Computation of the unitary group for the Rashba spin–orbit coupled operator, with application to point-interactions

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Abstract

We compute an explicit formula for the one-parameter unitary group of the single-particle Rashba spin–orbit coupled operator in dimension three. As an application, we derive the formula for the Green function for the two-particle operator, and then prove that the spin-dependent point-interaction is of class $H_{-4}$. The latter is thus the example of a supersingular perturbation for which no self-adjoint operator can be constructed.

Keywords: Rashba spin–orbit coupling, one-parameter unitary group, supersingular perturbation, cold molecule

1. Introduction

The fundamental object for describing quantum dynamics of a system governed by a Hamiltonian $h$ is the associated one-parameter unitary group $e^{iht} (t \in \mathbb{R})$. For $h$ lower semi-bounded, the unitary group is closely related to the semigroup $e^{-ith} (t > 0)$ in that $e^{-ith}$ is the strong limit of $e^{-i(t-i\epsilon)h}$ as $\epsilon \downarrow 0$. For example, the integral kernel (the free propagator) of the Schrödinger semigroup $e^{i\Delta t} |_{H^{2}(\mathbb{R}^3)}$ is well-known [1]:

$$K^0_t(x) = \frac{e^{-|x|^2}}{(4\pi t)^{3/2}} \quad \text{a.e. } x \in \mathbb{R}^3$$

(1.1)

and

$$e^{i\Delta t} |_{H^{2}(\mathbb{R}^3)} u = \text{l.i.m. } \int K^0_t (\cdot - y) u(y) \, dy$$

(1.2)
for \( u \in L^2(\mathbb{R}^3) \). Here and elsewhere \( \text{l.i.m.} \int_0^1 \text{l.i.m.} R_{r,s} \int_{|y| \leq R} \) implies the \( L^2 \)-norm convergent integral; the integral is just the convolution \( K_\mu^0 \ast u \) when \( u \in L^2 \cap L^1 \). For a comprehensive exposition of Schrödinger (semi)groups the reader may refer to [1–4].

In the first half of the present paper we obtain the formulas (theorem 3, corollary 4) analogous to (1.1) and (1.2) when \( h \) is the Rashba spin–orbit coupled operator considered in the presence of the out-of-plane magnetic field. To the best of our knowledge, no such formula has been derived previously. More specifically, we consider the operator \( h \) in \( \mathcal{H} = \mathfrak{h} \otimes \mathbb{C}^2 \), with \( \mathfrak{h} = L^2(\mathbb{R}^3) \), given by the operator sum

\[
\begin{align*}
   h &= h^0 + U, \\
   h^0 &= -\Delta |_{\mathcal{H}(\mathbb{R}^3)} \otimes \mathbb{I}_{\mathbb{C}^2} 
\end{align*}
\]  

(1.3a)

where the potential \( U \) (atom-light coupling) is the operator sum

\[
U = \alpha U^\alpha + \beta U^\beta, \quad \alpha, \beta \geq 0
\]  

(1.3b)

of the Rashba spin–orbit coupling term

\[
U^\alpha = D^- \otimes S^+ - D^+ \otimes S^-, \quad D^\pm = (\nabla_1 \pm i\nabla_2)|_{\mathcal{H}(\mathbb{R}^3)}
\]  

(1.3c)

(the overbar denotes the closure) and the Raman-coupling term

\[
U^\beta = 2\mathbb{I}_\mathfrak{h} \otimes S^3.
\]  

(1.3d)

The spin operators are

\[
S^i = \frac{1}{2} \sigma^i \quad \text{for} \quad i \in \{1, 2, 3\}; \quad S^\pm = S^1 \pm iS^2
\]  

(1.4)

where \((\sigma^i)\) are standard Pauli matrices.

In Bose–Einstein condensates or atomic Fermi gases, one commonly distinguishes between the Rashba spin–orbit coupling and the Dresselhaus spin–orbit coupling [5]. However, the two are unitarily equivalent [6], so we focus on the Rashba-type coupling in what follows.

By using a classic Nelson theorem for analytic vectors (see e.g. [7, theorem X.39]) we show that \( D^- \otimes S^+ - D^+ \otimes S^- \) is essentially self-adjoint and that the linear span \( \mathcal{D} \) of bounded elementary tensors \( u \otimes \varphi \), with \( u \in \mathcal{D}_h(D^+D^-) \) and \( \varphi \in \mathbb{C}^2 \), is the core for its closure \( U^\alpha \); see proposition 1 for the definition and [7, section X.6] and [8, section 7.4] for more details.

As a result, the operator \( h \) defined by (1.3) and (1.4) is self-adjoint. Of course, to show the self-adjointness of \( h \) it would suffice to notice that \( h^0 \) is self-adjoint and that \( U \) is relatively \( h^0 \)-bounded. However, it is \( \mathcal{D} \) itself that is more important to our investigation besides the self-adjointness.

It is known that \( h \geq -\Sigma \) is lower semibounded with \( \Sigma = \beta \) if \( 2\beta > \alpha^2 \) and \( \Sigma = (\beta/\alpha)^2 + (\alpha/2)^2 \) otherwise. Variant forms of \( h \) were studied by many authors. For example, the special case \( \alpha = 0 \) (but \( \beta \geq 0 \)) in various spatial dimensions can be found in [9–13]. A general case in three spatial dimensions is studied in [6, 14].

In the second half of the paper we use the computed unitary group for deriving the Green function for the two-particle operator

\[
H = h \otimes \mathbb{I}_\mathfrak{h} + \mathbb{I}_\mathfrak{h} \otimes h.
\]  

(1.5)

Since \( h \geq -\Sigma \) is self-adjoint in \( \mathcal{H} \), \( H \geq -2\Sigma \) is self-adjoint in \( \mathcal{H} \otimes \mathcal{H} \). We use the integral representation [15] of the resolvent \( R(z) \equiv (H - z\mathbb{I}_{\mathcal{H} \otimes \mathcal{H}})^{-1} \),

\[
R(z) = \pm i \int_0^\infty e^{\pm it} e^{\mp izH} dt, \quad e^{itH} = e^{it \mathfrak{h}} \otimes e^{it \mathfrak{h}}
\]  

(1.6)
where the upper (lower) sign is taken when $\Im z > 0$ ($\Im z < 0$). For $\alpha$ small, we give explicit formulas for the parts of Green function in propositions 8, 9, and A.1.

Our main motive for considering (1.5) is an attempt to understand eventually in a rigorous way the formation of cold molecules [16], provided that the interaction is short-range. The cold molecules available for experiments typically are diatomic molecules [17–20]. The atoms interact through the van der Waals potentials whose range at ultracold temperatures is much smaller than the de Broglie wavelength of atoms. As a consequence, the interatomic potentials can be replaced by short-range (or zero-range) potentials.

The main technical difficulty is that the two-particle operator $H$ does not admit the separation of variables in the center-of-mass coordinate system $Q = (x, X)$ unless $\alpha = 0$; here $x$ is the relative coordinate (the distance between the two atoms) and $X$ is the center-of-mass coordinate. The situation is clearly seen from the operator which is unitarily equivalent to $H$:

$$A \otimes 1_{B} + 1_{A} \otimes B + \alpha D$$

where the self-adjoint operators $A = A(x)$ and $B = B(X)$ are defined by

$$A = 2h^{0} + U, \quad B = \frac{1}{2}(h^{0} + U + \beta U^{B})$$

and the essentially self-adjoint operator $D = D(x, X)$ is defined by

$$D = (D^{+} \otimes 1_{C^{2}}) \otimes (1_{B} \otimes S^{-}) - (D^{-} \otimes 1_{C^{2}}) \otimes (1_{B} \otimes S^{+})$$

$$+ \frac{1}{2}[(1_{B} \otimes S^{+}) \otimes (D^{-} \otimes 1_{C^{2}}) - (1_{B} \otimes S^{-}) \otimes (D^{+} \otimes 1_{C^{2}})].$$

When $\alpha = 0$, (1.7) simplifies so that one can apply the theory of singular perturbations developed in [21] (and in particular in theorem 5.2.1 therein), since it was shown in [14] that the Dirac delta is of class $\mathcal{H}_{-3}(h) \subset \mathcal{H}_{-4}(h)$ for $h$, and hence for $A = 2h^{0} + \beta U^{B}$; as usual, $\mathcal{H}_{a}$ is the scale of Hilbert spaces associated with a self-adjoint operator. We assume that the two particles at positions $x_{1}$ and $x_{2}$ are interacting via the zero-range potential which is modeled by the Dirac distribution concentrated at $x = x_{1} - x_{2} = 0$.

When $\alpha > 0$, one cannot associate the $x$-dependent interaction potential to $A(x)$ alone because of $D(x, X)$; that is, the two-particle case no longer reduces to the single-particle one. Instead, one studies the restriction of (1.7) to $(H^{2}(\mathbb{R}^{3} \setminus \{0\}) \otimes \mathbb{C}^{2}) \otimes \text{dom } h$. Equivalently, one considers the singular perturbation concentrated at $(0, X)$ and associated to the total operator (1.7). Further results in this direction will be provided elsewhere. Here, we aim at considering the perturbation itself, and we show by using (1.6) that the perturbation is of class $\mathcal{H}_{-4}(H) \subset \mathcal{H}_{-5}(H)$; see theorem 11. A general theory of supersingular rank one perturbations is developed in [22, 23] (see also the list of references therein), where it is shown that the restricted operator does not have self-adjoint extensions, but the so-called regular ones. The results for finite rank perturbations, which is our case, are generalized naturally.

One can also obtain the Green function for (1.5) by using the single-particle Green function in [6]. Mimicking the proof of theorem 5 in [24], for $z \in \mathbb{C}$ and $\Re z < -2\Sigma$, the resolvent $R(z)$ of $H$ is the norm convergent integral $\int_{\mathbb{R}} r(z/2 - it) \otimes r(z/2 + it) \, dt/(2\pi)$, where $r(\cdot)$ is the resolvent of $h$. However, in this case we are restricted to $\Re z < -2\Sigma$, while considering singular perturbations we deal with $R(\pm i)$. Even if one shows that one can analytically relax the restriction, the exposition becomes highly complicated due to the hypergeometric origin of functions $G_{1}$ and $G_{2}$ in [6]; that is, the functions are linear combinations of hypergeometric series in three variables. On the other hand, we note in remark 5 without proof how the unitary group computed in the present paper relates to $G_{1}$ and $G_{2}$.
2. Preliminaries

Here and elsewhere:

- \( \nabla_i, i \in \{1, 2, 3\} \) is the gradient in the \( i \)th component of a three-dimensional position vector; the Laplacian \( \Delta = \sum_{i=1}^3 \nabla_i^2 \).

- \( \mathcal{S}_i = \mathfrak{h} \otimes \mathbb{C}^2, \mathfrak{h} = L^2(\mathbb{R}^3), \mathfrak{h}^* = L^2(\mathbb{R}^6), H^m (m \in \mathbb{N}) \) is the \((L^2-)Sobolev space of order \( m \) \)
[8, definition D.2], [25, definition 2.15.1], [26, section 3.2].

- The tensor product \( A \otimes B = A \otimes B \) of the operators \( A \) and \( B \) in Hilbert spaces \( \mathcal{S}_1 \) and \( \mathcal{S}_2 \), respectively, is the closure of the operator \( A \otimes B \) defined on the linear space spanned by elementary tensors \( u \otimes v (\text{conjugate-bilinear forms on } \mathcal{S}_1 \times \mathcal{S}_2) \), with \( u \in \text{dom } A \) and \( v \in \text{dom } B \): \( (A \otimes B)(u \otimes v) = Au \otimes Bv \). The tensor product \( \mathcal{S}_1 \otimes \mathcal{S}_2 \) of Hilbert spaces \( \mathcal{S}_1 \) and \( \mathcal{S}_2 \) is the completion of \( \mathcal{S}_1 \otimes \mathcal{S}_2 \) with respect to the cross norm, where \( \mathcal{S}_1 \otimes \mathcal{S}_2 \) is the linear space spanned by elementary tensors \( u \otimes v \), with \( u \in \mathcal{S}_1 \) and \( v \in \mathcal{S}_2 \).

Denote the standard basis of \( \mathbb{C}^2 \) by

\[
\left| \frac{1}{2} \right> = \left( \begin{array}{c} 1 \\ 0 \end{array} \right), \quad \left| - \frac{1}{2} \right> = \left( \begin{array}{c} 0 \\ 1 \end{array} \right).
\]

With this notation

\[
S^\pm |s\rangle = \delta_{s, \pm 1} \pm \frac{1}{2}, \quad S^0 |s\rangle = s |s\rangle
\]

for \( s \in \{- \frac{1}{2}, \frac{1}{2}\} \); \( \delta_{s, \pm 1} \) is the Kronecker symbol. The spin operators \( S^\pm \) are bounded in \( \mathbb{C}^2 \), with the adjoint ones \( (S^\pm)^* = S^\mp \).

By Gauss formula \[8, \text{theorem D.8}]\, the adjoint operators \( (D^\pm)^* = -D^\mp \) are densely defined in \( \mathfrak{h} \) and hence the \( D^\pm = D^{\mp} \) are closed. We therefore have that \( (D^\mp \otimes S^\pm)^* = -D^\pm \otimes S^\mp \).

By definition, \( \text{dom } (D^\mp \otimes S^\pm) \) is dense in \( \mathcal{S}_i \), hence so is \( \text{dom } (D^\mp \otimes S^\mp) \). Thus we have

\[
(D^- \otimes S^+ - D^+ \otimes S^-)^* \supseteq (D^- \otimes S^+)^* - (D^+ \otimes S^-)^* = D^- \otimes S^+ - D^+ \otimes S^-
\]
i.e. \( D^- \otimes S^+ - D^+ \otimes S^- \) is densely defined, symmetric, closable. In fact, a stronger property holds; see proposition 2.

**Proposition 1.** Let \( \mathcal{D}_b(D^+D^-) \) be the set of bounded vectors \( u \) for a self-adjoint operator \( D^+D^- \); that is, \( \| (D^+D^-)^n u \|_{\mathbb{C}^2} \leq C_n \) for some \( C_n > 0 \) and for \( n \in \mathbb{N} \). Let \( \mathcal{D} \) be the set spanned by elementary tensors \( u \otimes \varphi \), where \( u \in \mathcal{D}_b(D^+D^-) \) and \( \varphi \in \mathbb{C}^2 \). Then \( \mathcal{D} \subseteq \mathcal{S}_i \) densely.

**Proof.** Applying Gauss formula twice one finds that \( D^+D^- \) is self-adjoint. Therefore, by standard argument, \( \mathcal{D}_b(D^+D^-) \) is dense in \( \mathfrak{h} \) and \( \mathcal{D} \) is dense in \( \mathcal{S}_i \).

**Proposition 2.** The operator \( D^- \otimes S^+ - D^+ \otimes S^- \) is essentially self-adjoint, and \( \mathcal{D} \) is the core for its closure.

**Proof.** Consider an elementary tensor \( u \otimes \varphi \in \mathcal{D} \). Each \( \varphi \in \mathbb{C}^2 \) is of the form \( \varphi = \sum s \varphi_s |s\rangle \), with \( \varphi_s \in \mathbb{C} \). Let \( u_0 = (D^+D^-)^n u \). Using (2.1) we have by induction
\[(D^- \otimes S^+ - D^+ \otimes S^-)2^2(u \otimes \varphi) = (-1)^n u_n \otimes \varphi,
\]
\[(D^- \otimes S^+ - D^+ \otimes S^-)2^n+1(u \otimes \varphi) = (-1)^n D^+ u_n \otimes \varphi - \frac{1}{2}
\]
\(- (-1)^n D^+ u_n \otimes \varphi + \frac{1}{2}\)

for \(n \in \mathbb{N}_0\). Since \(\|u_n\|_b \leq C^n_u\) (see proposition 1), we have
\[
\| (D^- \otimes S^+ - D^+ \otimes S^-)2^n(u \otimes \varphi) \|_{\mathcal{D}} \leq \sqrt{C^{2n}_u}\|\varphi\|_{L^2}.
\]  

(2.2)

For odd powers we have
\[
\| (D^- \otimes S^+ - D^+ \otimes S^-)2^n+1(u \otimes \varphi) \|_{\mathcal{D}} \leq \frac{1}{2} \| D^- u_n \|_h + \| D^+ u_n \|_h.
\]

(2.3)

But
\[
0 \leq \| D^\pm u_n \|_h^2 = -\langle u_n, u_{n+1} \rangle_h \leq \| u_n \|_h \| u_{n+1} \|_h \leq C^{n+1}_u
\]

and hence
\[
\| (D^- \otimes S^+ - D^+ \otimes S^-)2^n+1(u \otimes \varphi) \|_{\mathcal{D}} \leq \sqrt{C^{n+1}_u}\|\varphi\| \left( \frac{1}{2} \right) + \left( \frac{1}{2} \right).\]

(2.3)

It follows from (2.2) and (2.3) that \(u \otimes \varphi \in \mathcal{D}\) is a bounded, hence analytic, vector for \(D^- \otimes S^+ - D^+ \otimes S^-\). Since \(\mathcal{D}\) is dense in \(\mathcal{D}\) by proposition 1, the set of analytic vectors for a symmetric operator \(D^- \otimes S^+ - D^+ \otimes S^-\) is also dense in \(\mathcal{D}\). Then, by Nelson theorem, \(D^- \otimes S^+ - D^+ \otimes S^-\) is essentially self-adjoint.

By proposition 2, the operator \(h\) on \(dom \ h = dom \ h^0\) is self-adjoint.

3. Integral kernel of the unitary group

Recall that the confluent Humbert function \(\Phi_3\) possesses the series representation [27, equation (40)]
\[
\Phi_3(a; b; x, y) = \sum_{m,n \in \mathbb{N}_0} \frac{(a)_m (x^n y^n)}{(b)_{m+n} m! n!}
\]

which is absolutely convergent for \(|x|, |y| < \infty\), provided that the Pochhammer symbols exist (i.e. \(-b \notin \mathbb{N}_0\)). The \(\Phi_3\) function is one of the seven confluent forms of the Appell \(F_1\) function; see also [28].

**Theorem 3.** For \(t > 0\) and \(u \otimes |s\rangle \in \mathcal{D}\)
\[
e^{-i t h}(u \otimes |s\rangle) = \sum_{p} \langle G^{p t} \ast u \rangle \otimes |s\rangle
\]  

(3.1)

where
\[
G^{p t}(x) = K^{p t}_0(x)[\delta_{s\cdot a, \Gamma(t - 2ib \beta)} + \frac{\alpha}{2t} b \delta_{s\cdot \frac{1}{2} x^{-1} x^{-1} - \delta_{s\cdot \frac{1}{2} x^{-1} x^{-1}}}]
\]

(3.2a)
\[ a_t = \Phi_3(1; 1/2; t(\alpha/2)^2, (\beta t/2)^2), \quad b_t = t\Phi_3(1; 3/2; t(\alpha/2)^2, (\beta t/2)^2) \]  
\quad \text{(3.2b)}

for a.e. \( x = (x^1, x^2, x^3) \in \mathbb{R}^3; \ x^\pm = x^1 \pm ix^2. \)

**Corollary 4.** For \( t \in \mathbb{R} \setminus \{0\} \) and \( u \otimes |s| \in D \)

\[ e^{-ih}(u \otimes |s|) = s - \lim_{\epsilon \downarrow 0} \sum_{i'} (G^{(i')}_{i+it} * u) \otimes |s'| \]
\quad \text{(3.3a)}

\[ = \sum_{i'} \text{l.i.m.} \int G^{(i')}_{i+it}(-y)u(y) \, dy \otimes |s'|. \]  
\quad \text{(3.3b)}

**Remark 5.**

1. Let \( U_t = e^{ih}|_D \). Then \( U_t \subseteq e^{ih} \Rightarrow U_t^* = e^{-ih} \Rightarrow U_t = e^{ih} \). Thus, the extension \( e^{ih} \) of \( U_t \) acts on \( u \in \mathfrak{h} \) by (3.3): For all \( \epsilon > 0 \) and a given \( f \in \mathfrak{f} \) one finds a \( g \in D \) such that \( \|f - g\|_{\mathfrak{f}} < \epsilon \), so \( \|e^{ih}f\|_{\mathfrak{f}} \leq \|U_tf\|_{\mathfrak{f}} + \epsilon \).

2. Using \( (h - z1_\mathfrak{h})^{-1} = \int_0^\infty e^{zt}e^{-ht} \, dt \) for \( \Re z < -\Sigma \), one shows that

\[ G_i(x; z) = \int_0^\infty e^{zt}K_i^0(x)b_t \, dt, \quad x \in \mathbb{R}^3, \]  
\quad \text{(3.4a)}

\[ D^\pm G_1(x; z) = -\frac{x^\pm}{2} \int_0^\infty e^{zt}K_i^0(x)b_t \, dt, \quad x \in \mathbb{R}^3 \setminus \{0\}, \]  
\quad \text{(3.4b)}

\[ G_2(x; z) = \int_0^\infty e^{zt}K_i^0(x)\alpha_t \, dt, \quad x \in \mathbb{R}^3 \setminus \{0\} \]  
\quad \text{(3.4c)}

provided that the hypergeometric series on the left exist (theorem 3.3 in [6]). Initially, relations in (3.4) are valid for a.e. \( x \), as it is seen from the comparison between the single-particle Green function in [6] and that derived by using (3.1). However, the direct computation of the integrals on the right shows that the equalities hold true for all \( x \). One therefore refers to (3.4) as the integral representations of the hypergeometric series \( G_1, D^\pm G_1, G_2. \)

(3) As \( \alpha \searrow 0 \)

\[ a_0 = \cos(\beta t) + \frac{2i}{\beta} (\alpha/2)^2 \sin(\beta t) + O(\alpha^4), \]
\quad \text{(3.5a)}

\[ b_0 = \frac{i}{\beta} \sin(\beta t) + \frac{2}{\beta^2} (\alpha/2)^2 (\cos(\beta t) - \frac{\sin(\beta t)}{\beta t}) + O(\alpha^4). \]  
\quad \text{(3.5b)}

If further \( \beta = 0 \), one assumes the limit \( \beta \searrow 0 \). Similar relations hold for \( \alpha \) arbitrary and \( \beta \) small. We use (3.5) for computing the two-particle Green function later on.

Now we give the proofs of the above results. The proof of theorem 3 relies on the two lemmas.

**Lemma 6.** For \( t > 0 \), the operator

\[ e^{\Delta_{|\mathfrak{g}^2(\alpha^2)}} \cosh(t\sqrt{-\alpha^2D^+D^- + \beta^21_\mathfrak{h}}) |_{D_{\mathfrak{g}}(D^+D^-)} \]
\quad \text{(3.6)}
in \( \mathfrak{h} \) admits the unique extension which is bounded in \( \mathfrak{h} \). The integral kernel \( k_i \) of the operator in (3.6) is given by

\[
k_i(x) = K^0_t(x)\Psi_3(1; 1/2; t(\alpha/2)^2, (\beta t/2)^2)
\]

for a.e. \( x \in \mathbb{R}^3 \).

**Lemma 7.** For \( t > 0 \), the operator

\[
e^{t\Delta|\cdot|_p^2} \sinh(t\sqrt{-\alpha^2D^+D^- + \beta^2I_\mathfrak{h}}) |D_\alpha(D^+D^-)
\]

(3.7)

in \( \mathfrak{h} \) admits the unique extension which is bounded in \( \mathfrak{h} \). The integral kernel \( l_i \) of the operator in (3.7) is given by

\[
l_i(x) = K^0_t(x)\Psi_3(1; 3/2; t(\alpha/2)^2, (\beta t/2)^2)
\]

for a.e. \( x \in \mathbb{R}^3 \).

**Proof of lemma 6.** Throughout, \( \| \cdot \|_p \) is the norm in \( L^p(\mathbb{R}^3) \) for \( 1 \leq p < \infty \); in particular \( \| \cdot \|_2 = \| \cdot \|_h \). Let \( p_1(-i\nabla) \) denote the operator in (3.6). First we show that \( p_1(-i\nabla) \) defines a continuous mapping \( D_h(D^+D^-) \rightarrow L^2(\mathbb{R}^3) \).

Using \( \cosh(\cdot) = s - \lim_{n \rightarrow \infty} \sum_{k=0}^{\infty} (\cdot)^{2k}/(2k)! \) on \( D_0(D^+D^-) \), and the binomial formula, we have for \( u \in D_0(D^+D^-) \)

\[
\|p_1(-i\nabla)u\|_2 = \| \sum_{n \in \mathbb{N}_0} \frac{(\beta t)^{2n}}{(2n)!} \sum_{m=0}^{n} \left( \begin{array}{c} n \\ m \end{array} \right) (-1)^m (\frac{\alpha}{\beta})^{2m} e^{t\Delta} u_m \|_2
\]

\[
\leq \sum_{n \in \mathbb{N}_0} \frac{(\beta t)^{2n}}{(2n)!} \sum_{m=0}^{n} \left( \begin{array}{c} n \\ m \end{array} \right) (\frac{\alpha}{\beta})^{2m} \| e^{t\Delta} u_m \|_2
\]

where \( u_m = (D^kD^-)^m u \). Since \( K^0_t \in L^1(\mathbb{R}^3) \), we have by Young inequality

\[
\| e^{t\Delta} u_m \|_2 = \| K^0_t * u_m \|_2 \leq\| K^0_t \|_1 \| u_m \|_2.
\]

(3.8)

But \( \|u_m\|_2 \leq C^0 u \) for some finite \( C^0 u > 0 \), and \( \| K^0_t \|_1 = 1 \), so

\[
\|p_1(-i\nabla)u\|_2 \leq \sum_{n \in \mathbb{N}_0} \frac{(\beta t)^{2n}}{(2n)!} \sum_{m=0}^{n} \left( \begin{array}{c} n \\ m \end{array} \right) (\frac{\alpha}{\beta})^{2m} C^0 u = \cosh(t\sqrt{\alpha^2C^0 u + \beta^2})
\]

showing that \( p_1(-i\nabla) \) is a continuous linear operator from \( D_0(D^+D^-) \) into \( L^2(\mathbb{R}^3) \). Since \( D_0(D^+D^-) \) is dense in \( L^2(\mathbb{R}^3) \), there exists the unique bounded operator in \( L^2(\mathbb{R}^3) \) that extends \( p_1(-i\nabla) \).

Next we compute \( k_t \). Since \( p_1(-i\nabla)u = k_t * u \) for \( u \in D_0(D^+D^-) \), we have

\[
k_t = p_1(-i\nabla)\delta
\]

(3.9)

in \( \mathcal{S}'(\mathbb{R}^3) \), where \( \delta \) is the Dirac distribution. Let \( \mathcal{F}_{x \rightarrow \xi}: \mathfrak{h} \rightarrow \mathfrak{h} \) be the Fourier transform; \( \xi = (\xi^1, \xi^2, \xi^3) \in \mathbb{R}^3 \). In the sense of Plancherel–Riesz theorem, for \( u \in \mathfrak{h} \)

\[
\mathcal{F}[D^k u] = i\xi^k \hat{u}, \quad \xi^\pm = \xi^1 \pm i\xi^2, \quad \hat{u} = \mathcal{F}[u].
\]

(3.10)
Using (3.10), \( p_t(-i\nabla) \) has the symbol
\[
p_t(\xi) = e^{-\imath \| \xi \|^2} \cosh(\sqrt{\alpha^2 + \xi^2} + \beta^2). \tag{3.11}
\]
The dot product denotes the standard scalar product of vectors in \( \mathbb{R}^3 \). Since the symbol \( p_t \in L^1(\mathbb{R}^3) \), relation (3.9) gives
\[
k_t(x) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} e^{\imath \| \xi \|^2} p_t(\xi) \, d\xi \quad \text{a.e.} \, x \in \mathbb{R}^3.
\tag{3.12}
\]
Rewrite \( \xi \) in (3.11) and (3.12) in spherical coordinates (\( \| \xi \| = \rho, \theta, \phi \)) and use the series representation of \( \cosh \). Then, expand \((\alpha^2 + \xi^2 + \beta^2)^n\) using binomial formula, apply the relations
\[
\int_0^\pi e^{\imath \rho \cos \theta} \sin^{2m+1} \theta \, d\theta = \frac{\sqrt{\pi} \, m!}{\Gamma(m + \frac{3}{2})} {}_0F_1\left(\frac{3}{2}; -\frac{|x|^2 \rho^2}{4}\right), \tag{3.13a}
\]
\[
\int_0^\infty \rho^{m+1/2} e^{-\rho} \, d\rho = \pi^{m+1} \Gamma\left(m + \frac{3}{2}\right)
\tag{3.13b}
\]
and get that
\[
k_t(x) = \frac{e^{-|x|^2}}{(4\pi)^{3/2}} a_t, \quad a_t = \sum_{n \in \mathbb{N}_0} \sum_{m = 0}^\infty \frac{(\beta t)^{2m}}{(2m)!} \sum_{n = 0}^m \frac{n!}{m!} \frac{(\alpha^2)^m}{(2)^{n-m}} t^{n-m}.
\]
It remains to compute \( a_t \). The formal double series
\[
\sum_{n \in \mathbb{N}_0} \sum_{m = 0}^\infty \Omega_{nm} = \sum_{n \in \mathbb{N}_0} \sum_{m = n}^\infty \Omega_{mn}
\]
provided that the sum exists. Using in addition that \( 1/\Gamma(k) = 0 \) for \(-k \in \mathbb{N}_0\), we get
\[
a_t = \sum_{n,m \in \mathbb{N}_0} \frac{(\beta t)^{2m}}{(2m)!} \frac{\alpha^2}{\beta^4} t^{-n-m} \frac{m!}{\Gamma(m - n + 1)}
\]
\[
= \sum_{n,m \in \mathbb{N}_0} \frac{|(\alpha/\beta)^2|/4^n}{n!} \frac{|(\beta t)^2|^m}{m!} \left[ \frac{(1)_n (1)_m (1)_m}{(1)_2 (1)_{m-n}} \right].
\]
Using Legendre’s duplication formula \((1)_2m = 4^m (\frac{1}{2})_m (1)_m\) and then replacing \( m \) by \( n + p \) for \( p \in \mathbb{N}_0 \) (since \( 1/(1)_p = 0 \) for \( -p \in \mathbb{N}_0 \)) we get
\[
a_t = \sum_{n, p \in \mathbb{N}_0} \frac{|(\alpha/\beta)^2|/4^n}{n!} \frac{|(\beta t)^2|^{n+p}}{(n + p)!} \left[ \frac{4^{-n-p} (1)_{n+p} (1)_n}{(\frac{1}{2})^{n+p} (1)_p} \right]
\]
\[
= \sum_{n, p \in \mathbb{N}_0} \frac{|(t/2)^2|^{n+p}}{n!} \frac{|(\beta/2)^2|^p}{p!} \left[ \frac{(1)_n}{(1/2)_{n+p}} \right]
\]
which is the confluent Humbert function \( \Phi_3(1/2; 1/2; t(\alpha/2)^2, (\beta t/2)^2) \). This completes the proof of the lemma. \( \square \)
Proof of lemma 7. Let \( p_t(-i\nabla) \) denote the operator in (3.7). First we show that \( p_t(-i\nabla) \) defines a continuous mapping \( \mathcal{D}_b(D^+D^-) \to L^2(\mathbb{R}^3) \).

Using \( \sinh(t) = s - \lim_{n \to \infty} \sum_{k=0}^{n} (-1)^k t^{2k+1} / (2k+1)! \) on \( \mathcal{D}_b(D^+D^-) \), and the binomial formula, we have for \( a \in \mathcal{D}_b(D^+D^-) \)

\[
\| p_t(-i\nabla)a \|_2 = \left\| \sum_{n \in \mathbb{N}_0} \frac{(\beta t)^{2n}}{(2n+1)!} \frac{1}{n} \binom{n}{m} (\alpha/\beta)^m e^{\Delta} u_m \right\|_2 \\
\leq t \sum_{n \in \mathbb{N}_0} \frac{(\beta t)^{2n}}{(2n+1)!} \frac{1}{n} \binom{n}{m} (\alpha/\beta)^m \| e^{\Delta} u_m \|_2
\]

where \( u_m = (D^+D^-)^m u \). It was shown in the proof of lemma 6 that \( \| e^{\Delta} u_m \|_2 \leq C^m \) for some finite \( C > 0 \), so

\[
\| p_t(-i\nabla)a \|_2 \leq \frac{\sinh(t\sqrt{\alpha^2 C + \beta^2})}{\sqrt{\alpha^2 C + \beta^2}}
\]

implying that \( p_t(-i\nabla) \) is a continuous linear operator from \( \mathcal{D}_b(D^+D^-) \) into \( L^2(\mathbb{R}^3) \). Since \( \mathcal{D}_b(D^+D^-) \) is dense in \( L^2(\mathbb{R}^3) \), there exists the unique bounded operator in \( L^2(\mathbb{R}^3) \) that extends \( p_t(-i\nabla) \).

The computation of \( l_t \) is pretty much the same as that of \( k_t \) in lemma 6. In this case the symbol of \( p_t(-i\nabla) \) is

\[
p_t(\xi) = e^{-it\xi} \frac{\sinh(t\sqrt{\alpha^2 \xi^2 + \beta^2})}{\sqrt{\alpha^2 \xi^2 + \beta^2}}, \quad p_t \in L^1(\mathbb{R}^3).
\]

Using the series representation of \( \sinh(t) \), (3.12), and (3.13), we get

\[
l_t(x) = \frac{e^{-|x|^2}}{(4\pi t)^{3/2}} b_t, \quad b_t = t \sum_{n \in \mathbb{N}_0} \frac{(\beta t)^{2n}}{(2n+1)!} \frac{1}{n} \binom{n}{m} (\alpha/\beta)^m t^{-m}.
\]

Proceeding exactly the same way as when equating \( a_t \) in the proof of lemma 6, we get \( b_t = t\Phi_3(1; 3/2; it(\alpha/2)^2, (\beta/2)^2) \) (the only difference is that now \((2m+1)! = (2m)! (1/2)_m(1)_m \). The proof of the lemma is accomplished. \( \square \)

We are in a position to accomplish the proof of the theorem.

Proof of theorem 3. Both \( e^{-th}|_\mathcal{D} \) and \( e^{-it\xi}|_\mathcal{D} \) are the strong limits of their Taylor series. Since \( \mathcal{D} \) is invariant under the action of \( e^{-th} \) (because of (3.8)) and \( e^{-it\xi} \) (by definition), the operators \( e^{-th} \) and \( e^{-it\xi} \) commute on \( \mathcal{D} \), and it holds

\[
e^{-th}|_\mathcal{D} = e^{-th} e^{-it\xi}|_\mathcal{D}.
\]

Next, using

\[
(S^\pm)^n = 0 \quad (n \in \mathbb{N}_{\geq 2}), \quad S^+ S^- + S^- S^+ = 1_{_{C^2}}, \quad S^\pm S^3 + S^3 S^\pm = 0
\]

we have by induction
for \( n \in \mathbb{N}_0 \) and \( u \otimes |s\rangle \in \mathcal{D} \). Therefore, by (3.14)
\[
e^{-ih} (u \otimes |s\rangle ) = (e^{i \Delta \alpha^2(s)} \otimes \mathds{1}_{C^2}) \sum_{n \in \mathbb{N}_0} \frac{(-i)^n}{n!} U^n(u \otimes |s\rangle)
\]
\[
= \sum_{n \in \mathbb{N}_0} \frac{(-i)^n}{(2n)!} e^{i \Delta \alpha^2(s)} (-\alpha^2 D^+ D^- + \beta^2 \mathds{1}_b)^n u \otimes |s\rangle
+ \sum_{n \in \mathbb{N}_0} \frac{(-i)^{2n+1}}{(2n+1)!} (e^{i \Delta \alpha^2(s)} (-\alpha^2 D^+ D^- + \beta^2 \mathds{1}_b)^n \otimes \mathds{1}_{C^2}) U(u \otimes |s\rangle).
\]

The first series is (equation (3.6)) \( u \otimes |s\rangle \) and the second one is \((-1) (\text{equation (3.7)}) \otimes \mathds{1}_{C^2}) U(u \otimes |s\rangle)\). Using the definition of \( U \), and then applying lemmas 6 and 7, and
\[
D^\pm h(x) = -\frac{x^\pm}{2i} h(x) \quad \text{a.e. } x \in \mathbb{R}^3
\]
one deduces (3.1) and (3.2). The proof of the theorem is complete. \(\square\)

**Proof of corollary 4.** For \( t \in \mathbb{R} \setminus \{0\} \), \( \epsilon > 0 \), \( u \otimes |s\rangle \in \mathcal{D} \), we have by theorem 3
\[
\|(e^{-i(t-\epsilon)h} - e^{-ih}) (u \otimes |s\rangle)\|_B = \| \sum_{s'} \varphi_{\epsilon'}^{s'} \otimes |s'\rangle \|_B = \left( \sum_{s'} \| \varphi_{\epsilon'}^{s'} \|_B^2 \right)^{1/2}
\]
where
\[
\varphi_{\epsilon'}^{s'} = G_{\epsilon'}^{s'} u - \delta_{\epsilon'} \epsilon' u.
\]

Further, using \( \lim_{t \to 0} a_t = 1 \) and \( \lim_{t \to 0} b_t = 0 \)
\[
\lim_{\epsilon \to 0} \| \varphi_{\epsilon}^{s'} \|_B = \delta_{\epsilon} \lim_{\epsilon \to 0} \| K_0^{s'} u - u \|_B.
\]

But
\[
\lim_{\epsilon \to 0} \| K_0^{s'} u - u \|_B = \lim_{\epsilon \to 0} \| e^{i \Delta \alpha^2} u - u \|_B = \lim_{\epsilon \to 0} \| \frac{1}{\epsilon} (e^{i \Delta \alpha^2} - \mathds{1}_b) u \|_B
= \lim_{\epsilon \to 0} \| \Delta u \|_B = 0
\]
and hence
\[
e^{-ih} (u \otimes |s\rangle) = \sum_{s' > 0} \lim_{\epsilon \to 0} e^{-i(t-\epsilon)h} (u \otimes |s\rangle) = \sum_{s' > 0} (G_{\epsilon'}^{s'} u) \otimes |s'\rangle.
\]

Now, by standard argument, instead of \( u \), consider the function \( u_R = 1_{\{x \mid |x| \leq R\}} u \). Then \( u_R \in \mathcal{D}_b(D^+ D^-) \cap L^1(\mathbb{R}^3) \) and one deduces (3.3). \(\square\)
4. Green function for the two-particle operator

In this section we study the resolvent of the two-particle operator \( H \) in (1.5) written in the center-of-mass coordinate system.

4.1. Bases

In what follows we find it convenient to identify \( \mathbb{C}^2 \otimes \mathbb{C}^2 \) with \( \mathbb{C}^3 \oplus \mathbb{C}^1 \), which basically says that the tensor product \( 2 \otimes 2 \) of \( SU_2 \)-irreducible representations of dimensions \( 2s + 1 = 2 \) reduces to the orthogonal sum \( 3 \oplus 1 \) of \( SU_2 \)-irreducible representations of dimensions \( 2s + 1 = 3 \) and \( 2s + 1 = 1 \). The basis of the space of the representation \( 3 \) is \( \{(|s\rangle)_{s \in \{-1,0,1\}}\} \), while the space of \( 1 \) is single-dimensional, with the basis \( |00\rangle \). This follows from the fact that the basis of \( \mathbb{C}^3 \oplus \mathbb{C}^1 \)

\[
\{(\sigma)_{\sigma \in S}\}, \quad S = \bigcup_{s \in \{0,1\}} \{|(S,s)\rangle | s \in \{-S,-S+1, \ldots, S\}\}
\]

is orthonormal and is related to the orthonormal basis

\[
\{(s_1s_2) = (|s_1\rangle \otimes |s_2\rangle)_{(s_1,s_2) \in \{-\frac{1}{2},\frac{1}{2}\}^2}\}
\]

of \( \mathbb{C}^2 \otimes \mathbb{C}^2 \) via the Clebsch–Gordan coefficient of \( SU_2 \) [29]:

\[
|Ss\rangle = \sum_{s_1,s_2} \left[ \frac{1}{s_1} \frac{1}{s_2} \frac{S}{s} \right]_{s_1s_2} |s_1s_2\rangle \quad (4.1)
\]

where the sum runs over \( (s_1,s_2) \in \{ -\frac{1}{2}, \frac{1}{2} \}^2 \) such that \( s_1 + s_2 = s \). Using (4.1) and the orthogonality condition for the Clebsch–Gordan coefficient, one represents the basis vector \( |s_1s_2\rangle \) of \( \mathbb{C}^2 \otimes \mathbb{C}^2 \) as a linear combination of the basis vectors \( |\sigma\rangle \) of \( \mathbb{C}^3 \oplus \mathbb{C}^1 \), with \( \sigma \) ranging over \( S \).

Given the orthonormal basis \( (e_i) \) of \( h \), the orthonormal basis of \( \mathfrak{h} \) is \( (e_i \otimes |\sigma\rangle) \) and the orthonormal basis of \( \mathfrak{h} \otimes \mathfrak{h} \) is \( ((e_i \otimes |s_1\rangle) \otimes (e_j \otimes |s_2\rangle)) \). The Hilbert space

\[
\mathcal{H} = (h \otimes h) \otimes (\mathbb{C}^3 \otimes \mathbb{C}^1)
\]

has orthonormal basis \( (e_i \otimes |\sigma\rangle) \), with \( e_{ij} = e_i \otimes e_j, \sigma = (S,s) \in S \). The map \( J : \mathfrak{h} \otimes \mathfrak{h} \to \mathcal{H} \) given by

\[
J : (e_i \otimes |s_1\rangle) \otimes (e_j \otimes |s_2\rangle) \mapsto \sum_{\sigma} \left[ \frac{1}{s_1} \frac{1}{s_2} \frac{S}{s} \right] e_{ij} \otimes |\sigma\rangle
\]

is unitary, and so \( \mathcal{H} \) is isomorphic to \( \mathfrak{h} \otimes \mathfrak{h} \).

4.2. Center-of-mass coordinate system

Let \( x_1 \in \mathbb{R}^3 \), \( x_2 \in \mathbb{R}^3 \) be the position-vectors of the two atoms, and put \( q = (x_1,x_2) \) and \( Q = (x,X) \), where \( x = x_1 - x_2 \) and \( X = (x_1 + x_2)/2 \). Then

\[
Kq = Q, \quad K = \begin{pmatrix} 1 & -1 \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}.
\]

The coordinate transformation \( K \) gives rise to the unitary transformation \( \mathcal{U} \) in the Hilbert space \( \mathcal{H}' = L^2(\mathbb{R}^6) \), \( \mathcal{U} : \mathcal{H}' \to \mathcal{H}' \), \( f(q) \mapsto f(Kq) \).
Now consider the unitary isomorphisms $\tau: h \otimes h \rightarrow h^c, e_{ij} \mapsto e_i(x_1)e_j(x_2)$, and
\[
\tilde{\tau} = UT \otimes 1_{C^* \otimes C^*}: \mathcal{R} \rightarrow \mathcal{R}^c = h^c \otimes (C^3 \oplus C^1).
\]
Note that $UT \in B(h \otimes h, h^c)$ is bounded, so $(UT \otimes 1_{C^* \otimes C^*})^* = (UT)^* \otimes 1_{C^* \otimes C^*}$. Define
\[
R^c(z) = LR(z)L^*, \quad z \in \text{res } H = C \setminus [-2\Sigma, \infty)
\]
(4.2)
where the unitary map
\[
L = \tilde{\tau} J: \hat{J} \otimes \hat{J} \rightarrow \hat{R}^c,
\]
\[
[(e_i \otimes |s_1\rangle) \otimes (e_j \otimes |s_2\rangle)] \mapsto \sum_{s, s'} \left[ \frac{1}{s_1} \frac{1}{s} \right] S |s\rangle e_i(x) e_j(x) \otimes |s_1\rangle.
\]
Note that $J \in B(\hat{J} \otimes \hat{J}, \mathcal{R})$, so $(\tilde{\tau} J)^* = J^\ast \tilde{\tau}^\ast$. The bounded operator $R^c(z) \in B(\mathcal{R}^c)$ is the resolvent $(H^c - z 1_{\mathcal{R}^c})^{-1}$ of the self-adjoint operator
\[
H^c = LHL^*, \quad \text{dom } H^c = L \text{dom } H
\]
which represents the two-particle Hamiltonian (1.5) written in the center-of-mass coordinate system $Q$. The operator $H$ is unitarily equivalent to (1.7), and the unitary self-map is given by $J^* [\tau^* UT \otimes 1_{C^* \otimes C^*}] J$.

4.3. Resolvent

By (1.6), (3.3), and (4.2), the resolvent $R^c(z)$ acts on $f \otimes |\sigma\rangle \in h^c \otimes (C^3 \oplus C^1)$ as follows:
\[
R^c(z)(f(\sigma) \otimes |\sigma\rangle) = \sum_{\sigma'} \text{l.i.m. } \int R^c_{\sigma', \sigma}(z)(Q - Q') f(Q') dQ' \otimes |\sigma'\rangle.
\]
(4.3)
For a.e. $Q = (x, X) \in \mathbb{R}^6$, the element $R^c_{\sigma', \sigma}(z)(Q)$ of the Green function is given by the improper Riemann integral ($\int_0^\infty \equiv \lim_{t \rightarrow 0} \int_t^\infty$)
\[
R^c_{\sigma', \sigma}(z)(x, X) = \pm i \int_0^\infty e^{-i\epsilon t} \sum_{\ell, j} \left[ \frac{1}{s_1} \frac{1}{s} \right] S |s\rangle G_{\pm \ell, \sigma'}^{(\epsilon)}(x) G_{\pm \ell, \sigma}^{(\epsilon)}(X) dt
\]
(4.4)
with the upper (lower) sign taken for $\Im z > 0$ ($\Im z < 0$). Relations (4.3) and (4.4) follow from the fact that the integrand $(\cdot)$ in (4.4) is not Lebesgue summable, since $(\cdot)$ is of the form $\exp(\pm i(z + Q^2/(4t)))e^{-i\ell t}$ containing the powers $t^\ell$ for $n \in \mathbb{Z}$. Therefore, in order to apply the Fubini theorem for changing the order of integration with respect to $Q'$ and $t$, one introduces the factor $e^{-\epsilon t}$ so that $\int_0^\infty e^{-\epsilon t} \otimes |\sigma\rangle dt = \int_{\epsilon > 0} \otimes |\sigma\rangle dt$. The latter holds true because $e^{-\epsilon t} \rightarrow 0$ as $t \rightarrow 0$ for all $n \in \mathbb{Z}$, which further amounts to $\int_0^\infty e^{-\epsilon t} \otimes |\sigma\rangle dt \rightarrow 0$ as $\epsilon \downarrow 0$ (see also the proof of proposition 8).

We compute (4.4) for $\alpha \geq 0$ small.

**Proposition 8.** For $\Im z \neq 0$ and $\alpha = 0$
\[
R^c_{\sigma', \sigma}(z)(Q) = -\frac{\delta_{\sigma', \sigma}}{8\pi^2 \epsilon^2} \left[ \delta_{\alpha 0} K_2(|Q| \sqrt{-\epsilon + z}) + \delta_{\alpha 1} [K_2(|Q|) \sqrt{2\beta - z}]ight. \left. + \delta_{\alpha 1} (z + 2\beta) K_2(|Q|) \sqrt{-2\beta - z}) \right]
\]
(4.5)
for a.e. $Q \in \mathbb{R}^6$. If in addition $\beta = 0$ then
\[ R_\sigma' (z)(Q) = -\delta_\sigma' \frac{zK_3(|Q| \sqrt{-z})}{8\pi^2 Q^2} \]  

\( R_\sigma' \) is the Macdonald function of order \( \nu \). More generally, we have proposition 9.

**Proposition 9.** For \( \Im z \neq 0 \) and \( \alpha \gg 0 \) arbitrarily small, the diagonal element

\[ R_\sigma' (z) = R_\sigma'(z)_{\alpha=0} + \alpha^2 \Delta_\sigma (z) + O(\alpha^4) \]  

where \( R_\sigma'(z)_{\alpha=0} \) is given by (4.5), and the correction term

\[ \Delta_\sigma (z)(Q) = \frac{\mp i}{8\pi^2 |Q|^2} \left( \delta_0 z^{3/2}K_3(|Q| \sqrt{-z}) - \frac{1}{2} (z + 2\beta) \frac{3/2 K_3(|Q| \sqrt{-2\beta - z}) - \frac{1}{2} (z - 2\beta) \frac{3/2 K_3(|Q| \sqrt{2\beta - z})}{8 |Q|} \right) \]

\[ \cdot \left( 2z^2 K_4(|Q| \sqrt{-z}) - (z + 2\beta) z K_4(|Q| \sqrt{-2\beta - z}) - (z - 2\beta) z K_4(|Q| \sqrt{2\beta - z}) \right) \]

\[ + \left( \delta_{\lambda i} [z (z - 2\beta) \frac{3/2 K_3(|Q| \sqrt{2\beta - z}) - z^{3/2} K_3(|Q| \sqrt{-z})}{8 |Q|} \right) \]

\[ + \delta_{\lambda,-1} [z (z + 2\beta) \frac{3/2 K_3(|Q| \sqrt{-2\beta - z}) - z^{3/2} K_3(|Q| \sqrt{-z})}{8 |Q|} \right) \]

\[ + i \beta |Q| (z + 2\beta) K_2(|Q| \sqrt{-2\beta - z}) \]  

for a.e. \( Q = (x, X) \in \mathbb{R}^6 \): the upper (lower) sign is taken when \( \Im z > 0 \) (\( \Im z < 0 \)). When in addition \( \beta = 0 \), one assumes the limit \( \beta \searrow 0 \) in (4.8).

\( X^\pm \) is defined similar to \( x^\pm \). For the purposes of the present paper, the computation of the diagonal elements of the two-particle Green function is sufficient. However, for completeness, we list non-diagonal elements in the appendix.

We close the section by giving the proofs of the above propositions.

**Proof of proposition 8.** Using (3.2) and (3.5)

\[ G^\nu (x) = \delta_{\nu,0} K_{\lambda i}^0 (x) (\cos(\beta t) - 2i \sin(\beta t)) \]  

a.e. \( x \in \mathbb{R}^3 \)

and hence by (4.4)

\[ R_\sigma' (z)(Q) = \pm i \delta_\sigma' \int_0^\infty e^{\pm izt} K_{\lambda i}^0 (x) K_{\pm,0}^0 (X) \]

\[ \cdot \left( \delta_{\nu,0} + \delta_{\lambda i} [\delta_{\lambda i} e^{2\beta t} + \delta_{\lambda,-1} e^{2\beta t}] \right) dt \]  

for a.e. \( Q = (x, X) \in \mathbb{R}^6 \). The improper Riemann integrals

\[ \int_0^\infty e^{\pm izt} K_{\lambda i}^0 (x) K_{\pm,0}^0 (X) t^{-n} dt \approx \lim_{\epsilon \searrow 0} \int_0^\infty e^{\pm izt} \exp \left( \frac{\pm izt}{\epsilon} \right) t^{-n} dt \]  

(4.10a)
\[
\lim_{\delta \to 0} \int_{-\epsilon}^{\epsilon} e^{i tz + Q/z} dt = 0
\]
for \( n \in \mathbb{Z} \); the upper (lower) sign is for \( \Im z > 0 \) (\( \Im z < 0 \)). To show the second equality, let us define

\[
I_\epsilon = \int_0^\infty e^{i [t+Q/t] - \epsilon} t^n dt
\]
for \( \Im z > 0, \|Q\| > 0, \epsilon > 0, n \in \mathbb{Z} \). Making the substitution \( t \to t - \epsilon \) and then using the decomposition \( I_\epsilon^\infty = \int_\epsilon^\infty + \int_0^\infty \) for \( \delta > \epsilon \), we get \( I_\epsilon = I_{\epsilon,\delta}^{(1)} + I_{\epsilon,\delta}^{(2)} \) where

\[
I_{\epsilon,\delta}^{(1)} = \int_\epsilon^\infty e^{i [(t-\epsilon)+(Q/t)]} - \epsilon/(t-\epsilon) (t-\epsilon)^n dt,
\]
\[
I_{\epsilon,\delta}^{(2)} = \int_0^\delta e^{i [(t-\epsilon)+(Q/t)]} - \epsilon/(t-\epsilon) (t-\epsilon)^n dt.
\]

In the limit, the second integral

\[
\lim_{\delta \to 0} \lim_{\epsilon \to 0} I_{\epsilon,\delta}^{(2)} = \lim_{\delta \to 0} \int_0^\infty e^{i [(t-\epsilon)+(Q/t)]} - \epsilon/(t-\epsilon) (t-\epsilon)^n dt
\]

\[
= \int_0^\infty e^{i [t+Q/t] - \epsilon} t^n dt
\]

because \( t \geq \delta > \epsilon \). The first integral

\[
I_{\epsilon,\delta}^{(1)} = \int_0^\delta e^{i [t+Q/t] - \epsilon} t^n dt.
\]

Since \( e^{-\epsilon/t^n} \to 0 \) as \( t \to 0 \), we have in the limit

\[
\lim_{\delta \to 0} \lim_{\epsilon \to 0} I_{\epsilon,\delta}^{(1)} = 0
\]

which, together with the above result, shows the equality (4.10a) \( \to \) (4.10b) for \( \Im z > 0 \); the proof for \( \Im z < 0 \) is analogous.

Relation (4.10c) follows from (4.10b) by using e.g. [30, equation (9.42)]. Substitute (4.10c) with \( n = 0 \) in (4.9) and deduce (4.5). Passing to the limit \( \beta \searrow 0 \) one gets (4.6).

\textbf{Proof of proposition 9.} We have by (4.4)

\[
K_{\sigma \tau} (z, X) = \pm i \int_0^\infty e^{\pm izc} K_{\pm \pm}^0 (x) K_{\pm \pm}^0 (x) \left( \delta_{\tau 0} a_{\pm \pm}^2 - \beta^2 b_{\pm \pm}^2 \right)
\]

\[
- (-1)^\delta \frac{\alpha_\| b_{\pm \pm}^2}{8t^2} \left( x^- X^+ + x^+ X^- \right)
\]

\[
+ \delta_{\tau 1} \left[ \delta_{\nu} (a_{\pm \pm} - \beta b_{\pm \pm})^2 + \delta_{\nu -1} (a_{\pm \pm} + \beta b_{\pm \pm})^2 \right] dt
\]

(4.11)
and by (3.5)
\[ a_n^2 - \beta^2 b_n^2 = 1 + \frac{i\alpha^2}{2\beta^2} (1 - \cos(2\beta t)) + O(\alpha^4), \quad (4.12a) \]
\[ (a_n \pm \beta b_n)^2 = e^{\pm 2\beta t} + \frac{\alpha^2}{2\beta^2} (e^{\pm 2\beta t}(i \pm 2\beta t) - i) + O(\alpha^4) \quad (4.12b) \]
as \alpha \searrow 0. In view of (4.9) and using \( a_{-\nu} = a_\nu \) (and similarly for \( b_{-\nu} \)) and the exponentiation of sine and cosine functions, substitute (4.12) in (4.11), and then apply (4.10c) for \( n \in \{0, 1, 2\} \), and deduce (4.7) and (4.8).

5. Supersingular perturbation

When considering the two atoms interacting via the zero-range potential which depends on the relative coordinate \( x \in \mathbb{R}^3 \), one follows a usual procedure and restricts the initial self-adjoint operator (Hamiltonian) \( H^c \) to the set of functions vanishing at \( x = 0 \), and then looks for possible self-adjoint extensions of the obtained symmetric operator. One should keep in mind that \( H^c \) is non-separable in \( Q \) for \( \alpha > 0 \).

Equivalently, one defines the singular distribution \( \psi_\sigma (\sigma \in S) \) concentrated at \( Q_0 = (0, X) \) via the duality pairing
\[ \langle \psi_\sigma, f \rangle = N_\sigma f_\sigma (Q_0) \quad (5.1) \]
for
\[ f = \sum_\sigma f_\sigma \otimes |\sigma \rangle \in C^\infty(\mathbb{R}^6) \odot (\mathbb{C}^3 \oplus \mathbb{C}^4) \]
and some normalization constant \( N_\sigma > 0 \). Since \( C^\infty_0(\mathbb{R}^6) \subseteq C^\infty \) and \( C^\infty_0 \) is dense in \( H^c \), the restricted operator is thus the operator \( H^c \) subject to the boundary condition \( \langle \psi_\sigma, f \rangle = 0 \) for \( f \in \text{dom } H^c \) and all \( Q_0 \). Using the scale \( (H_n = H_n(H^c))_{n \in \mathbb{Z}} \) associated with \( H^c \), \( \text{dom } H^c = \mathcal{H}_2 \), i.e. \( H^c \) defines a mapping \( \mathcal{H}_2 \to \mathcal{H}_0 = \mathbb{R}^6 \); the reader may refer to [21] for more details.

When \( \psi_\sigma \in \mathcal{H}_
 \neq \mathcal{H}_0 \) for some \( n \in \mathbb{N} \), the duality pairing in (5.1) is equivalently defined via the scalar product \( \langle \cdot, \cdot \rangle_0 \) in \( \mathcal{H}_0 \):
\[ \langle \psi_\sigma, f \rangle = \langle (|\mathbb{H}|^2 + 1)^{-n/2} \psi_\sigma, (|H^c| + 1)^n f \rangle_0 \quad (5.2) \]
with \( f \in \mathcal{H}_n \). Here \( \mathbb{I} = 1 \mathbb{R}^6 \) and \( (|\mathbb{H}|^2 + 1)^{-n/2} \) is an extension of \( (|H^c| + 1)^{-n/2} \) when considered as a mapping from \( \mathcal{H}_n \) onto \( \mathcal{H}_0 \). The duality pairing is well-defined since when we have \( \langle \psi_\sigma, f \rangle \rangle_0 \leq \| \psi_\sigma \| \cdot \| f \|_n \). We remark the following:

**Proposition 10.** The operator \( \mathbb{H}^c \) is a continuation of \( H^c : \mathcal{H}_2 \to \mathcal{H}_0 \) as a bounded operator from \( \mathcal{H}_0 \) into \( \mathcal{H}_n \).

**Proof.** Relation \( \psi_\sigma \in \mathcal{H}_n \) implies \( h_\sigma = (|\mathbb{H}|^2 + 1)^{-n/2} \psi_\sigma \in \mathcal{H}_0 \) and hence
\[ \| \psi_\sigma \|_n = \| h_\sigma \|_0 = \| (|\mathbb{H}|^2 + 1)^{-1} (|H^c| + 1) h_\sigma \|_0 = \| (|\mathbb{H}|^2 + 1) h_\sigma \|^{-2} \]
i.e. \( \mathbb{H}^c \) defines a mapping \( \mathcal{H}_0 \to \mathcal{H}_n \). \( \Box \)
Thus, the task is to find \( n \in \mathbb{N} \) for which \( \psi_\sigma \in \mathcal{H}_{-n} \) holds. It suffices to verify the relation for \( \mathcal{H}_c \) parametrized by \( \alpha = \beta = 0 \), because both \( \mathcal{H}^0 \) and \( h \) are self-adjoint on their common domain of definition; the Green function is given by (4.6) for such \( \mathcal{H}_c \). On the other hand, in order to use the Krein formula [23] for calculating eigenvalues later on (see also the discussion in section 6), we have to compute the normalization constant \( N_\sigma \), and we do so for \( \alpha \) small (and \( \beta \) arbitrary).

**Theorem 11.** We have \( \psi_\sigma \in \mathcal{H}_{-4} \setminus \mathcal{H}_{-3} \). Moreover, if \( ((\mathbb{H}_c)^2 + 1)^{-1} \psi_\sigma \in \mathcal{H}_0 \) is the unit vector, then, for \( \alpha \gg 0 \) arbitrarily small, the normalization constant satisfies the relation

\[
N_\sigma^{-2} = \frac{1}{512 \pi^4} \left( \delta_{\alpha, 0} + 2 \delta_{\alpha} \left[ \delta_{\alpha}(2 \beta + \theta, (1 + 4 \beta^2)) - \delta_{\alpha-1}(2 \beta + (\pi - \theta, (1 + 4 \beta^2))) \right] \right.
\]

\[
+ \frac{\alpha^2}{1536 \pi^4 \beta^2} \left( \frac{1}{4} \delta_{\alpha}(2 \beta \pi(5 + 4 \beta^2) - 1) \theta, 4 \beta(2 - 3 \beta \theta) \right)
\]

\[
- 4 \log(1 + 4 \beta^2) + \beta \sqrt{1 + 4 \beta^2}(4 \beta(\pi - \theta) - \log(1 + 4 \beta^2)) \cos \theta \beta
\]

\[
+ 2(\pi - \theta + \beta \log(1 + 4 \beta^2)) \sin \theta \beta
\]

\[
+ \delta_{\alpha}(8 \beta^2(1 - 2 \beta \theta) + \log(1 + 4 \beta^2))
\]

\[
\left( \delta_{\alpha-1}(8 \beta^2(1 + 2 \beta(\pi - \theta)) + \log(1 + 4 \beta^2)) \right) + O(\alpha^4)
\]

(5.3)

with \( \theta \beta = \arg(2 \beta + i) \) (\( \arg \) is the principal value of the argument). When \( \beta = 0 \), one assumes the limit \( \beta \searrow 0 \) in (5.3).

**Remark 12.** For \( \alpha = \beta = 0 \), relation (5.3) gives \( N_\sigma = N \) and \( \sqrt{N} = 2c \), where \( c = 2\sqrt{2}\sqrt{\pi} \) is the normalization constant for the functionals of class \( \mathcal{H}_{-2}(h^0) \) [21, section 2.3].

**Proof.** We use lemma 13 to show that \( \psi_\sigma \notin \mathcal{H}_{-3} \).

**Lemma 13.** If \( \phi \in \mathcal{H}_{-3} \setminus \mathcal{H}_{-2} \) then

\[
2^6 \|\phi\|^2 \geq 2 \|\phi, \left\{ \frac{3i}{2}((\mathbb{H}_c + i 1) - ((\mathbb{H}_c - i 1) - 2) \right. \]

\[
+ ((\mathbb{H}_c + i 1) - 1)^3 + ((\mathbb{H}_c - i 1) - 1)^3 \phi \rangle |.
\]

(5.4)

**Proof.** We have

\[
[([\mathbb{H}_c - i 1])^{-1} + ([\mathbb{H}_c + i 1])^{-1}] = 2\mathbb{H}_c([\mathbb{H}_c]^2 + 1)^{-1} \phi \in \mathcal{H}_{-2},
\]

\[
([\mathbb{H}_c - i 1])^{-1} - ([\mathbb{H}_c + i 1])^{-1} \phi = 2 i ([\mathbb{H}_c]^2 + 1)^{-1} \phi \in \mathcal{H}_0
\]

because \( ([\mathbb{H}_c]^2 + 1)^{-1}: \mathcal{H}_{-4} \to \mathcal{H}_0, \mathcal{H}_{-3} \subset \mathcal{H}_{-4} \) densely, and \( \mathbb{H}_c : \mathcal{H}_0 \to \mathcal{H}_{-2} \) by proposition 10. Now, all we need is to apply \( ([\mathbb{H}_c]^2 + 1)^{-1} \geq 2^{-1} |\mathbb{H}_c|^3 (([\mathbb{H}_c]^2 + 1)^{-1} \) (see e.g. the proof of theorem 3.1 in [31]) thrice to get

\[
\|\phi\|^2 \geq 2^{-6} \|([\mathbb{H}_c - i 1])^{-1} + ([\mathbb{H}_c + i 1])^{-1}] \phi, (\mathbb{H}_c - i 1)^{-2} \phi + (\mathbb{H}_c + i 1)^{-2} \phi
\]

\[
- i([\mathbb{H}_c - i 1])^{-1} - ([\mathbb{H}_c + i 1])^{-1} \phi \rangle |.\]
Transferring \([([\mathbb{H}^c + i \mathbb{I})^{-1} + (\mathbb{H}^e + i \mathbb{I})^{-1}])\) in the latter scalar product from left to right gives the result as claimed.

Assume that \(\psi_\sigma \in \mathcal{H}_{-3} \setminus \mathcal{H}_{-2}\). In view of (5.4)

\[
\{ \frac{3i}{2} [(\mathbb{H}^c + i \mathbb{I})^{-2} + (\mathbb{H}^e + i \mathbb{I})^{-2}] + (\mathbb{H}^c - i \mathbb{I})^{-3} + (\mathbb{H}^e - i \mathbb{I})^{-3} \} \psi_\sigma \in \mathcal{H}_3.
\]

Since \(\mathcal{H}_3 \subset \mathcal{H}_0 \subset \mathcal{H}_{-3}\) densely, for \(f = \sum_\sigma \psi_\sigma \otimes \sigma \in \mathcal{H}_0\)

\[
\{ \frac{3i}{2} [(\mathbb{H}^c + i \mathbb{I})^{-2} + (\mathbb{H}^e + i \mathbb{I})^{-2}] + (\mathbb{H}^c - i \mathbb{I})^{-3} + (\mathbb{H}^e - i \mathbb{I})^{-3} \} \psi_\sigma, f \}
\]

\[
= \psi_\sigma \{ \frac{3i}{2} [(\mathbb{H}^c - i \mathbb{I})^{-2} - (\mathbb{H}^e - i \mathbb{I})^{-2}] + (\mathbb{H}^c - i \mathbb{I})^{-3} + (\mathbb{H}^e - i \mathbb{I})^{-3} \} f
\]

\[
= \psi_\sigma \{ \frac{3i}{2} [P(i) - P(-i)] + \frac{1}{2} P(i)' + \frac{1}{2} P(-i)'' \} f
\]

where in the last step we also use the relations

\[
R^e(z)' = \frac{\partial}{\partial w} R^e(w)|_{w=z}, \quad R^e(z)'' = \frac{\partial^2}{\partial w^2} R^e(w)|_{w=z}
\]

for \(z \in \text{res } \mathbb{H}^e\). Thus, by (4.3) and (5.1)

\[
\{ \frac{3i}{2} [(\mathbb{H}^c + i \mathbb{I})^{-2} - (\mathbb{H}^e - i \mathbb{I})^{-2}] + (\mathbb{H}^c + i \mathbb{I})^{-3} + (\mathbb{H}^e - i \mathbb{I})^{-3} \} \psi_\sigma, f \}
\]

\[
= N_\sigma \sum_{\sigma'} \lim_{Q \to Q_0} \int \{ - \frac{3i}{2} [R^e_\sigma \sigma'(i) (Q_0 - Q) - R^e_\sigma \sigma'(-i) (Q_0 - Q)']
\]

\[
+ \frac{1}{2} R^e_\sigma \sigma'(i) (Q_0 - Q)'' + \frac{1}{2} R^e_\sigma \sigma'(-i) (Q_0 - Q)'' \} dQ
\]

(5.5)

where

\[
R^e_\sigma \sigma'(z)(Q)' = \frac{\partial}{\partial w} R^e_\sigma \sigma'(w)(Q)|_{w=z}, \quad R^e_\sigma \sigma'(z)(Q)'' = \frac{\partial^2}{\partial w^2} R^e_\sigma \sigma'(w)(Q)|_{w=z}
\]

for \(\Im z \neq 0\). But

\[
\overline{R^e_\sigma \sigma'(z)(Q)} = R^e_\sigma \sigma'(\overline{z})(-Q)
\]

by (4.4), and hence

\[
\{ \frac{3i}{2} [(\mathbb{H}^c + i \mathbb{I})^{-2} - (\mathbb{H}^e - i \mathbb{I})^{-2}] + (\mathbb{H}^c + i \mathbb{I})^{-3} + (\mathbb{H}^e - i \mathbb{I})^{-3} \} \psi_\sigma
\]

\[
= N_\sigma \sum_{\sigma'} \{ 3i [R^e_\sigma \sigma'(-i)(-Q_0)' - R^e_\sigma \sigma'(i)(-Q_0)']
\]

\[
+ R^e_\sigma \sigma'(-i)(-Q_0)'' + R^e_\sigma \sigma'(i)(-Q_0)'' \} \otimes |\sigma'\rangle
\]

(5.6)

a.e. on \(\mathbb{R}^6\). When deriving (5.6) from (5.5) we have also used the following property: Since the Lebesgue integral \(\int_\mathbb{R}^6\) on the left-hand side of (5.5) exists by hypothesis on \(\psi_\sigma\), it coincides with the improper Riemann integral \(\lim_{\mathcal{F}_{\sigma'}, \sigma' \to \mathcal{F}_{\sigma'}} \int_{|Q| \leq R}\).

By (5.1) and (5.6), the duality pairing on the right-hand side of (5.4) with \(\phi = \psi_\sigma\) is therefore given by
\[
\frac{N^2}{2} \lim_{|Q| \to 0} \left( 3i[R^c_{\sigma\sigma}(-i)(Q)' - R^c_{\sigma\sigma}(i)(Q)'] + R^c_{\sigma\sigma}(-i)(Q)'' + R^c_{\sigma\sigma}(i)(Q)'' \right).
\]

It suffices to take \( R^c_{\sigma\sigma}(\pm i) \) as in (4.6) to show the non-existence of (5.7):
\[
3i[R^c_{\sigma\sigma}(-i)(Q)' - R^c_{\sigma\sigma}(i)(Q)'] + R^c_{\sigma\sigma}(-i)(Q)'' + R^c_{\sigma\sigma}(i)(Q)'' = O(\log |Q|) \quad \text{as} \quad |Q| \searrow 0
\]

i.e. \( \psi_\sigma \not\in \mathcal{H}_{-3} \).

Assume that \( \psi_\sigma \in \mathcal{H}_{-4} \). Then
\[
\|\psi_\sigma\|_{-4} \lesssim \|\psi_\sigma\|_{-4}^* = \|(i(\mathbb{H}^c)^2 + \mathbb{I})^{-1}\psi_\sigma\|_0 = \frac{1}{2} \|((\mathbb{H}^c - i\mathbb{I})^{-1} - (\mathbb{H}^c + i\mathbb{I})^{-1})\psi_\sigma\|.
\]

By rearranging the terms within the equivalent norm \( \|\psi_\sigma\|_{-4}^* \) we get that
\[
\|\psi_\sigma\|_{-4}^* = \frac{1}{4} \langle \psi_\sigma, \{i[(\mathbb{H}^c + i\mathbb{I})^{-1} - (\mathbb{H}^c - i\mathbb{I})^{-1}] - (\mathbb{H}^c + i\mathbb{I})^{-2} - (\mathbb{H}^c - i\mathbb{I})^{-2} \} \psi_\sigma \rangle.
\]

Then, repeating the steps that were used for obtaining (5.6) we get that
\[
\|\psi_\sigma\|_{-4}^* = \frac{N^2}{4} \lim_{|Q| \to 0} (i[R^c_{\sigma\sigma}(-i)(Q) - R^c_{\sigma\sigma}(i)(Q)] - R^c_{\sigma\sigma}(-i)(Q)' - R^c_{\sigma\sigma}(i)(Q)').
\]

Again, taking \( R^c_{\sigma\sigma}(\pm i) \) as in (4.6), we get that \( \|\psi_\sigma\|_{-4}^* = N_\sigma/(16\sqrt{2}\pi) \); hence \( \psi_\sigma \in \mathcal{H}_{-4} \).

Using proposition 9, the above formula gives (5.3). This accomplishes the proof of the theorem.

\[\square\]

6. Concluding remarks and discussion

In the paper, in theorem 3 and corollary 4, we present the integral kernel of the one-parameter unitary group for the Rashba spin–orbit coupled operator in dimension three. The main motive for considering the unitary group is to derive the Green function, (4.3) and (4.4), for the corresponding two-particle operator, which is necessary for the spectral analysis of spin–orbit coupled cold molecules. For \( \alpha \geq 0 \) small, we compute explicitly the elements of the two-particle Green function in propositions 8, 9 and A.1.

The interatomic interaction is zero-range and therefore we apply the singular perturbation theory. We show that, since the two-particle Hamiltonian in the center-of-mass coordinate system is non-separable for \( \alpha > 0 \), the perturbation associated to the total Hamiltonian is supersingular (theorem 11). As a result, no self-adjoint operator can be constructed for describing the formation of spin–orbit coupled molecules with point-interaction. Instead, one considers the so-called regular operators whose spectrum is known to be pure real. The spectral properties of the regular operators are described by the generalized Krein Q-function; in particular, the zeroes of the function represent the singular points of the resolvent [23, equation (4.15)]. For small spin–orbit-coupling strength, the Q-function can be found analytically by using the two-particle Green function derived in the present paper.

For example, assume that \( \beta = 0 \) and \( \alpha \) is so small that we can practically put \( \alpha = 0 \). Formally, the problem reduces to the analysis of the operator \( -2\Delta_x + \frac{1}{\lambda} \Delta_x \) (which is separable) plus the \( \lambda \)-dependent singular perturbation. Using (4.6), the resolvent formula in [23], and the normalization constant \( 16\sqrt{2}\pi \) (see (5.3)), the singular points \( \lambda \) of the restricted
(to the original Hilbert space) two-particle resolvent of the one-parameter regular operator satisfy the relation

$$0 = (1 + \lambda)[2(1 + 3\lambda) + \pi(\gamma(1 + \lambda) - 1)] - 4\lambda^2 \log(-\lambda)$$

for some non-uniquely defined real parameter \(\gamma\); hence \(\lambda < 0\) necessarily. On the other hand, when we associate the perturbation to \(-2\Delta_x\), we have the two-particle case described in [21, theorems 5.2.1 and 5.2.2]. Namely, one solves the eigenvalue problem for the single-particle operator \(-2\Delta + 2c\delta\), with \(c\) as in remark 12, for which it is well-known that there is the single eigenvalue below 0. The question, which was raised in [23] in a much more general setting, is whether there exists the similarity operator that transforms the non-self-adjoint case to the self-adjoint one.

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**Appendix. Non-diagonal elements of Green function**

Here we list non-diagonal elements \(R_{\sigma'\sigma}(z)\) of the two-particle Green function up to \(O(\alpha^4)\); recall (4.4).

**Proposition A.1.** For \(\Im z \neq 0\) and \(\alpha \geq 0\) arbitrarily small, the non-diagonal element \((\sigma' \neq \sigma)\)

$$R_{\sigma'\sigma}(z) = \alpha \Delta_{\sigma'\sigma}^{(1)}(z) + \alpha^2 \Delta_{\sigma'\sigma}^{(2)}(z) + \alpha^3 \Delta_{\sigma'\sigma}^{(3)}(z) + O(\alpha^4) \quad (A.1)$$

where

$$\Delta_{\sigma'\sigma}^{(1)}(z)(Q) = \frac{\pm i}{16\sqrt{2\pi}^3 \beta |Q|^3} \left( (\delta_{\nu'\nu} \delta_{\nu'1} \delta_{\nu0}[X^- - (-1)^{s'}x^-] \
- \delta_{\nu'0} \delta_{\nu1} \delta_{\nu0} [X^+ - (-1)^{s'}x^+]) \right)^{3/2} \mathcal{K}_3(|Q| \sqrt{-z}) \\nonumber$$

$$- (z - 2\beta)^{3/2} \mathcal{K}_3(|Q| \sqrt{2\beta - z}) \\nonumber$$

$$+ (\delta_{\nu'0} \delta_{\nu1} \delta_{\nu1} [(-1)^{s'}X^- - x^-] - \delta_{\nu'1} \delta_{\nu1} \delta_{\nu0} [(-1)^{s'}X^+ - x^+]) \\nonumber$$

$$\times [z^{1/2} \mathcal{K}_3(|Q| \sqrt{-z}) - (z + 2\beta)^{1/2} \mathcal{K}_3(|Q| \sqrt{2\beta - z})] \quad (A.2a)$$

$$\Delta_{\sigma'\sigma}^{(2)}(z)(Q) = - \frac{1}{64\sqrt{2\pi}^3 \beta^2 |Q|^4} \left( 2\delta_{\nu'S} \delta_{\nu1} \delta_{\nu'-1} [x^- X^- + \delta_{\nu'-1} x^+ X^+] \\nonumber$$

$$+ (-1)^{s'} \delta_{\nu'0} \delta_{\nu1} [X^- x^+ - x^+ X^-]) \mathcal{K}_4(|Q| \sqrt{-z}) \\nonumber$$

$$- (z + 2\beta)^2 \mathcal{K}_4(|Q| \sqrt{2\beta - z}) - (z - 2\beta)^2 \mathcal{K}_4(|Q| \sqrt{2\beta - z}) \right), \quad (A.2b)$$
\[ \Delta^{(3)}_{\sigma',\sigma}(z)(Q) = \frac{1}{32 \sqrt{2\pi^3 \beta^3}} \times \left( \delta_{\sigma',1} \delta_{S1} \delta_{a0} [X^- - (-1)^S x^-] 
\quad - \delta_{\sigma',0} \delta_{S1} [X^+ - (-1)^S x^+] [3(z - 2\beta)^2 K_4(|Q| \sqrt{2\beta - z}) 
\quad - 4\beta K_4(|Q| \sqrt{2\beta - z}) + (z + 2\beta)^2 K_4(|Q| \sqrt{2\beta - z}) 
\quad \pm 2i \beta |Q| (z - 2\beta)^{3/2} K_3(|Q| \sqrt{2\beta - z}) 
\quad + (\delta_{\sigma',0} \delta_{S1} [-1]^{\frac{S}{2}} X^- - x^-] - \delta_{\sigma',-1} \delta_{S1} [(-1)^S X^+ - X^+]) \right) \times \left[ 3(z + 2\beta)^2 K_4(|Q| \sqrt{2\beta - z}) - 4\beta K_4(|Q| \sqrt{2\beta - z}) 
\quad + (z - 2\beta)^2 K_4(|Q| \sqrt{2\beta - z}) \right] \times (A.2c) \]

for a.e. \( Q = (x, X) \in \mathbb{R}^6 \); the upper (lower) sign is taken when \( \Im z > 0 \) (\( \Im z < 0 \)). When in addition \( \beta = 0 \), one assumes the limit \( \beta \xrightarrow{\leftarrow} 0 \) in the above expressions.

**Proof.** We have by (4.4)

\[ R_{S',\sigma}(z)(x,X) = \int_0^\infty e^{\pm iz} K^0_{\pm,\pm}(x)K^0_{\pm,\pm}(X) \times \left( \frac{\alpha}{2\sqrt{2\pi t}} b_{\pm}(a_{\pm} - \beta b_{\pm}) \delta_{\sigma',1} \delta_{S1} \delta_{a0} [X^- - (-1)^S x^-] 
\quad - \delta_{\sigma',0} \delta_{S1} [X^+ - (-1)^S x^+] (a_{\pm} + \beta b_{\pm}) 
\quad - \delta_{\sigma',-1} \delta_{S1} [(-1)^S X^- - x^-] - \delta_{\sigma',1} \delta_{S1} [(-1)^S X^+ - X^+] \right) \times \left[ 3(z + 2\beta)^2 K_4(|Q| \sqrt{2\beta - z}) - 4\beta K_4(|Q| \sqrt{2\beta - z}) 
\quad + (z - 2\beta)^2 K_4(|Q| \sqrt{2\beta - z}) \right] \times \left( -1 \right)^S \delta_{\sigma',0} (1 - \delta_{S,3}) [x^- X^+ - x^+ X^-] \right) dt \times (A.3) \]

for \( \sigma' \neq \sigma \). Using \( a_{-\nu} = \overline{a_{\nu}} \) (and similarly for \( b_{-\nu} \)) and the exponentiation of sine and cosine functions, substitute (3.5) in (A.3), and then apply (4.10c) for \( n \in \{1, 2\} \), and deduce (A.1) and (A.2a).

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