Analytical coupled-channels treatment of two-body scattering in the presence of three-dimensional isotropic spin-orbit coupling

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It is shown that the single-particle spin-orbit coupling terms, which—in the cold atom context—are associated with synthetic gauge fields, can significantly and non-trivially modify the phase accumulation at small interparticle distances even if the length scale $(k_{so})^{-1}$ associated with the spin-orbit coupling term is significantly larger than the van der Waals length $r_{vdW}$ that characterizes the two-body interaction potential. A theoretical framework, which utilizes a generalized local frame transformation and accounts for the phase accumulation analytically, is developed. Comparison with numerical coupled-channels calculations demonstrates that the phase accumulation can, to a very good approximation, be described over a wide range of energies by the free-space scattering phase shifts—evaluated at a scattering energy that depends on $k_{so}$—and the spin-orbit coupling strength $k_{so}$.

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The tunability of low-energy scattering parameters such as the $s$-wave scattering length $a_s$ and $p$-wave scattering volume $V_p$ by means of application of an external magnetic field in the vicinity of a Feshbach resonance [1] has transformed the field of ultracold atom physics, providing experimentalists with a knob to “dial in” the desired Hamiltonian. This tunability has afforded the investigation of a host of new phenomena including the BEC-BCS crossover [2, 3]. Most theoretical treatments of these phenomena are formulated in terms of a few scattering quantities such as $a_s$ and $V_p$, which properly describe the low-energy behavior of the two-body system.

The recent realization of spin-orbit coupled cold atom systems [4] is considered another milestone, opening the door for the observation of topological properties and providing a new platform with which to study scenarios typically encountered in condensed matter systems with unprecedented control [5–7]. An assumption that underlies most theoretical treatments of cold atom systems with synthetic gauge fields is that the spin-orbit coupling term, i.e., the Raman laser that couples the different internal states or the shaking of the lattice that couples different bands, leaves the atom-atom interactions “untouched”. More specifically, mean-field treatments “simply” add the single-particle spin-orbit coupling term to the mean-field Hamiltonian and parameterize the atom-atom interactions via contact potentials with coupling strengths that are calculated for the two-body van der Waals potential without the spin-orbit coupling terms [4–8].

Consistent with such mean-field approaches, most two-body scattering studies derive observables based on the assumption that the two-body Bethe-Peierls boundary condition, derived in the absence of single-particle spin-orbit coupling terms, remains unaffected by the spin-orbit coupling terms, provided an appropriate “basis transformation” is accounted for [9–11]. The underlying premise of these two-body and mean-field treatments is rooted in scale separation, which suggests that the free-space scattering length $a_s$ and scattering volume $V_p$ remain good quantities provided $(k_{so})^{-1}$ is larger than the two-body van der Waals length $r_{vdW}$. Indeed, model calculations for a square-well potential in the presence of three-dimensional isotropic spin-orbit coupling suggest that the above reasoning holds, provided $1/a_s$ and $V_p$ are small [17].

This work revisits the question of how to obtain and parameterize two-body scattering observables in the presence of three-dimensional isotropic spin-orbit coupling. Contrary to what has been reported in the literature, our calculations for Lennard-Jones and square-well potentials show that the three-dimensional isotropic spin-orbit coupling terms can impact the phase accumulation in the small interparticle distance region where the two-body interaction potential cannot be neglected even if $(k_{so})^{-1}$ is notably larger than $r_{vdW}$. We observe non-perturbative changes of the scattering observables when $k_{so}$ changes by a small amount. An analytical treatment, which reproduces the full coupled-channels results such as the energy-dependent two-body cross sections for the finite-range potentials with high accuracy, is developed. Our analytical treatment relies, as do previous treatments [9–13, 12–17], on separating the short- and large-distance regions. The short-distance Hamiltonian is treated by applying a gauge transformation, followed by a rotation, that “replaces” the $p$-dependent spin-orbit coupling term by an $r$- and $p$-independent diagonal matrix ($r$ and $p$ denote the relative position and momentum vectors, respectively). The diagonal terms, which can be interpreted as shifting the scattering energy in each channel, can introduce non-perturbative changes in the scattering observables for small changes in $k_{so}$, especially when $V_p$ is large. We note that our derivation of the short-distance Hamiltonian, although similar in spirit, differs in subtle but important ways from what is presented in Ref. [10, 12].

Our analytical framework also paves the way for designing energy-dependent zero-range or $\delta$-shell pseudo-
potentials applicable to systems with spin-orbit coupling. While energy-dependent pseudo-potentials have proven useful in describing systems without spin-orbit coupling [18, 19], generalizations to systems with spin-orbit coupling are non-trivial due to the more intricate nature of the dispersion curves. Our results suggest a paradigm shift in thinking about spin-orbit coupled systems with non-vanishing two-body interactions. While the usual approach is to assume that the short-distance behavior or the effective coupling strengths are not impacted by the spin-orbit coupling terms, our results suggest that they can be for specific parameter combinations. Even though our analysis is carried out for the case of three-dimensional isotropic spin-orbit coupling, our results point toward a more general conclusion, namely that spin-orbit coupling terms may, in general, notably modify the phase accumulation in the short-distance region.

We consider two particles with position vectors \( r_1 \) and masses \( m_j \) \((j = 1 \text{ and } 2)\) interacting through a spherically symmetric two-body potential \( V_{\text{int}}(r) = |r_1 - r_2| \). Both particles feel the isotropic spin-orbit coupling term with strength \( k_{so} \), \( V_{so}^{(j)} = h k_{so} \sigma_j \cdot \mathbf{r}/m_j \), where \( \sigma_j \) denotes the canonical momentum operator of the \( j \)-th particle and \( \mathbf{r} \) the vector that contains the three Pauli matrices \( \sigma_x^{(j)}, \sigma_y^{(j)} \) and \( \sigma_z^{(j)} \) for the \( j \)-th particle. Throughout, we assume that the expectation value of the total momentum operator \( \mathbf{P} \) of the two-body system vanishes. In this case, the total angular momentum operator \( \mathbf{J} = \mathbf{I} + \mathbf{S} \), of the two-particle system commutes with the system Hamiltonian and the scattering solutions can be labeled by the quantum numbers \( J \) and \( M_J \); \( M_J \) denotes the projection quantum number, \( \mathbf{I} \) is the relative orbital angular momentum operator, and \( \mathbf{S} = \hbar (\sigma_1 + \sigma_2)/2 \).

Separating off the center of masses degrees of freedom, the relative Hamiltonian \( \tilde{H} = \mathbf{H} + V_{so} \), \( \mathbf{H} = \mathbf{H}_{fs} + V_{so} \), where \( \mathbf{H}_{fs} = \left[ \frac{\mathbf{P}^2}{2\mu} + V_{\text{int}}(r) \right] \mathbf{I}_1 \otimes \mathbf{I}_2 \) (1)

and \( V_{so} = \hbar k_{so} \Sigma \cdot \mathbf{p}/\mu \) with \( \Sigma = (m_2 \sigma^{(1)} \otimes \mathbf{I}_2 - m_1 \mathbf{I}_1 \otimes \sigma^{(2)})/M \). Here, \( \mathbf{I}_1 \) denotes the 2 \times 2 identity matrix that spans the spin degrees of freedom of the \( j \)-th particle and \( M \) the total mass, \( M = m_1 + m_2 \). For each \( (J, M_J) \) channel, the \( r \)-dependent eigensolutions \( \tilde{\Psi}^{(J, M_J)}(r) \) are expanded as [13, 14, 16]

\[
\tilde{\Psi}^{(J, M_J)}(r) = \sum_{l,S} r^{-1} u^{(J)}_{l,S}(k, r) |J, M_J; l, S>,
\]

where the sum goes over \( (l, S) = (0, 0) \) and \( (1, 1) \) for \( (J, M_J) = (0, 0) \) and over \( (l, S) = (J, 0), (J, 1), (J - 1, 1) \), and \( (J + 1, 1) \) for \( J > 0 \). In the \( |J, M_J; l, S> \) basis (using the order of the states just given), the scaled radial set of differential equations for fixed \( J \) and \( M_J \) reads \( \hbar^{(J)} u^{(J)} = E^{(J)} u^{(J)} \), where \( \hbar^{(J)} \) denotes the scaled radial Hamiltonian for a given \( J \) (note that the Hamiltonian is independent of the \( M_J \) quantum number). For \( r > r_{\text{max}} \), the interaction potential \( V_{\text{int}} \) can be neglected and \( \tilde{u}^{(J)}(J) \) is matched to the analytic asymptotic \( \tilde{V}_{\text{int}} = 0 \)

\[
\tilde{u}^{(J)} \xrightarrow{r > r_{\text{max}}} \mathcal{K}^{(J)}(J) \left( \mathcal{G}^{(J)}(J) - \mathcal{A}^{(J)}(J) \right),
\]

where \( \mathcal{G}^{(J)}(J) \) and \( \mathcal{A}^{(J)}(J) \) are matrices that contain the regular and irregular solutions for finite \( k_{so} \) (for \( J = 0 \) and 1, explicit expressions are given in Ref. [16]). Defining the logarithmic derivative matrix \( \mathcal{L}^{(J)}(J) \) through \( (\tilde{u}^{(J)})'(J)(\tilde{u}^{(J)})^{-1} \), where the prime denotes the partial derivative with respect to \( r \), the K-matrix is given by

\[
\mathcal{K}^{(J)}(J) = \left[ (r \mathcal{G}^{(J)}(J))' - \mathcal{L}^{(J)}(J) \left( r \mathcal{G}^{(J)}(J) \right) \right] \times
\]

\[
\left[ (r \mathcal{G}^{(J)}(J))' - \mathcal{L}^{(J)}(J) \left( r \mathcal{G}^{(J)}(J) \right) \right] \bigg|_{r = r_{\text{max}}},
\]

the S-matrix by \( S^{(J)}(J) = (I + i \mathcal{K}^{(J)}(J))/(I - i \mathcal{K}^{(J)}(J))^{-1} \), where \( I \) denotes the identity matrix, and the cross sections by \( \sigma_{\alpha\beta} = 2\pi |S^{(J)}_{\alpha\beta} - \delta_{\alpha\beta}|^2/k_{so}^2 \), with \( \alpha \) and \( \beta \) each take the values 1, 2, \ldots .

In general, the K-matrix has to be determined numerically via coupled-channels calculations. In what follows, we address the question whether \( \mathcal{K} \) can, at least approximatively, be described in terms of the logarithmic derivative matrix of the free-space Hamiltonian \( \tilde{H}_{fs} \). If the spin-orbit coupling term \( V_{so} \) vanished in the small \( r \) limit, one could straightforwardly apply a projection or frame transformation approach [21–24] that would project the inner small \( r \) solution, calculated assuming that \( V_{so} \) vanishes in the inner region, onto the outer large \( r \) solution, calculated assuming that \( V_{\text{int}} \) vanishes in the outer region [25]. The fact that \( V_{so} \) does not vanish in the small \( r \) limit requires, as we shall show below, a generalization of the frame transformation approach.

We start with the Hamiltonian \( \tilde{H} \) and define a new Hamiltonian \( \tilde{H} \) through \( T^{-1} \tilde{H} T \), where \( T \) is an operator to be determined. The solution \( \tilde{\Psi} \) of the new Hamiltonian is related to the solution \( \Psi \) of \( \tilde{H} \) through \( \tilde{\Psi} = T^{-1} \Psi \); here and in what follows we drop the superscripts "\( (J, M_J) \)" and "\( (J) \)" for notational convenience. The operator \( T \) reads \( RU \), where \( R = \exp(-it_{so} \Sigma \cdot \mathbf{r}) \); the form of \( U \) is introduced later. To calculate \( H_R = R^{-1} \tilde{H} R \), we use

\[
R^{-1} \tilde{H} R = H_{fs} - V_{so} - E_{so} \left[ \Sigma \cdot \mathbf{r}, \Sigma \cdot \nabla \right] + \mathcal{O}(r)
\]

and

\[
R^{-1} V_{so} R = V_{so} + 2 \left[ \Sigma \cdot \mathbf{r}, \Sigma \cdot \nabla \right] + \mathcal{O}(r),
\]

where \( -ih \nabla = \mathbf{p} \) and \( E_{so} = \hbar^2 k_{so}^2/(2\mu) \) and where the notation \( \mathcal{O}(r) \) indicates that terms of order \( r \) and higher are neglected (\( r \) "counts" as being of order \( r \) and \( \mathbf{p} \) as being of order \( r^{-1} \)). Adding Eqs. [15] and [16] and neglecting the \( \mathcal{O}(r) \) terms, we find that the spin-orbit coupling
term $V_{so}$ is replaced by a commutator that arises from the fact that the operator $\Sigma \cdot \mathbf{p}$ does not commute with the exponent of $R$,

$$H^s_R = H_{fs} + E_{so} [\Sigma \cdot \mathbf{r}, \Sigma \cdot \nabla].$$ (7)

Here, the superscript “sr” indicates that this Hamiltonian is only valid for small $r$.

Our goal is now to evaluate the second term on the right-hand side of Eq. (7). Defining the scaled short-distance Hamiltonian $h^s_R$ through $rH^s_Rr^{-1}$ and expressing $h^s_R$ in the $|J, M_J; l, S \rangle$ basis, we find

$$h^s_R = \left( \frac{-\hbar^2}{2\mu} \frac{\partial^2}{\partial r^2} + V_{int}(r) \right) I_1 \otimes I_2 + \mathbf{\mathcal{L}} + \mathbf{\mathcal{U}},$$ (8)

where $\mathbf{\mathcal{L}}$ is a diagonal matrix with diagonal elements $-3E_{so}$ and $E_{so}$. For $J > 0$, in contrast, the 11 and 22 elements are, in general, coupled:

$$\mathbf{\mathcal{L}} = E_{so} \begin{pmatrix} -3 & c/M^2 & 0 & 0 \\ c/M^2 & -(\Delta M/M)^2 & 0 & 0 \\ 0 & 0 & d_1/M^2 & 0 \\ 0 & 0 & 0 & d_2/M^2 \end{pmatrix},$$ (9)

where $\Delta M = m_1 - m_2$, $c = 2\sqrt{J(J+1)(m_2^2 - m_1^2)}$, $d_1 = -JM^2 - (J + 1)\Delta M^2$, and $d_2 = 4m_1m_2 - d_1$. Since the $r$-dependent 11 and 22 elements of $\mathbf{\mathcal{L}}$ are identical (recall $l = J$ for these two elements), the matrix $\mathbf{\mathcal{U}}$, which is defined such that $\mathbf{\mathcal{U}}^{-1} \mathbf{\mathcal{L}} \mathbf{\mathcal{U}}$ is diagonal, also diagonalizes $h^s_R$, i.e., the short-range Hamiltonian $h^s_R = \mathbf{\mathcal{U}}^{-1} h^s_R \mathbf{\mathcal{U}}$ is diagonal. This implies that the scaled radial short-distance Schrödinger equation $h^s_R \mathbf{\mathcal{L}} = E \mathbf{\mathcal{L}}$ can be solved using standard propagation schemes such as the Johnson algorithm [26]. This Schrödinger equation differs from the “normal” free-space Schrödinger equation by channel-specific energy shifts. These shifts introduce a non-trivial modification of the phase accumulation in the short-distance region and—if a zero-range or $\delta$-shell pseudo-potential description was used—of the boundary condition. While the energy shifts do, in many cases, have a negligible effect, our analysis below shows that they can introduce non-perturbative corrections in experimentally relevant parameter regimes. The channel-specific energy shifts are not taken into account in Ref. [12].

To relate the logarithmic derivative matrix $\mathbf{\mathcal{L}}^s_R(r)$ to the logarithmic derivative matrix $\mathbf{\mathcal{L}}(r)$, the “$T$-operation” needs to be “undone”. Assuming that the short-distance Hamiltonian provides a faithful description, i.e., assuming that the higher-order correction terms can, indeed, be neglected for $r < r_{max}$, we obtain

$$\mathbf{\mathcal{L}}(r_{max}) \approx \left\{ T^s_R \mathbf{\mathcal{L}}^s_R(r)^{-1} - T^{-1} \right\} \bigg|_{r=r_{max}}.$$ (10)

To illustrate the results, we focus on the $J = 0$ subspace. Denoting the usual free-space phase shifts at scattering energy $\hbar^2k^2/(2\mu)$ for the interaction potential $V_{int}$ for the $s$-wave and $p$-wave channels by $\delta_s(k)$ and $\delta_p(k)$, respectively, the short-range K-matrix $K^s$ for the Hamiltonian $h^s_R$ has the diagonal elements $\tan(\delta_s(k_s))$ and $\tan(\delta_p(k_p))$, where $\hbar^2k^2_s/(2\mu) = E + 3E_{so}$ and $\hbar^2k^2_p/(2\mu) = E - E_{so}$. If we now, motivated by the concept of scale separation, make the assumption that the phase shifts $\tan(\delta_s(k_s))$ and $\tan(\delta_p(k_p))$ are accumulated at $r = 0$ and correspondingly take the $r_{max} \to 0$ limit of Eq. (10) with $\mathbf{\mathcal{L}}^{(J)}$ given by the right-hand side of Eq. (4), we obtain the following zero-range K-matrix,

$$K_s^s = \frac{-a_s(k_s)}{k_+ - k_-} \begin{bmatrix} k^2_+ & k_+k_- & k^2_- \\ k_+k_- & k_+ - k_- & k^2_- \\ k^2_- & k_-k_+ & k^2_+ \end{bmatrix} - \frac{V_p(k_p)}{k_+ - k_-} \begin{bmatrix} k^2_+ & (k_+ - k_so)^2 & k_+k_- - k_so(k_+ - k_-) \\ (k_+ - k_so)^2 & k_-k_+ & k^2_- - k_so^2 \\ k_+k_- - k_so(k_+ - k_-) & k_-k_+ & k^2_- - k_so^2 \end{bmatrix},$$ (11)

where $\hbar k_{\perp} = \pm \sqrt{2\mu(E + E_{so}) - \hbar k_{so}}$.

To validate our analytical results, we perform numerical coupled-channels calculations. Since the wave function in the $J = 0$ subspace is anti-symmetric under the simultaneous exchange of the spatial and spin degrees of freedom of the two particles, the solutions apply to two identical fermions. The Schrödinger equation for the Lennard-Jones potential $V_{LJ}(r) = C_{12}/r^{12} - C_6/r^6$, with $C_6$ and $C_{12}$ denoting positive coefficients, is solved numerically [27]. The solid lines in Figs. 1 and 2 show the partial cross section $\sigma_{22}$ and the K-matrix element $K_{22}$ as a function of $k_{so}$ for vanishing scattering energy $E$ for a two-body potential with large $a_s(0)$ and large $V_p(0)$, respectively. The dashed lines show the results predicted by our zero-range model that accounts for the spin-orbit coupling induced energy shifts. This model provides an excellent description of the numerical results for the Lennard-Jones potential, provided the length $(k_{so})^{-1}$ associated with the spin-orbit coupling term is not too small compared to the van der Waals length $r_{vdW}$, where $r_{vdW}$ is given by $(2\mu C_6/\hbar^2)^{1/4}$ (in Figs. 1 and 2, the largest $k_{so}r_{vdW}$ considered corresponds to 0.4913 and 0.4171, respectively).

The dash-dotted lines in Figs. 1 and 2 show $\sigma_{22}$ and $K_{22}$ for the zero-range model when we set the spin-orbit coupling induced energy shifts artificially to zero. In this
case, the divergence in the $K_{22}$ matrix element at finite $k_{so}$ is not reproduced. For large $a_s(0)$ [see Fig. 1(a)], the model without energy shifts introduces deviations at the few percent level in the cross section $\sigma_{22}$. For large $V_p(0)$ [see Fig. 2(a)], in contrast, the model without the energy shifts provides a quantitatively and qualitatively poor description of the cross section $\sigma_{22}$ even for relatively small $k_{so}$ ($k_{so}a_s(0) \gtrsim 0.05$). Figures 1(c) and 2(c) demonstrate that the divergence of the $K_{22}$ matrix element occurs when the free-space scattering length $a_s(k_s)$, calculated at energy $3E_{so}$, or the free-space scattering volume $V_p(k_p)$, calculated at energy $-E_{so}$, diverge. We find that this occurs roughly when $a_s(0)k_{so} \approx 10$ and $(V_p(0))^{1/3}k_{so} \approx 0.21$; we checked that this holds quite generally, i.e., not only for the parameters considered in the figures. In Figs. 1(c) and 2(c), the “critical” $k_{so}$ values correspond to $k_{so}r_{vdW} = 0.1423$ and $k_{so}r_{vdW} = 0.1462$, respectively. For comparison, using the $k_{so}$ value for the one-dimensional realization of Ref. 4 and assuming $r_{vdW} = 100a_0$, one finds $k_{so}r_{vdW} \approx 0.03$. This suggests that the phenomena discussed in the context of Figs. 1 and 2 should be relevant to future realizations of three-dimensional isotropic spin-orbit coupling experiments.

To further explore the two-particle scattering properties in the presence of spin-orbit coupling for short-range potentials with large free-space scattering volume $V_p(0)$, Figs. 3(a) and 3(b) show the partial cross section $\sigma_{22}$ as a function of the scattering energy $-E_{so} \leq E \leq 0$ and $0 \leq E \leq 400E_{so}$, respectively, for $a_s(0)/V_p(0) = 0.3213$ and $a_s(0)k_{so} = 0.07673$. The results for the Lennard-Jones potential (dashed line) and square-well potential (solid line) are essentially indistinguishable on the scale shown. To assess the accuracy of our zero-range model, we focus on the Lennard-Jones potential and compare the numerically determined partial cross section $(\sigma_{22})^{\text{exact}}$ with the partial cross section $(\sigma_{22})^{\text{tr}}$ predicted using Eq. (11). Solid lines in Figs. 3(c) and 3(d) show the normalized difference $\Delta$, defined through $\Delta = |(\sigma_{22})^{\text{tr}} - (\sigma_{22})^{\text{exact}}|/(\sigma_{22})^{\text{exact}}$. The deviations are smaller than 1.3% for the scattering energies considered. Neglecting the spin-orbit coupling induced energy shifts in our zero-range model and calculating the normalized difference, we obtain the dashed lines in Figs. 3(c) and 3(d). Clearly, the zero-range model provides a faith-

FIG. 1: (Color online) Large $a_s(0)$ case. The black solid line shows (a) the scaled partial cross section $\sigma_{22}(k_{so})^2/(2\pi)$ and (b) the K-matrix element $K_{22}$ for $E = 0$ as a function of $k_{so}a_s(0)$ for the Lennard-Jones potential with $a_s(0)/r_{vdW} = 24.42$ and $V_p(0)/(r_{vdW})^3 = -0.2380$ (this potential supports two $s$-wave bound states in free space). The red dashed line shows the result for the zero-range model developed in this work [see Eq. (11)]; the numerical results for the Lennard-Jones potential and the model are indistinguishable on the scale shown. To illustrate the importance of the energy shifts, the blue dash-dotted line shows the results for the zero-range model that artificially neglects the energy shifts. The solid line in (c) shows the scaled energy-dependent $s$-wave scattering length $a_s(k_s)/a_s(0)$, where $\hbar^2k_s^2 = 6\mu E_{so}$.

FIG. 2: (Color online) Large $V_p(0)$ case. The black solid line shows (a) the scaled partial cross section $\sigma_{22}(k_{so})^2/(2\pi)$ and (b) the K-matrix element $K_{22}$ for $E = 0$ as a function of $k_{so}a_s(0)$ for the Lennard-Jones potential with $a_s(0)/r_{vdW} = 0.9591$ and $V_p(0)/(r_{vdW})^3 = 26.61$, corresponding to $a_s(0)/(V_p(0))^{1/3} = 0.3213$ (this potential supports four $s$-wave bound states in free space). The red dashed line shows the result for the zero-range model developed in this work [see Eq. (11)]; the model reproduces the numerical results excellently for $k_{so}a_s(0) \lesssim 0.3$. The blue dash-dotted line shows the results for the zero-range model that artificially neglects the energy shifts. The solid line in (c) shows the scaled energy-dependent $p$-wave scattering volume $V_p(k_p)/V_p(0)$, where $\hbar^2k_p^2 = -2\mu E_{so}$. The green circles mark three of the four $k_{so}a_s(0)$ values considered in Fig. 3.
V Jones potential as that used in Figs. 2 and 3 for four different values of the energy for the same Lennard-Jones potential, respectively, as a function of the energy $E$.

For both potentials, we have $a_s(0)/(V_p(0))^{1/3} = 0.3213$ [for $V_p(0) > 0$] and $k_{so} a_s(0) = 0.07673$. The length scale associated with the spin-orbit coupling is notably larger than the range of the potential ($k_{so} r_{vdW} = 0.08$ for the Lennard-Jones potential and $k_{so} r_{vdW} = 0.07676$ for the square-well potential).

(c) and (d): The solid and dashed lines show the normalized difference $\Delta$ (see text) between the cross section for the Lennard-Jones potential and the zero-range model, obtained using Eq. (11), and between that for the Lennard-Jones potential and the zero-range model that neglects the spin-orbit coupling induced energy shifts, respectively. The zero-range model derived in this work (solid line) provides an excellent description (the deviations are smaller than 1.3% for the data shown) over the entire energy regime. Panels (a) and (c) cover negative $E$ (linear scale) while panels (b) and (d) cover positive $E$ (logarithmic scale).

Figure 4 demonstrates that the non-quadratic single-particle dispersion relations. Restricting ourselves to three-dimensional isotropic spin-orbit coupling terms and spin-independent central two-body interactions, we developed an analytical coupled-channels theory that connects the short- and large-distance eigenfunctions using a generalized frame transformation. A key, previously overlooked result of our treatment is that the gauge transformation that converts the short-distance Hamiltonian to the “usual form” (i.e., a form without linear momentum dependence) introduces channel-dependent energy shifts. These energy shifts were then shown to appreciably alter the low-energy scattering observables, especially in the regime where the free-space scattering volume is large. To illustrate this, the $(J, M_J) = (0, 0)$ channel was considered exemplarily. Our framework provides the first complete analytical description that consistently accounts for all partial wave channels. Moreover, the first numerical coupled-channels results for two-particle Hamiltonian with realistic Lennard-Jones potentials in the presence of spin-orbit coupling terms were presented. The influence of the revised zero-range formulation put forward in this paper on two- and few-body bound states and on mean-field and beyond mean-field studies will be the topic of future publications.

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