cdot\boldsymbol{p}_1}{16m_a^2m_b}-\frac{4\boldsymbol{p}_1^2+3\boldsymbol{q}^2+6\boldsymbol{q}\cdot\boldsymbol{p}_1}{16m_b^3}\right),\\
g_6^{\rm NR}&=-g_P^a g_S^b\mu\frac{\boldsymbol{q}^2+2\boldsymbol{q}\cdot\boldsymbol{p}_1}{8m_a^3},\\
g_7^{\rm NR}&=g_S^a g_P^b\mu\frac{\boldsymbol{q}^2+2\boldsymbol{q}\cdot\boldsymbol{p}_1}{8m_b^3},\\
g_8^{\rm NR}&=0,
\end{aligned} \quad (32)$$

and

$$\begin{aligned}
g_9^{\rm NR}&=-g_P^a g_P^b\frac{\mu^2}{4m_am_b}\left(1-\frac{4\boldsymbol{p}_1^2+3\boldsymbol{q}^2+6\boldsymbol{q}\cdot\boldsymbol{p}_1}{8m_a^2}\right.\\
&\quad\left.-\frac{4\boldsymbol{p}_1^2+3\boldsymbol{q}^2+6\boldsymbol{q}\cdot\boldsymbol{p}_1}{8m_b^2}\right)-g_S^a g_S^b\mu^2\frac{\boldsymbol{p}_1^2}{16m_a^2m_b^2},\\
g_{10}^{\rm NR}&=g_S^a g_S^b\mu^2\frac{\boldsymbol{q}\cdot\boldsymbol{p}_1}{16m_a^2m_b^2}+g_P^a g_P^b\mu^2\frac{\boldsymbol{q}^2+2\boldsymbol{q}\cdot\boldsymbol{p}_1}{16m_a^3m_b},\\
g_{11}^{\rm NR}&=g_S^a g_S^b\mu^2\frac{\boldsymbol{q}\cdot\boldsymbol{p}_1}{16m_a^2m_b^2}+g_P^a g_P^b\mu^2\frac{\boldsymbol{q}^2+2\boldsymbol{q}\cdot\boldsymbol{p}_1}{16m_am_b^3},\\
g_{12}^{\rm NR}&=-g_S^a g_S^b\mu^2\frac{\boldsymbol{q}^2}{16m_a^2m_b^2},\\
g_{13}^{\rm NR}&=-g_S^a g_P^b\mu^3\left(\frac{1}{8m_a^2m_b}-\frac{6\boldsymbol{p}_1^2+3\boldsymbol{q}^2+6\boldsymbol{q}\cdot\boldsymbol{p}_1}{64m_a^4m_b}\right.\\
&\quad\left.-\frac{4\boldsymbol{p}_1^2+3\boldsymbol{q}^2+6\boldsymbol{q}\cdot\boldsymbol{p}_1}{64m_a^2m_b^3}\right)\\
&\quad+g_P^a g_S^b\mu^3\left(\frac{1}{8m_am_b^2}-\frac{4\boldsymbol{p}_1^2+3\boldsymbol{q}^2+6\boldsymbol{q}\cdot\boldsymbol{p}_1}{64m_a^3m_b^2}\right.\\
&\quad\left.-\frac{6\boldsymbol{p}_1^2+3\boldsymbol{q}^2+6\boldsymbol{q}\cdot\boldsymbol{p}_1}{64m_am_b^4}\right),\\
g_{14}^{\rm NR}&=g_S^a g_P^b\mu^3\frac{\boldsymbol{q}^2+2\boldsymbol{q}\cdot\boldsymbol{p}_1}{32m_a^2m_b^3}-g_P^a g_S^b\mu^3\frac{\boldsymbol{q}^2+2\boldsymbol{q}\cdot\boldsymbol{p}_1}{32m_a^3m_b^2},\\
g_{15}^{\rm NR}&=\frac{g_P^a g_S^b\mu\boldsymbol{q}\cdot\boldsymbol{p}_1}{8m_am_b^2},\\
g_{16}^{\rm NR}&=-\frac{g_P^a g_S^b\mu\boldsymbol{q}^2}{8m_am_b^2}.
\end{aligned} \quad (33)$$

We would like to mention that the on-shell conditions are not applied in the above calculation, namely the off-shell effects are kept in the results of equations (32) and (33). By imposing the on-shell condition, one will get

$$\boldsymbol{q}\cdot\boldsymbol{p}_1 = -\tfrac{1}{2}\boldsymbol{q}^2, \tag{34}$$

and the potential can then take a different form when higher-order contributions are considered.

3. Non-relativistic potential in the coordinate space

Although it is straightforward to calculate the relativistic potential in the momentum space, such as those in equations (29) and (30), there is still no viable way to get its counterpart in the coordinate space. In contrast, the NR potential in coordinate space can be derived by performing the standard Fourier transformation. For the LO NR potential, the effects of the long-range part have been discussed in [2, 7, 22], and the effects of the short-range part are analyzed in [7, 22]. To make a direct comparison with the potential in [2], we will first revisit the long-range part of $\overline{V}^{\mathrm{I,NR}}$ as discussed in the former reference. As an improvement, the higher-order contributions from the full relativistic and off-shell effects will be taken into account. More importantly, we will also perform Fourier transformation of the potentials in the new basis introduced in section 2.3 and derive their expressions in the coordinate space by simultaneously keeping the short-range and long-range parts.

3.1. Long-range potential in coordinate space for the hybrid representation

In [2], the variable $\boldsymbol{P}/m_a$ in the long-range potential part of $\overline{V}^{\mathrm{I,NR}}$ (20) is interpreted as the classical velocity, which remains unaffected by the Fourier transformation with respect to $\boldsymbol{q}$. Meanwhile, the former reference only focuses on the long-range potential between two macroscopic objects, in which the short-range parts are not so relevant.

It is mentioned that most of the $\boldsymbol{q}^2$ terms in equation (21), except the one in f_2 (otherwise it will vanish), will be neglected when performing the Fourier transformation in the study of the hybrid representation. This is a valid approximation for a large class of models, since after the Fourier transformation $\boldsymbol{q}^2$ gives a factor of m_0^2/m_a^2, which is strongly suppressed due to the tiny mass m_0 of the exchanged spin-0 particle. Furthermore, since $\boldsymbol{P}/m_a$ is considered to be a classic velocity, instead of an operator, the spin- and $\boldsymbol{r}$-dependent structures for the on-shell parts of the potentials in coordinate space will remain the same with the LO ones as given in [2]. The relativistic corrections manifest in some global factors related to the velocity squared. While, for the off-shell parts, different structures with spin and $\boldsymbol{r}$ dependences will appear.

The explicit expressions in the coordinate space can be obtained via the Fourier transformation

$$\begin{aligned} V^{\mathrm{I,NR}}(\boldsymbol{r},\boldsymbol{P}) &\equiv \int \frac{\mathrm{d}^3\boldsymbol{q}}{(2\pi)^3}\overline{V}^{\mathrm{I,NR}}(\boldsymbol{q},\boldsymbol{P})\mathrm{e}^{\,\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \\ &\equiv \sum V_i^{\mathrm{I,NR}} \\ &\equiv \sum V_{i,\mathrm{on}}^{\mathrm{I,NR}} + V_{i,\mathrm{off}}^{\mathrm{I,NR}}. \end{aligned} \tag{35}$$

Utilizing the properties of Fourier transformation delineated in Appendix B, one can match from the corresponding potentials of equation (20) in momentum space to the forms in the coordinate space, and the terms with relativistic corrections that survive in the on-shell condition are found to be

$$\begin{aligned} V_{1,\mathrm{on}}^{\mathrm{I,NR}} &= -g_S^a g_S^b\left[1-\frac{\boldsymbol{P}^2}{2m_a^2}-\frac{\boldsymbol{P}^2}{2m_b^2}\right]V_0, \\ V_{2,\mathrm{on}}^{\mathrm{I,NR}} &= -\boldsymbol{\sigma}^a\cdot\boldsymbol{\sigma}^b g_S^a g_S^b\frac{m_0^2\boldsymbol{P}^2}{16m_a^2m_b^2r}V_0, \\ V_{3,\mathrm{on}}^{\mathrm{I,NR}} &= [\boldsymbol{\sigma}^a\cdot\boldsymbol{\sigma}^b C_1-(\boldsymbol{\sigma}^a\cdot\bar{\boldsymbol{r}})(\boldsymbol{\sigma}^b\cdot\bar{\boldsymbol{r}})C_2] \\ &\quad\times\left[-g_S^a g_S^b\frac{\boldsymbol{P}^2}{16m_b^2}+g_P^a g_P^b\left(-\frac{m_a}{4m_b}+\frac{m_a\boldsymbol{P}^2}{8m_b^3}\right.\right. \\ &\quad\left.\left.+\frac{\boldsymbol{P}^2}{8m_am_b}\right)\right]\frac{1}{m_a^2r^2}V_0, \\ V_{4,\mathrm{on}}^{\mathrm{I,NR}} &= (\boldsymbol{\sigma}^a+\boldsymbol{\sigma}^b)\cdot(\boldsymbol{P}\times\bar{\boldsymbol{r}})g_S^a g_S^b\left(\frac{1}{4}+\frac{m_a^2}{4m_b^2}\right. \\ &\quad\left.-\frac{3m_a^2\boldsymbol{P}^2}{16m_b^4}-\frac{\boldsymbol{P}^2}{4m_b^2}-\frac{3\boldsymbol{P}^2}{16m_a^2}\right)\frac{C_1}{2m_a^2r}V_0, \\ V_{5,\mathrm{on}}^{\mathrm{I,NR}} &= -(\boldsymbol{\sigma}^a-\boldsymbol{\sigma}^b)\cdot(\boldsymbol{P}\times\bar{\boldsymbol{r}})g_S^a g_S^b\left(\frac{1}{4}-\frac{m_a^2}{4m_b^2}\right. \\ &\quad\left.+\frac{3m_a^2\boldsymbol{P}^2}{16m_b^4}-\frac{3\boldsymbol{P}^2}{16m_a^2}\right)\frac{C_1}{2m_a^2r}V_0, \\ V_{8,\mathrm{on}}^{\mathrm{I,NR}} &= (\boldsymbol{\sigma}^a\cdot\boldsymbol{P})(\boldsymbol{\sigma}^b\cdot\boldsymbol{P})g_S^a g_S^b\frac{m_0^2}{16m_a^2m_b^2r}V_0, \\ V_{9,\mathrm{on}}^{\mathrm{I,NR}} &= (\boldsymbol{\sigma}^a+\boldsymbol{\sigma}^b)\cdot\bar{\boldsymbol{r}}\left[g_S^a g_P^b\left(\frac{m_a}{2m_b}-\frac{m_a\boldsymbol{P}^2}{4m_b^3}\right.\right. \\ &\quad\left.\left.-\frac{\boldsymbol{P}^2}{4m_am_b}\right)-g_P^a g_S^b\left(\frac{1}{2}-\frac{\boldsymbol{P}^2}{4m_a^2}-\frac{\boldsymbol{P}^2}{4m_b^2}\right)\right]\frac{C_1}{2m_ar}V_0, \\ V_{10,\mathrm{on}}^{\mathrm{I,NR}} &= (\boldsymbol{\sigma}^a-\boldsymbol{\sigma}^b)\cdot\bar{\boldsymbol{r}}\left[g_S^a g_P^b\left(\frac{m_a}{2m_b}-\frac{m_a\boldsymbol{P}^2}{4m_b^3}\right.\right. \\ &\quad\left.\left.-\frac{\boldsymbol{P}^2}{4m_am_b}\right)+g_P^a g_S^b\left(\frac{1}{2}-\frac{\boldsymbol{P}^2}{4m_a^2}-\frac{\boldsymbol{P}^2}{4m_b^2}\right)\right]\frac{C_1}{2m_ar}V_0, \\ V_{14,\mathrm{on}}^{\mathrm{I,NR}} &= -(\boldsymbol{\sigma}^a\times\boldsymbol{\sigma}^b)\cdot\boldsymbol{P}(g_S^a g_P^b m_b+g_P^a g_S^b m_a) \\ &\quad\times\frac{m_0^2}{16m_a^2m_b^2r}V_0, \\ V_{15,\mathrm{on}}^{\mathrm{I,NR}} &= -[\boldsymbol{\sigma}^a\cdot(\boldsymbol{P}\times\bar{\boldsymbol{r}})\boldsymbol{\sigma}^b\cdot\bar{\boldsymbol{r}}+\boldsymbol{\sigma}^a\cdot\bar{\boldsymbol{r}}\boldsymbol{\sigma}^b\cdot(\boldsymbol{P}\times\bar{\boldsymbol{r}})] \\ &\quad\times\left(g_S^a g_P^b\frac{m_a}{8m_b}-g_P^a g_S^b\frac{m_a^2}{8m_b^2}\right)\frac{1}{2m_a^3r^2}C_2V_0, \end{aligned} \tag{36}$$

and the terms contributed by the off-shell effects are given by

$$\begin{aligned}
V_{1,\mathrm{off}}^{\mathrm{I,NR}} &= \frac{5g_S^a g_S^b(m_a^4+m_b^4)}{32m_a^4m_b^4r^2}[C_1\boldsymbol{P}^2 - C_2(\boldsymbol{P}\cdot\bar{\boldsymbol{r}})^2]V_0,\\
V_{2,\mathrm{off}}^{\mathrm{I,NR}} &= -\boldsymbol{\sigma}^a\cdot\boldsymbol{\sigma}^b\frac{g_S^a g_S^b}{16m_a^2m_b^2r^2}[C_1\boldsymbol{P}^2 - C_2(\boldsymbol{P}\cdot\bar{\boldsymbol{r}})^2]V_0,\\
V_{6,\mathrm{off}}^{\mathrm{I,NR}} &= [2C_1\boldsymbol{\sigma}^a\cdot\boldsymbol{P}\boldsymbol{\sigma}\cdot\boldsymbol{P} - C_2\boldsymbol{P}\cdot\bar{\boldsymbol{r}}(\boldsymbol{\sigma}^a\cdot\bar{\boldsymbol{r}}\boldsymbol{\sigma}^b\cdot\boldsymbol{P}\\
&\quad + \boldsymbol{\sigma}^a\cdot\boldsymbol{P}\boldsymbol{\sigma}^b\cdot\bar{\boldsymbol{r}})]\frac{g_S^a g_S^b m_a m_b + g_P^a g_P^b(m_a^2+m_b^2)}{16m_a^3m_b^3r^2}V_0,\\
V_{7,\mathrm{off}}^{\mathrm{I,NR}} &= (\boldsymbol{\sigma}^a\cdot\boldsymbol{P}\boldsymbol{\sigma}^b\cdot\bar{\boldsymbol{r}} - \boldsymbol{\sigma}^a\cdot\bar{\boldsymbol{r}}\boldsymbol{\sigma}^b\cdot\boldsymbol{P})\\
&\quad\times\frac{g_P^a g_P^b(m_a^2-m_b^2)}{16m_a^3m_b^3r^2}C_2\boldsymbol{P}\cdot\bar{\boldsymbol{r}}V_0,\\
V_{11,\mathrm{off}}^{\mathrm{I,NR}} &= (\boldsymbol{\sigma}^a\cdot\boldsymbol{P} + \boldsymbol{\sigma}^b\cdot\boldsymbol{P})\frac{-g_S^a g_P^b m_a^3 + g_P^a g_S^b m_b^3}{8m_a^3m_b^3r}C_1\boldsymbol{P}\cdot\bar{\boldsymbol{r}}V_0,\\
V_{12,\mathrm{off}}^{\mathrm{I,NR}} &= (\boldsymbol{\sigma}^a\cdot\boldsymbol{P} - \boldsymbol{\sigma}^b\cdot\boldsymbol{P})\frac{g_S^a g_P^b m_a^3 + g_P^a g_S^b m_b^3}{8m_a^3m_b^3r}C_1\boldsymbol{P}\cdot\bar{\boldsymbol{r}}V_0,\\
V_{13,\mathrm{off}}^{\mathrm{I,NR}} &= [C_2\boldsymbol{P}\cdot\bar{\boldsymbol{r}}(\boldsymbol{\sigma}^a\times\boldsymbol{\sigma}^b)\cdot\bar{\boldsymbol{r}} - C_1(\boldsymbol{\sigma}^a\times\boldsymbol{\sigma}^b)\cdot\boldsymbol{P}]\\
&\quad\times\frac{g_S^a g_P^b m_b + g_P^a g_S^b m_a}{16m_a^2m_b^2r^2}V_0,
\end{aligned}\tag{37}$$

with $r\equiv|\boldsymbol{r}|$, $\bar{\boldsymbol{r}}=\boldsymbol{r}/r$ and

$$\begin{aligned}
V_0 &\equiv \frac{1}{4\pi r}\mathrm{e}^{-m_0 r},\\
C_1 &= m_0 r + 1,\\
C_2 &= m_0^2r^2 + 3m_0 r + 3.
\end{aligned}\tag{38}$$

By neglecting the higher-order contributions featured by the $\boldsymbol{P}^2$ and $\boldsymbol{P}\cdot\bar{\boldsymbol{r}}$ terms in the aforementioned expressions, we can exactly recover the results presented in equations (3.6, 3.8, 4.6, and 4.7) of [2], with the exception of a global factor of $\frac{1}{2}$ in V_{15} that already exists in the momentum space. It is noticed that eight terms, $V_{2,6,7,8,11,12,13,14}^{\mathrm{I}}$, which are zero at LO [2], receive non-vanishing higher-order contributions from the relativistic and off-shell effects. It is also interesting to point out that the NLO and NNLO corrections are absent for V_{15}, though it receives contribution at LO. In contrast, contributions that depend on the square of the velocity emerge for the other potentials. These new contributions may provide further insights for laboratory experiments, enabling more comprehensive analyses.

3.2. NR potential in coordinate space for the new operator basis

In the study of [2], the variable $\boldsymbol{P}/m_a$ is simply interpreted as the velocity. Strictly speaking, for the Hamiltonian of a two-particle system in coordinate space, $\hat{\boldsymbol{p}}_1$ represents the momentum operator $-\mathrm{i}\frac{\partial}{\partial\boldsymbol{r}}$, with $\boldsymbol{r}$ the relative position vector pointing from particle 1 to particle 2, and $\langle\hat{\boldsymbol{p}}_1\rangle/m_1$ corresponds to the velocity of particle 1. Furthermore, in the Fourier transformation, the operator $\hat{\boldsymbol{p}}_1$ in potentials in the coordinate space should be placed at the far right of the expressions [21]. Since $\boldsymbol{P}$ is a mixture of $\boldsymbol{p}_1$ and $\boldsymbol{q}$, the operator $\hat{\boldsymbol{P}}$ can not be positioned freely in the coordinate space. Therefore, the optimal approach is to use $\boldsymbol{p}_1$ and $\boldsymbol{q}$ as variables, instead of $\boldsymbol{q}$ and $\boldsymbol{P}$ as proposed in [2], to express the potential in momentum space and then transfer them to coordinate space. When discussing both the short-range and long-range potentials for the atomic systems, the counterpart of the terms with $\boldsymbol{q}\cdot\boldsymbol{p}_1$ in momentum space will be retained in our calculation when performing the Fourier transformation. The potential in the coordinate space is written as

$$\begin{aligned}
V(\boldsymbol{r},\hat{\boldsymbol{p}}_1) \to V^{\mathrm{III,NR}} &\equiv \sum_{i=1}^{16}V_i^{\mathrm{III,NR}}\\
&\equiv \sum_{i=1}^{16}\mathcal{O}_i^{\mathrm{III}}(\boldsymbol{r},\hat{\boldsymbol{p}}_1)h_i^{\mathrm{NR}}(\boldsymbol{r},\hat{\boldsymbol{p}}_1),
\end{aligned}\tag{39}$$

where the operator basis of $\mathcal{O}_i^{\mathrm{III}}(\boldsymbol{r},\hat{\boldsymbol{p}}_1)$ has one-to-one correspondence with $\mathcal{O}_i^{\mathrm{II}}$ in equations (25) and (26). The spin-independent and one-spin-dependent operators are

$$\begin{aligned}
&\mathcal{O}_1^{\mathrm{III}} \equiv 1,\\
&\mathcal{O}_2^{\mathrm{III}} \equiv \frac{1}{\mu}\boldsymbol{\sigma}^a\cdot\hat{\boldsymbol{L}},\ \mathcal{O}_3^{\mathrm{III}} \equiv \frac{1}{\mu}\boldsymbol{\sigma}^b\cdot\hat{\boldsymbol{L}},\\
&\mathcal{O}_4^{\mathrm{III}} \equiv \boldsymbol{\sigma}^a\cdot\bar{\boldsymbol{r}},\ \mathcal{O}_5^{\mathrm{III}} \equiv \boldsymbol{\sigma}^b\cdot\bar{\boldsymbol{r}},\\
&\mathcal{O}_6^{\mathrm{III}} \equiv \frac{\mathrm{i}}{\mu}\boldsymbol{\sigma}^a\cdot\hat{\boldsymbol{p}}_1,\ \mathcal{O}_7^{\mathrm{III}} \equiv \frac{\mathrm{i}}{\mu}\boldsymbol{\sigma}^b\cdot\hat{\boldsymbol{p}}_1,
\end{aligned}\tag{40}$$

and the two-spin-dependent operators are

$$\begin{aligned}
&\mathcal{O}_8^{\mathrm{III}} \equiv \boldsymbol{\sigma}^a\cdot\boldsymbol{\sigma}^b,\\
&\mathcal{O}_9^{\mathrm{III}} \equiv \boldsymbol{\sigma}^a\cdot\bar{\boldsymbol{r}}\boldsymbol{\sigma}^b\cdot\bar{\boldsymbol{r}},\\
&\mathcal{O}_{10}^{\mathrm{III}} \equiv \frac{\mathrm{i}}{\mu}\boldsymbol{\sigma}^b\cdot\bar{\boldsymbol{r}}\boldsymbol{\sigma}^a\cdot\hat{\boldsymbol{p}}_1,\\
&\mathcal{O}_{11}^{\mathrm{III}} \equiv \frac{\mathrm{i}}{\mu}\boldsymbol{\sigma}^a\cdot\bar{\boldsymbol{r}}\boldsymbol{\sigma}^b\cdot\hat{\boldsymbol{p}}_1,\\
&\mathcal{O}_{12}^{\mathrm{III}} \equiv \frac{1}{\mu^2}\boldsymbol{\sigma}^a\cdot\hat{\boldsymbol{p}}_1\boldsymbol{\sigma}^b\cdot\hat{\boldsymbol{p}}_1,\\
&\mathcal{O}_{13}^{\mathrm{III}} \equiv \frac{1}{\mu}\boldsymbol{\sigma}^a\cdot\hat{\boldsymbol{L}}\boldsymbol{\sigma}^b\cdot\bar{\boldsymbol{r}},\\
&\mathcal{O}_{14}^{\mathrm{III}} \equiv \frac{\mathrm{i}}{\mu^2}\boldsymbol{\sigma}^a\cdot\hat{\boldsymbol{L}}\boldsymbol{\sigma}^b\cdot\hat{\boldsymbol{p}}_1,\\
&\mathcal{O}_{15}^{\mathrm{III}} \equiv (\boldsymbol{\sigma}^a\times\boldsymbol{\sigma}^b)\cdot\bar{\boldsymbol{r}},\\
&\mathcal{O}_{16}^{\mathrm{III}} \equiv \frac{1}{\mu}(\boldsymbol{\sigma}^a\times\boldsymbol{\sigma}^b)\cdot\hat{\boldsymbol{p}}_1\ ,
\end{aligned}\tag{41}$$

with $\hat{\boldsymbol{L}}\equiv\boldsymbol{r}\times\hat{\boldsymbol{p}}_1$. We clarify that the operator $\hat{\boldsymbol{p}}_1$ in the potential is understood to operate solely on the wave function and does not act on r or $\bar{\boldsymbol{r}}$ in the potential. The coefficients $h_i^{\mathrm{NR}}(\boldsymbol{r},\hat{\boldsymbol{p}}_1)$ in equation (39) can be decomposed as

$$\begin{aligned}
h_i^{\mathrm{NR}}(\boldsymbol{r},\hat{\boldsymbol{p}}_1) &\equiv h_{i,1}^{\mathrm{NR}} + h_{i,2}^{\mathrm{NR}}\hat{\boldsymbol{p}}_1^2 + \mathrm{i}h_{i,3}^{\mathrm{NR}}\bar{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}}_1\\
&\quad + \pi\delta^3(\bar{\boldsymbol{r}})(h_{i,4}^{\mathrm{NR}} + h_{i,5}^{\mathrm{NR}}\hat{\boldsymbol{p}}_1^2 + \mathrm{i}h_{i,6}^{\mathrm{NR}}\bar{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}}_1),
\end{aligned}\tag{42}$$

where $h_{i,j}^{\mathrm{NR}}$ are only dependent on r, whose expressions are presented in Appendix A.

Employing equations (39–42) and the expressions for $h_{i,j}^{\mathrm{NR}}$ in Appendix A, one can readily derive the potential in the forms utilized in [7, 22]. As an illustrative example, upon expanding the coefficients $h_{i,j}^{\mathrm{NR}}$ in terms of a joint expansion of $1/m_a$ and $1/m_b$ to second order, one obtains

$$\begin{aligned} V_{pp} = & -\frac{g_P^a g_P^b W}{4 m_a m_b r^3}\{\mathcal{O}_8^{\rm III}[C_1 - 4\pi r^3\delta^3(\boldsymbol{r})] \\ & - \mathcal{O}_9^{\rm III}[C_2 - 16\pi r^3\delta^3(\boldsymbol{r})] \\ & - \mathcal{O}_{12}^{\rm III}\frac{m_a^2+m_b^2}{2(m_a+m_b)^2}[C_1 - 4\pi r^3\delta^3(\boldsymbol{r})]\} \\ = & -\frac{g_P^a g_P^b W}{4 m_a m_b r^3}\{\mathcal{O}_8^{\rm III}[C_1 + \frac{4\pi}{3} r^3\delta^3(\boldsymbol{r})] \\ & - \mathcal{O}_9^{\rm III} C_2 - \mathcal{O}_{12}^{\rm III}\frac{m_a^2+m_b^2}{2(m_a+m_b)^2}[C_1 - 4\pi r^3\delta^3(\boldsymbol{r})]\}, \end{aligned} \quad (43)$$

wherein the relations in equation (B.5) has been used. In equation (43), the first two terms are identical to those presented in equation (3) of [22], while the third term is new and corresponds to the NLO relativistic contribution. Analogously, we further derive other types of potentials contributed by different combinations of $g_S^{(a,b)}$ and $g_P^{(a,b)}$ couplings:

$$\begin{aligned} V_{ss} = & -g_S^a g_S^b W\{\mathcal{O}_1^{\rm III}\Big[\frac{1}{r} \\ & + \frac{(m_a^2+m_b^2)[-4\mathrm{i}C_1\bar{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}}_1 - 4r\hat{\boldsymbol{p}}_1^2 - 4\pi r^2\delta^3(\boldsymbol{r}) + m_0^2 r]}{8 m_a^2 m_b^2 r^2}\Big] \\ & + \mathcal{O}_2^{\rm III}\frac{\mu C_1}{4 m_a^2 r^2} + \mathcal{O}_3^{\rm III}\frac{\mu C_1}{4 m_b^2 r^2} + \mathcal{O}_{12}^{\rm III} \\ & \times \frac{\mu^2[C_1 - C_2 - 12\pi r^3\delta^3(\boldsymbol{r})]}{16 m_a^2 m_b^2 r^3}\}, \\ V_{sp} = & g_S^a g_P^b W\{\mathcal{O}_5^{\rm III}\frac{C_1}{2 m_b r^2} + \mathcal{O}_7^{\rm III} \\ & \times \Big[\frac{\mu[2\mathrm{i}C_1 m_a^2 r\bar{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}}_1 + 2C_1 m_b^2 + (6C_1 - C_2)m_a^2]}{8 m_a^2 m_b^3 r^3} \\ & - \frac{\pi\mu(m_a^2+m_b^2)\delta^3(\boldsymbol{r})}{m_a^2 m_b^3}\Big] \\ & + \mathcal{O}_{13}^{\rm III}\frac{\mu[C_2 - 16\pi r^3\delta^3(\boldsymbol{r})]}{8 m_a^2 m_b r^3} \\ & - \mathcal{O}_{16}^{\rm III}\frac{\mu[C_1 - 4\pi r^3\delta^3(\boldsymbol{r})]}{8 m_a^2 m_b r^3}\}, \\ V_{ps} = & -g_P^a g_S^b W\{\mathcal{O}_4^{\rm III}\frac{C_1}{2 m_a r^2} + \mathcal{O}_6^{\rm III} \\ & \times \Big[\frac{\mu[2\mathrm{i}C_1 m_b^2 r\bar{\boldsymbol{r}}\cdot\hat{\boldsymbol{p}}_1 + 2C_1 m_a^2 + (6C_1 - C_2)m_b^2]}{8 m_a^3 m_b^2 r^3} \\ & - \frac{\pi\mu(m_a^2+m_b^2)\delta^3(\boldsymbol{r})}{m_a^3 m_b^2}\Big] \\ & + \mathcal{O}_{13}^{\rm III}\frac{\mu[C_2 - 16\pi r^3\delta^3(\boldsymbol{r})]}{8 m_a m_b^2 r^3} \\ & + \mathcal{O}_{16}^{\rm III}\frac{\mu[C_1 - C_2 + 12\pi r^3\delta^3(\boldsymbol{r})]}{8 m_a m_b^2 r^3}\}. \end{aligned} \quad (44)$$

The newly calculated potentials in equation (44) and the updated one in equation (43) are ready for use to conduct the laboratory experimental analyses in future.

4. Summary

In this study, we carry out an in-depth calculation of the interaction potentials with spin-0 particle exchange between two spin-$1/2$ fermions. Our calculation is based on the framework of Bethe–Salpeter equation, in conjunction with scattering amplitude analysis. Relativistic contributions and off-shell effects are carefully taken into account. The potentials in both momentum- and coordinate-space representations are calculated. The on-shell results at LO in the non-relativistic expansion in our study coincide with those reported in [2], with the exception of a global factor $\frac{1}{2}$ in $V_{15}^{\rm I}$. It is found that several terms in the potential receive non-vanishing corrections from the relativistic and off-shell contributions.

Apart from the revised calculation along the line of [2], we propose a different operator basis to construct the interaction potential, in order to conveniently calculate the potential in the coordinate space. Both relativistic and off-shell effects are included to derive the interaction potentials with the new operator basis in the momentum and coordinate spaces. These NLO relativistic corrections are generally much smaller than the LO contributions. However, we naively expect that experimental systems involving high-speed objects may still receive contributions. Furthermore, certain types of potentials that are zero at LO but nonzero at NLO suggest that experimental datasets should be analyzed carefully.

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Appendix A Expressions for $h_{i,j}^{\rm NR}$

In this Appendix, we list the expressions for $h_{i,j}^{\rm NR}$ defined in equation (42). The coefficients $h_{1,j}^{\rm NR}$ take the form

$$\begin{aligned} h_{1,1}^{\rm NR} &= -g_S^a g_S^b\frac{m_0^2(m_a^2+m_b^2) + 8m_a^2 m_b^2}{8 m_a^2 m_b^2 r}, \\ h_{1,2}^{\rm NR} &= g_S^a g_S^b\frac{m_a^2+m_b^2}{2m_a^2 m_b^2 r}, \\ h_{1,3}^{\rm NR} &= g_S^a g_S^b\frac{(m_a^2+m_b^2)C_1}{2m_a^2 m_b^2 r^2}, \\ h_{1,4}^{\rm NR} &= g_S^a g_S^b\frac{m_a^2+m_b^2}{2m_a^2 m_b^2}, \\ h_{1,5}^{\rm NR} &= 0, \\ h_{1,6}^{\rm NR} &= 0. \end{aligned} \quad (A.1)$$

The coefficients $h_{2,j}^{\rm NR}$ are given by

$$\begin{aligned} h_{2,1}^{\rm NR} &= -g_S^a g_S^b\frac{\mu[m_0^2(m_a^2+3m_b^2) + 8m_a^2 m_b^2]C_1}{32 m_a^4 m_b^2 r^2}, \\ h_{2,2}^{\rm NR} &= g_S^a g_S^b\frac{\mu(2m_a^2+3m_b^2)C_1}{16 m_a^4 m_b^2 r^2}, \\ h_{2,3}^{\rm NR} &= g_S^a g_S^b\frac{\mu(2m_a^2+3m_b^2)C_2}{16 m_a^4 m_b^2 r^3}, \\ h_{2,4}^{\rm NR} &= g_S^a g_S^b\frac{3\mu(m_a^2+3m_b^2)}{8 m_a^4 m_b^2 r}, \\ h_{2,5}^{\rm NR} &= 0, \\ h_{2,6}^{\rm NR} &= -g_S^a g_S^b\frac{\mu(2m_a^2+3m_b^2)}{m_a^4 m_b^2}. \end{aligned} \quad (A.2)$$

The coefficients $h_{3,j}^{\mathrm{NR}}$ are given by

$$\begin{aligned}
h_{3,1}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{S}}^{b} \frac{\mu[m_0^2(3m_a^2+m_b^2)+8m_a^2m_b^2]C_1}{32m_a^2m_b^4r^2},\\
h_{3,2}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{S}}^{b} \frac{\mu(3m_a^2+2m_b^2)C_1}{16m_a^2m_b^4r^2},\\
h_{3,3}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{S}}^{b} \frac{\mu(3m_a^2+2m_b^2)C_2}{16m_a^2m_b^4r^3},\\
h_{3,4}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{S}}^{b} \frac{3\mu(3m_a^2+m_b^2)}{8m_a^2m_b^4r},\\
h_{3,5}^{\mathrm{NR}} &= 0,\\
h_{3,6}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{S}}^{b} \frac{\mu(3m_a^2+2m_b^2)}{m_a^2m_b^4}.
\end{aligned} \tag{A.3}$$

The coefficients $h_{4,j}^{\mathrm{NR}}$ are given by

$$\begin{aligned}
h_{4,1}^{\mathrm{NR}} &= -g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{[m_0^2(m_a^2+3m_b^2)+8m_a^2m_b^2]C_1}{16m_a^3m_b^2r^2},\\
h_{4,2}^{\mathrm{NR}} &= g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{(m_a^2+m_b^2)C_1}{4m_a^3m_b^2r^2},\\
h_{4,3}^{\mathrm{NR}} &= g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{(2m_a^2+3m_b^2)C_2}{8m_a^3m_b^2r^3},\\
h_{4,4}^{\mathrm{NR}} &= g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{3(m_a^2+3m_b^2)}{4m_a^3m_b^2r},\\
h_{4,5}^{\mathrm{NR}} &= 0,\\
h_{4,6}^{\mathrm{NR}} &= -g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{2(2m_a^2+3m_b^2)}{m_a^3m_b^2}.
\end{aligned} \tag{A.4}$$

The coefficients $h_{5,j}^{\mathrm{NR}}$ are given by

$$\begin{aligned}
h_{5,1}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{[m_0^2(3m_a^2+m_b^2)+8m_a^2m_b^2]C_1}{16m_a^2m_b^3r^2},\\
h_{5,2}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{(m_a^2+m_b^2)C_1}{4m_a^2m_b^3r^2},\\
h_{5,3}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{(3m_a^2+2m_b^2)C_2}{8m_a^2m_b^3r^3},\\
h_{5,4}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{3(3m_a^2+m_b^2)}{4m_a^2m_b^3r},\\
h_{5,5}^{\mathrm{NR}} &= 0,\\
h_{5,6}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{(4m_b^2+6m_a^2)}{m_b^3m_a^2}.
\end{aligned} \tag{A.5}$$

The coefficients $h_{6,j}^{\mathrm{NR}}$ are written as

$$\begin{aligned}
h_{6,1}^{\mathrm{NR}} &= -g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{\mu[2m_a^2C_1+m_b^2(-m_0^2r^2+3m_0r+3)]}{8m_a^3m_b^2r^3},\\
h_{6,2}^{\mathrm{NR}} &= 0,\\
h_{6,3}^{\mathrm{NR}} &= -g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{\mu C_1}{4m_a^3r^2},\\
h_{6,4}^{\mathrm{NR}} &= g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{\mu(m_a^2+m_b^2)}{m_a^3m_b^2},\\
h_{6,5}^{\mathrm{NR}} &= 0,\\
h_{6,6}^{\mathrm{NR}} &= 0.
\end{aligned} \tag{A.6}$$

The coefficients $h_{7,j}^{\mathrm{NR}}$ are given by

$$\begin{aligned}
h_{7,1}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{\mu[m_a^2(m_0^2r^2-3m_0r-3)-2m_b^2C_1]}{8m_a^2m_b^3r^3},\\
h_{7,2}^{\mathrm{NR}} &= 0,\\
h_{7,3}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{\mu C_1}{4m_b^3r^2},\\
h_{7,4}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{\mu(m_a^2+m_b^2)}{m_a^2m_b^3},\\
h_{7,5}^{\mathrm{NR}} &= 0,\\
h_{7,6}^{\mathrm{NR}} &= 0.
\end{aligned} \tag{A.7}$$

The coefficients $h_{8,j}^{\mathrm{NR}}$ are given by

$$\begin{aligned}
h_{8,1}^{\mathrm{NR}} &= -g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{(3m_0^2(m_a^2+m_b^2)+8m_a^2m_b^2)C_1}{32m_a^3m_b^3r^3},\\
h_{8,2}^{\mathrm{NR}} &= -\frac{g_{\mathrm{S}}^{a} g_{\mathrm{S}}^{b} C_1}{16m_a^2m_b^2r^3} + g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{(m_a^2+m_b^2)C_1}{8m_a^3m_b^3r^3},\\
h_{8,3}^{\mathrm{NR}} &= g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{3(m_a^2+m_b^2)C_2}{16m_a^3m_b^3r^4},\\
h_{8,4}^{\mathrm{NR}} &= g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{m_a^2(3m_0^2r^2+8m_b^2r^2+9)+3m_b^2(m_0^2r^2+3)}{8m_a^3m_b^3r^2},\\
h_{8,5}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{S}}^{b} \frac{1}{4m_a^2m_b^2} - g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{m_a^2+m_b^2}{2m_a^3m_b^3},\\
h_{8,6}^{\mathrm{NR}} &= -g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{3(m_a^2+m_b^2)}{m_a^3m_b^3r}.
\end{aligned} \tag{A.8}$$

The coefficients $h_{9,j}^{\mathrm{NR}}$ are given by

$$\begin{aligned}
h_{9,1}^{\mathrm{NR}} &= g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{[3m_0^2(m_a^2+m_b^2)+8m_a^2m_b^2]C_2}{32m_a^3m_b^3r^3},\\
h_{9,2}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{S}}^{b} \frac{C_2}{16m_a^2m_b^2r^3} - g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{(m_a^2+m_b^2)C_2}{8m_a^3m_b^3r^3},\\
h_{9,3}^{\mathrm{NR}} &= -g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{3(m_a^2+m_b^2)(m_0^3r^3+6m_0^2r^2+15m_0r+15)}{16m_a^3m_b^3r^4},\\
h_{9,4}^{\mathrm{NR}} &= -g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{m_a^2(12m_0^2r^2+32m_b^2r^2+45)+3m_b^2(4m_0^2r^2+15)}{8m_a^3m_b^3r^2},\\
h_{9,5}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{S}}^{b} \frac{1}{m_a^2m_b^2} + g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{2(m_a^2+m_b^2)}{m_a^3m_b^3},\\
h_{9,6}^{\mathrm{NR}} &= g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{69(m_a^2+m_b^2)}{4m_a^3m_b^3r}.
\end{aligned} \tag{A.9}$$

The coefficients $h_{10,j}^{\mathrm{NR}}$ are given by

$$\begin{aligned}
h_{10,1}^{\mathrm{NR}} &= g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{\mu[3m_a^2C_2+m_b^2(-m_0^3r^3+2m_0^2r^2+9m_0r+9)]}{16m_a^3m_b^3r^4},\\
h_{10,2}^{\mathrm{NR}} &= 0,\\
h_{10,3}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{S}}^{b} \frac{\mu C_2}{16m_a^2m_b^2r^3} + g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{\mu C_2}{8m_a^3m_br^3},\\
h_{10,4}^{\mathrm{NR}} &= -g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{3\mu(4m_a^2+3m_b^2)}{4m_a^3m_b^3r},\\
h_{10,5}^{\mathrm{NR}} &= 0,\\
h_{10,6}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{S}}^{b} \frac{\mu}{m_a^2m_b^2} - g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{2\mu}{m_a^3m_b}.
\end{aligned} \tag{A.10}$$

The coefficients $h_{11,j}^{\mathrm{NR}}$ are given by

$$\begin{aligned}
h_{11,1}^{\mathrm{NR}} &= -g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{\mu[m_a^2(m_0^3r^3 - 2m_0^2r^2 - 9m_0r - 9) - 3m_b^2C_2]}{16m_a^3m_b^3r^4},\\
h_{11,2}^{\mathrm{NR}} &= 0,\\
h_{11,3}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{S}}^{b} \frac{\mu C_2}{16m_a^2m_b^2r^3} + g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{\mu C_2}{8m_am_b^3r^3},\\
h_{11,4}^{\mathrm{NR}} &= -g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{3\mu(3m_a^2 + 4m_b^2)}{4m_a^3m_b^3r},\\
h_{11,5}^{\mathrm{NR}} &= 0,\\
h_{11,6}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{S}}^{b} \frac{\mu}{m_a^2m_b^2} - g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{2\mu}{m_am_b^3}.
\end{aligned} \tag{A.11}$$

The coefficients $h_{12,j}^{\mathrm{NR}}$ are given by

$$\begin{aligned}
h_{12,1}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{S}}^{b} \frac{\mu^2(m_0^2r^2 + 2m_0r + 2)}{16m_a^2m_b^2r^3} + g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{\mu^2(m_a^2 + m_b^2)C_1}{8m_a^3m_b^3r^3},\\
h_{12,2}^{\mathrm{NR}} &= 0,\\
h_{12,3}^{\mathrm{NR}} &= 0,\\
h_{12,4}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{S}}^{b} \frac{3\mu^2}{4m_a^2m_b^2} - g_{\mathrm{P}}^{a} g_{\mathrm{P}}^{b} \frac{\mu^2(m_a^2 + m_b^2)}{2m_a^3m_b^3},\\
h_{12,5}^{\mathrm{NR}} &= 0,\\
h_{12,6}^{\mathrm{NR}} &= 0.
\end{aligned} \tag{A.12}$$

The coefficients $h_{13,j}^{\mathrm{NR}}$ are given by

$$\begin{aligned}
h_{13,1}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{\mu[3m_0^2(m_a^2 + m_b^2) + 8m_a^2m_b^2]C_2}{64m_a^4m_b^3r^3}\\
&\quad - g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{\mu[3m_0^2(m_a^2 + m_b^2) + 8m_a^2m_b^2]C_2}{64m_a^3m_b^4r^3},\\
h_{13,2}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{\mu(2m_a^2 + 3m_b^2)C_2}{32m_a^4m_b^3r^3} + g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{\mu(3m_a^2 + 2m_b^2)C_2}{32m_a^3m_b^4r^3},\\
h_{13,3}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{3\mu(m_a^2 + m_b^2)(m_0^3r^3 + 6m_0^2r^2 + 15m_0r + 15)}{32m_a^4m_b^3r^4}\\
&\quad + g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{3\mu(m_a^2 + m_b^2)(m_0^3r^3 + 6m_0^2r^2 + 15m_0r + 15)}{32m_a^3m_b^4r^4},\\
h_{13,4}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{\mu[m_a^2(12m_0^2r^2 + 32m_b^2r^2 + 45) + 3m_b^2(4m_0^2r^2 + 15)]}{16m_a^4m_b^3r^2}\\
&\quad + g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{\mu[m_a^2(12m_0^2r^2 + 32m_b^2r^2 + 45) + 3m_b^2(4m_0^2r^2 + 15)]}{16m_a^3m_b^4r^2},\\
h_{13,5}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{\mu(2m_a^2 + 3m_b^2)}{2m_a^4m_b^3} - g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{\mu(3m_a^2 + 2m_b^2)}{2m_a^3m_b^4},\\
h_{13,6}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{69\mu(m_a^2 + m_b^2)}{8m_a^4m_b^3r} - g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{69\mu(m_a^2 + m_b^2)}{8m_a^3m_b^4r}.
\end{aligned} \tag{A.13}$$

The coefficients $h_{14,j}^{\mathrm{NR}}$ are given by

$$\begin{aligned}
h_{14,1}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{\mu^2[m_a^2(m_0^3r^3 - 2m_0^2r^2 - 9m_0r - 9) - 3m_b^2C_2]}{32m_a^4m_b^3r^4}\\
&\quad - g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{\mu^2[3m_a^2C_2 + m_b^2(-m_0^3r^3 + 2m_0^2r^2 + 9m_0r + 9)]}{32m_a^3m_b^4r^4},\\
h_{14,2}^{\mathrm{NR}} &= 0,\\
h_{14,3}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{\mu^2C_2}{16m_a^2m_b^3r^3} - g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{\mu^2C_2}{16m_a^3m_b^2r^3},\\
h_{14,4} &= -g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{3\mu^2(3m_a^2 + 4m_b^2)}{8m_a^4m_b^3r} + g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{3\mu^2(4m_a^2 + 3m_b^2)}{8m_a^3m_b^4r},\\
h_{14,5}^{\mathrm{NR}} &= 0,\\
h_{14,6}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{\mu^2}{m_a^2m_b^3} + g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{\mu^2}{m_a^3m_b^2}.
\end{aligned} \tag{A.14}$$

The coefficients $h_{15,j}^{\mathrm{NR}}$ are given by

$$\begin{aligned}
h_{15,1}^{\mathrm{NR}} &= 0,\\
h_{15,2}^{\mathrm{NR}} &= 0,\\
h_{15,3}^{\mathrm{NR}} &= g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{C_2}{8m_am_b^2r^3},\\
h_{15,4}^{\mathrm{NR}} &= 0,\\
h_{15,5}^{\mathrm{NR}} &= 0,\\
h_{15,6}^{\mathrm{NR}} &= -g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{2}{m_am_b^2}.
\end{aligned} \tag{A.15}$$

The coefficients $h_{16,j}^{\mathrm{NR}}$ are given by

$$\begin{aligned}
h_{16,1}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{\mu[3m_0^2(m_a^2 + m_b^2) + 8m_a^2m_b^2]C_1}{64m_a^4m_b^3r^3}\\
&\quad + g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b}\\
&\quad \times \frac{\mu[3m_0^3r(m_a^2 + m_b^2) + m_0^2(8m_b^2m_a^2r^2 + 3m_a^2 + 3m_b^2) + 16m_0m_a^2m_b^2r + 16m_a^2m_b^2]}{64m_a^3m_b^4r^3},\\
h_{16,2}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{\mu(2m_a^2 + 3m_b^2)C_1}{32m_a^4m_b^3r^3}\\
&\quad - g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{\mu(3m_a^2 + 2m_b^2)C_1}{32m_a^3m_b^4r^3},\\
h_{16,3}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{3\mu(m_a^2 + m_b^2)C_2}{32m_a^4m_b^3r^4}\\
&\quad - g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{3\mu(m_a^2 + m_b^2)C_2}{32m_a^3m_b^4r^4},\\
h_{16,4}^{\mathrm{NR}} &= g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{\mu[m_a^2(3m_0^2r^2 + 8m_b^2r^2 + 9) + 3m_b^2(m_0^2r^2 + 3)]}{16m_a^4m_b^3r^2}\\
&\quad - g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{3\mu[m_a^2(m_0^2r^2 + 8m_b^2r^2 + 3) + m_b^2(m_0^2r^2 + 3)]}{16m_a^3m_b^4r^2},\\
h_{16,5}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{\mu(2m_a^2 + 3m_b^2)}{8m_a^4m_b^3}\\
&\quad + g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{\mu(3m_a^2 + 2m_b^2)}{8m_a^3m_b^4},\\
h_{16,6}^{\mathrm{NR}} &= -g_{\mathrm{S}}^{a} g_{\mathrm{P}}^{b} \frac{3\mu(m_a^2 + m_b^2)}{2m_a^4m_b^3r}\\
&\quad + g_{\mathrm{P}}^{a} g_{\mathrm{S}}^{b} \frac{3\mu(m_a^2 + m_b^2)}{2m_a^3m_b^4r}.
\end{aligned} \tag{A.16}$$

Appendix B Useful formulas in Fourier transformation

The potential in coordinate space is defined as

$$\begin{aligned}
V[\boldsymbol{r}, -\mathrm{i}\tfrac{\partial}{\partial \bar{\boldsymbol{r}}}] &\equiv \mathcal{F}[\overline{V}(\boldsymbol{q}, \boldsymbol{p}_1)]\\
&\equiv \left[\int \frac{\mathrm{d}^3\boldsymbol{q}}{(2\pi)^3} \mathrm{e}^{\,\mathrm{i}\boldsymbol{q}\cdot\bar{\boldsymbol{r}}}\overline{V}(\boldsymbol{q}, \boldsymbol{p}_1)\right]\Big|_{\text{place } \boldsymbol{p}_1 \text{ at far right and replace } \boldsymbol{p}_1 \text{ with } -\mathrm{i}\frac{\partial}{\partial \bar{\boldsymbol{r}}}}.
\end{aligned} \tag{B.1}$$

Some useful formulas for the Fourier transformation are

$$\begin{aligned}
\mathcal{F}[\tfrac{1}{\boldsymbol{q}^2 + m_0^2}] &= \tfrac{1}{4\pi r}\mathrm{e}^{-m_0 r} \equiv W\tfrac{1}{r},\\
\mathcal{F}[\tfrac{\boldsymbol{q}_i}{\boldsymbol{q}^2 + m_0^2}] &= iWr^2C_1\bar{\boldsymbol{r}}_i,\\
\mathcal{F}[\tfrac{\boldsymbol{q}_i\boldsymbol{q}_j}{\boldsymbol{q}^2 + m_0^2}] &= Wr^3[C_{21}T_{ij,1} + C_{22}T_{ij,2}],\\
\mathcal{F}[\tfrac{\boldsymbol{q}_i\boldsymbol{q}_j\boldsymbol{q}_k}{\boldsymbol{q}^2 + m_0^2}] &= iWr^4[C_{31}T_{ijk,1} + C_{32}T_{ijk,2}],\\
\mathcal{F}[\tfrac{\boldsymbol{q}_i\boldsymbol{q}_j\boldsymbol{q}_k\boldsymbol{q}_l}{\boldsymbol{q}^2 + m_0^2}] &= Wr^5[C_{41}T_{ijkl,1} + C_{42}T_{ijkl,2} + C_{43}T_{ijkl,3}],
\end{aligned} \tag{B.2}$$

where $W=\frac{1}{4\pi}e^{-m_0 r}$, and the coefficients are expressed as

$$\begin{aligned}
C_{21} &= -C_2 + 16\pi r^3\delta^3(\boldsymbol{r}),\\
C_{22} &= C_1 - 4\pi r^3\delta^3(\boldsymbol{r}),\\
C_{31} &= -[m_0^3 r^3 + 6m_0^2 r^2 + 15m_0 r + 15r]\\
&\quad + 92\pi r^3\delta^3(\boldsymbol{r}),\\
C_{32} &= -C_{21},\\
C_{41} &= [m_0^4 r^4 + 10m_0^3 r^3 + 45m_0^2 r^2 + 105m_0 r + 105]\\
&\quad - [44(m_0^2 r^2 + 1) + 704]\pi r^3\delta^3(\boldsymbol{r}),\\
C_{42} &= C_{31} + 4\pi m_0^2 r^5\delta^3(\boldsymbol{r}),\\
C_{43} &= -C_{21},
\end{aligned} \tag{B.3}$$

with $C_{1,2}$ defined in equation (38). The tensor structures in equation (B.2) are defined as

$$\begin{aligned}
T_{ij,1} &\equiv \bar{\boldsymbol{r}}_i\bar{\boldsymbol{r}}_j,\\
T_{ij,2} &\equiv \delta_{ij},\\
T_{ijk,1} &\equiv \bar{\boldsymbol{r}}_i\bar{\boldsymbol{r}}_j\bar{\boldsymbol{r}}_k,\\
T_{ijk,2} &\equiv \bar{\boldsymbol{r}}_i\delta_{jk} + \bar{\boldsymbol{r}}_j\delta_{ik} + \bar{\boldsymbol{r}}_k\delta_{ij},\\
T_{ijkl,1} &\equiv \bar{\boldsymbol{r}}_i\bar{\boldsymbol{r}}_j\bar{\boldsymbol{r}}_k\bar{\boldsymbol{r}}_l,\\
T_{ijkl,2} &\equiv \bar{\boldsymbol{r}}_i\bar{\boldsymbol{r}}_j\delta_{kl} + \bar{\boldsymbol{r}}_i\bar{\boldsymbol{r}}_k\delta_{jl}\\
&\quad + \bar{\boldsymbol{r}}_i\bar{\boldsymbol{r}}_l\delta_{jk} + \bar{\boldsymbol{r}}_j\bar{\boldsymbol{r}}_k\delta_{il}\\
&\quad + \bar{\boldsymbol{r}}_j\bar{\boldsymbol{r}}_l\delta_{ik} + \bar{\boldsymbol{r}}_k\bar{\boldsymbol{r}}_l\delta_{ij},\\
T_{ijkl,3} &\equiv \delta_{ij}\delta_{kl} + \delta_{ik}\delta_{kl} + \delta_{il}\delta_{jl}.
\end{aligned} \tag{B.4}$$

Furthermore, the following relations hold:

$$\begin{aligned}
&\int \delta^3(\boldsymbol{r})T_{ij,1}\mathrm{d}\Omega = \frac{1}{3}\int \delta^3(\boldsymbol{r})T_{ij,2}\mathrm{d}\Omega,\\
&\int \delta^3(\boldsymbol{r})T_{ijk,\alpha}\mathrm{d}\Omega = \int \delta^3(\boldsymbol{r})T_{ijk,1\alpha}Y_{1m}Y_{1m'}^*\mathrm{d}\Omega = 0,\\
&\int \delta^3(\boldsymbol{r})T_{ijkl,1}\mathrm{d}\Omega = \frac{1}{15}\int \delta^3(\boldsymbol{r})T_{ijkl,3}\mathrm{d}\Omega,\\
&\int \delta^3(\boldsymbol{r})T_{ijkl,2}\mathrm{d}\Omega = \frac{2}{3}\int \delta^3(\boldsymbol{r})T_{ijkl,3}\mathrm{d}\Omega,
\end{aligned} \tag{B.5}$$

with $\alpha = 1, 2$.

For the atomic systems, the properties of the radial components of the wave functions impose specific constraints on the contributions of various terms Specifically, $\delta^3(\boldsymbol{r})T_{ij,\alpha}$ contributes exclusively to S-wave states, $\delta^3(\boldsymbol{r})T_{ijk,\alpha}$ contributes to S-wave and P-wave states, and $\delta^3(\boldsymbol{r})T_{ijkl,\alpha}$ contributes to S-, P-, and D-wave states. Consequently, one can express:

$$\begin{aligned}
\delta^3(\boldsymbol{r})T_{ij,1} &= \frac{1}{3}\delta^3(\boldsymbol{r})T_{ij,2},\\
\delta^3(\boldsymbol{r})T_{ijk,\alpha} &= 0.
\end{aligned} \tag{B.6}$$

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