

**Anisotropic pseudopotential for polarized dilute quantum gases**

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An anisotropic pseudopotential arising in the context of collisions of two particles polarized by an external field is rigorously derived and its properties are investigated. Such a low-energy pseudopotential may be useful in describing collective properties of dilute quantum gases, such as molecules polarized by an electric field or metastable  $^3P_2$  atoms polarized by a magnetic field. The pseudopotential is expressed in terms of the reactance ( $K$ ) matrix and derivatives of the Dirac  $\delta$  function. In most applications, it may be represented as a sum of a traditional spherically symmetric contact term and an anisotropic part. The former contribution may be parameterized by a generalized scattering length. The anisotropic part of the pseudopotential may be characterized by the off-diagonal scattering length for dipolar interactions and off-diagonal scattering volume for quadrupolar interactions. The two-body matrix element of the pseudopotential in a basis of plane waves is also derived.

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**I. INTRODUCTION AND PROBLEM SETUP**

The concept of a pseudopotential, i.e., full interparticle interaction being replaced by some less complicated “effective” potential, plays an important role in many subfields of physics [1]. In particular, the properties of traditional Bose-Einstein condensates (BEC) may be well understood just in terms of a  $\delta$ -function potential, with its strength determined by a single parameter—scattering length [2,3] that characterizes low-energy scattering between two particles. A rigorous derivation of a pseudopotential for spherically symmetric interactions has been carried out by Huang and Yang [4]. Here I extend their derivation to *anisotropic* interactions. I also evaluate a matrix element of the derived anisotropic pseudopotential in the basis of plane waves; this matrix element may be useful in studies of many-body properties of quantum degenerate gasses.

Unusual collective properties of bosons and fermions with anisotropic interactions have generated a considerable interest over the last few years, see, e.g., Refs. [5–14]. Below I enumerate several systems where the results of my analysis may be applicable. First, Yi and You [5] considered an application of strong electric field to an atomic condensate. The electric field induces atomic electric dipoles and thus anisotropic dipole-dipole interactions between the atoms. Another novel systems where the anisotropic interactions dominate at large separations are heteronuclear molecules [8]. Here an application of electric field is required to freeze the rotations of the molecules and to align the intrinsic molecular dipole moments with the field. *Magnetic* dipole-dipole interactions are present even for well-studied alkali-metal atoms. These interactions may be amplified for more complex atoms such as europium and chromium [15–17] with larger magnetic momenta of the ground atomic state. The influence of such magnetic dipolar interactions on the condensate properties was discussed in Ref. [9]. New systems where the anisotropy of interactions may be also of interest are metastable  $^3P_2$  alkaline-earth-metal atoms placed in external magnetic field.

Here the long-range forces are dominated by interactions of atomic quadrupoles [18]. It should be noted that the application of external magnetic or electric field is important in all these examples—the field fixes quantization axis and a condensate may be described in terms of a single order parameter.

In all the enumerated examples the collision process may be formalized using Fig. 1. Here we show a pair of identical particles interacting in the presence of an external uniform field. The  $z$  axis is chosen along the direction of the field and angle  $\theta$  determines the orientation of collision (interatomic) axis  $\hat{r}$  with respect to the field. At large separations  $r$  the particles are polarized along the direction of the field. In the most general case, as a result of a collision, a change in polarization may occur (e.g. dipole moment of a molecule could end up pointing in the direction opposite to the field). We will disregard these nonadiabatic collisions. Then the interaction between the particles may be described by a unique potential  $V(r, \theta)$ . Without loss of generality, this axially symmetric potential may be expanded into Legendre polynomials  $P_L(\cos \theta)$

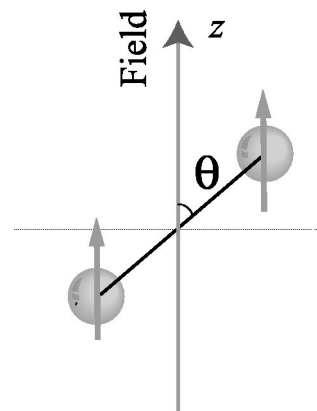


FIG. 1. Geometry of collision process. At large separations colliding particles are polarized along external field. During the collision the particles are assumed to follow a unique adiabatic potential.

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$$V(r, \theta) = V_{\text{sph}}(r) + V_{\text{anis}}(r, \theta), \quad (1)$$

$$V_{\text{anis}}(r, \theta) = \sum_{L=2,4,\dots} V_L(r) P_L(\cos \theta). \quad (2)$$

Here  $V_{\text{sph}}(r)$  and  $V_{\text{anis}}(r, \theta)$  are spherically symmetric ( $L=0$ ) and nonspherical contributions respectively. Although all even  $L$  contribute, at sufficiently large  $r$  the anisotropic contribution may be dominated by a single  $L$  term. In particular, we will focus on two practically interesting cases—dipolar ( $L=2$ )

$$V_{\text{anis}}(r, \theta) \rightarrow V_{\text{DD}} = \frac{C_3}{r^3} P_2(\cos \theta), \quad r \rightarrow \infty, \quad (3)$$

and quadrupolar ( $L=4$ )

$$V_{\text{anis}}(r, \theta) \rightarrow V_{\text{QQ}} = \frac{C_5}{r^5} P_4(\cos \theta), \quad r \rightarrow \infty \quad (4)$$

interactions. In the above equations constants  $C_{L+1}$  parametrize strengths of interactions and are proportional to the squares of respective multipole moments (e.g., molecular dipole moment).

Realistic interaction potentials  $V(\mathbf{r})$  are singular at small interparticle separations and this singularity leads to well-known problems [19] in formulating perturbative expansion for many-body properties. In particular, the matrix element of the interaction in basis of free-particle is divergent. To remedy this problem, the full interaction potential  $V$  is usually replaced by a pseudopotential  $\hat{V}$ . A rigorous derivation of the pseudopotential for spherically symmetric interactions has been carried out by [4]. Here I extend their method to anisotropic interactions.

Previously, for anisotropic dipolar interactions, Yi and You [5] proposed the following pseudopotential:

$$\hat{V}_{\text{DD}}^{\text{YY}} = g \delta(\mathbf{r}) + \frac{C_3}{r^3} P_2(\cos \theta). \quad (5)$$

Here the first term is related to the spherically symmetric part of the full potential (2) and the second contribution is simply the long-range dipolar interaction (3). This pseudopotential has been employed in a large number of studies of the properties of BECs with dipolar interactions, see, e.g., Refs. [5–12]. Although straightforward to work with in applications, the pseudopotential (5) has certain shortcomings. For example, it is not valid in the vicinity of resonances. The pseudopotential derived here resolves these shortcomings.

The goal of this work is to consistently develop a pseudopotential method for nonspherical interaction potentials. It will be required that two-body wave functions obtained with the pseudopotential  $\hat{V}$  and full original potential  $V$  to be equal at large interparticle separations. The derivation of this pseudopotential is carried out in Sec. II. Certain properties of the derived pseudopotential are discussed in Sec. III and we specialize the discussion to dipolar and quadrupolar interactions in Sec. IV. The matrix element of the pseudopotential in

free-particle basis is evaluated in Sec. V. Finally, the Appendix contains a derivation of certain low-energy limits of the  $K$  matrix in the Born approximation.

## II. ANISOTROPIC PSEUDOPOTENTIAL

We consider a solution of the Schrödinger equation for a relative motion of two particles interacting through a potential  $V(\mathbf{r})$

$$\frac{\hbar^2}{2\mu} (\nabla^2 + k^2) \Phi(\mathbf{r}) = V(\mathbf{r}) \Phi(\mathbf{r}), \quad (6)$$

where  $\mu$  is the reduced mass of the pair and  $\mathbf{k}$  is the relative linear momentum. We assume that at sufficiently large separations  $r > r_c$ ,  $r^2 V(\mathbf{r}) \rightarrow 0$  for any direction  $\hat{r}$ . We also assume that the particles are contained in some large volume with the characteristic size much larger than the extent of the potential  $r_c$ . Some arbitrary boundary conditions may be imposed on the surface of the enclosing volume. At  $r \gg r_c$  the wave function  $\Phi(\mathbf{r})$  may be expanded in free-particle solutions

$$\Phi_{\infty}(\mathbf{r}) = \sum_{lm} [\alpha_{lm} j_l(kr) - \beta_{lm} n_l(kr)] Y_{lm}(\theta, \varphi), \quad (7)$$

where  $j_l(kr)$  and  $n_l(kr)$  are spherical Bessel and Neumann functions, respectively, and  $\alpha_{lm}$  and  $\beta_{lm}$  are integration constants.

Following Ref. [4] the pseudopotential is determined by acting with  $\hbar^2/2\mu(\nabla^2 + k^2)$  on the asymptotic form (7)

$$\hat{V} \Phi_{\infty}(\mathbf{r}) = -\frac{\hbar^2}{2\mu} \sum_{lm} \beta_{lm} Y_{lm}(\theta, \varphi) \frac{(2l-1)!!(l+1)}{k^{l+1}} \frac{\delta(r)}{r^{l+2}}. \quad (8)$$

Thus the original potential  $V(\mathbf{r})$  is replaced by a sum over “lumped” multipole sources placed at  $\mathbf{r}=0$ . To complete the construction of the pseudopotential, we need to determine coefficients  $\beta_{lm}$  in terms of  $\Phi(\mathbf{r})$ . First we relate the integration constants  $\alpha_{lm}$  and  $\beta_{lm}$  by requiring the complete solution  $\Phi$  to be regular at  $r=0$

$$\beta_{lm} = \sum_{l'm'} \mathcal{K}_{lm}^{l'm'} \alpha_{l'm'}. \quad (9)$$

Here  $\mathcal{K}_{lm}^{l'm'}$  are the elements of the reactance (or  $K$ ) matrix used to parametrize multichannel scattering [20]. It is worth noting that the entire dependence of the pseudopotential on the original potential will be encapsulated in matrix elements of the  $K$  matrix.

Let us review some properties of the  $K$  matrix. First it is related to more familiar scattering matrix  $S$  via  $S = (1 + i\mathcal{K})(1 - i\mathcal{K})^{-1}$  and further to transmission or  $T$  matrix through  $S = 1 - iT$ . For low-energy collisions  $\mathcal{K} \approx -\frac{1}{2}T$ . The  $K$  matrix is real and symmetric

$$\mathcal{K}_{lm}^{l'm'}(k) = \mathcal{K}_{l'm'}^{lm}(k). \quad (10)$$

For identical bosons (fermions) only even (odd) partial waves need to be considered. The  $K$  matrix is diagonal in  $l$  and  $m$  for spherically symmetric potentials

$$[\mathcal{K}_{\text{sph}}]_{lm}^{l'm'} = \delta_{ll'} \delta_{mm'} \tan \delta_l, \quad (11)$$

where  $\delta_l$  is the phase shift for partial wave  $l$ . Compared to spherically symmetric case, *anisotropic* potentials additionally couple different partial waves. For example, dipolar interactions, Eq. (3), couple  $s$  and  $d$  waves so that  $[\mathcal{K}_{\text{DD}}]_{00}^{20} \neq 0$  and quadrupolar interactions (4) couple  $s$  and  $g$  waves. The scalar part  $V^{\text{sph}}(r)$  of the potential (2) assures nonvanishing  $\mathcal{K}_{00}^{00}$ . In practice, the  $K$  matrix for nonspherical interactions may be found from a solution of coupled radial equations [21]. In particular, it may be shown that for potentials parametrized by Eq. (2),  $\mathcal{K}_{lm}^{l'm'} \propto \delta_{mm'}$ , i.e., the  $K$  matrix is diagonal with respect to magnetic quantum numbers. In Appendix, I derive some elements of the  $K$  matrix in the Born approximation for dipolar and quadrupolar interaction.

At this point, we related the integration constants  $\alpha_{lm}$  and  $\beta_{lm}$  via elements of the  $K$  matrix, Eq. (9). Further, in the low-energy limit  $kr_c \ll 1$ , the integration constants  $\alpha_{lm}$  may be expressed in terms of  $\Phi_\infty(\mathbf{r})$  [4],

$$\alpha_{lm} = \frac{1}{2^l l!} \frac{1}{k^l} \left[ \left( \frac{d}{dr} \right)^{2l+1} \left( r^{l+1} \int Y_{lm}^*(\Omega) \Phi_\infty(\mathbf{r}) d\Omega \right) \right]_{r=0}. \quad (12)$$

Finally, combining Eqs. (8)–(12) we arrive at a generalization of pseudopotential  $\hat{\mathcal{V}}$  for anisotropic interactions,

$$\hat{\mathcal{V}}\Phi(\mathbf{r}) = -\frac{\hbar^2}{M} \sum_{lm'l'm'} \xi_{lm}^{l'm'}(k) [\hat{v}_{lm}^{l'm'} \Phi(\mathbf{r})], \quad (13)$$

where

$$\begin{aligned} \hat{v}_{lm}^{l'm'} \Phi(\mathbf{r}) &= \frac{(2l)!(l+1)}{2^{l+l'} l'! l!} Y_{lm}(\theta, \varphi) \frac{\delta(r)}{r^{l+2}} \\ &\times \left[ \left( \frac{d}{dr} \right)^{2l'+1} \left( r^{l'+1} \int Y_{l'm'}^*(\Omega) \Phi(r, \Omega) d\Omega \right) \right]_{r=0}, \end{aligned} \quad (14)$$

$$\xi_{lm}^{l'm'}(k) = \frac{\mathcal{K}_{lm}^{l'm'}}{k^{l+l'+1}}, \quad (15)$$

and  $M = 2\mu$  is a mass of the collision partner.

### III. SOME PROPERTIES OF A PSEUDOPOTENTIAL

The derived anisotropic pseudopotential (13) is one of the main results of this work. The spherically symmetric pseudopotential of Huang and Yang [4] is subsumed in this equation. Indeed, for spherically symmetric interactions the  $K$  matrix is diagonal in  $l, l'$  and  $m, m'$  and is expressed in terms

of conventional phase shifts, Eq. (11). Upon substitution of Eq. (11) into pseudopotential (13) we recover as a limiting case the result of Ref. [4]. As the pseudopotential of Huang and Yang [4] the anisotropic pseudopotential is non-Hermitian and velocity dependent.

The pseudopotential (13) may be separated into spherically symmetric  $\hat{\mathcal{V}}_{\text{sph}}$  and anisotropic  $\hat{\mathcal{V}}_{\text{anis}}$  parts,

$$\hat{\mathcal{V}} = \hat{\mathcal{V}}_{\text{sph}} + \hat{\mathcal{V}}_{\text{anis}}, \quad (16)$$

where

$$\hat{\mathcal{V}}_{\text{sph}} = -\frac{\hbar^2}{M} \sum_{lm} \xi_{lm}^{lm}(k) \hat{v}_{lm}^{lm} \quad (17)$$

and

$$\hat{\mathcal{V}}_{\text{anis}} = -\frac{\hbar^2}{M} \sum_{(lm) > (l'm')} \xi_{lm}^{l'm'}(k) (\hat{v}_{lm}^{l'm'} + \hat{v}_{l'm'}^{lm}). \quad (18)$$

In simplifying the anisotropic part we used symmetry property (10) of the  $K$  matrix.

Let us focus first on the spherically symmetric part of the pseudopotential and in the following section we will consider the anisotropic part of the pseudopotential for dipolar and quadrupolar interactions. We expect that as in traditional BECs of dilute atomic gasses with spherically symmetric interactions, the effect of  $\hat{\mathcal{V}}_{\text{sph}}$  on collective properties will be determined mainly by the  $s$  wave contribution, i.e.,  $l=0, m=0$  term in Eq. (17),

$$\hat{\mathcal{V}}_{\text{sph}} \approx -\frac{\hbar^2}{M} \frac{\mathcal{K}_{00}^{00}}{k} \hat{v}_{00}^{00}.$$

It may be shown that for realistic potentials the following low-energy limit is finite:

$$a_{ss} = -\lim_{k \rightarrow 0} \frac{\mathcal{K}_{00}^{00}(k)}{k}, \quad (19)$$

this quantity is a generalized scattering length. With this definition, the truncated pseudopotential reduces to

$$\hat{\mathcal{V}}_{\text{sph}} \Phi(\mathbf{r}) \approx 4\pi \frac{\hbar^2}{M} a_{ss} \delta(\mathbf{r}) \frac{\partial}{\partial r} [r \Phi(\mathbf{r})],$$

where we used  $\delta(\mathbf{r}) = \delta(r)/(4\pi r^2)$  consistent with Ref. [4]. Finally, for sufficiently slowly varying wave function,  $|d \ln \Phi / d \ln r| \ll 1$ , we recover a conventional contact pseudopotential

$$\hat{\mathcal{V}}_{\text{sph}} \approx 4\pi \frac{\hbar^2}{M} a_{ss} \delta(\mathbf{r}) \quad (20)$$

widely employed in studies of BECs.

Having discussed the spherically symmetric part of the pseudopotential, in the following section we consider the anisotropic part of pseudopotential (18) for dipolar and quadrupolar interactions.

#### IV. DIPOLAR AND QUADROPOLAR INTERACTIONS

At this point we derived an anisotropic pseudopotential, Eq. (13). We separated the pseudopotential into spherically symmetric and anisotropic contributions. We found that the spherically symmetric contribution reduces to a familiar contact term (20), widely employed in studies of Bose condensates; the only modification being an introduction of generalized scattering length (19). In this section we focus on the anisotropic contribution and illustrate some of its properties for dipolar and quadrupolar interactions of identical bosons. These interactions were defined in the introductory section as potentials that at large separations  $r$  are dominated by

$$V_{\text{anis}}^{\text{DD}}(r, \theta) \rightarrow \frac{C_3}{r^3} P_2(\cos \theta) \quad (21)$$

for dipolar interactions and

$$V_{\text{anis}}^{\text{QQ}}(r, \theta) \rightarrow \frac{C_5}{r^5} P_4(\cos \theta) \quad (22)$$

for quadrupolar interactions.

Anisotropic interactions mix different partial waves ( $lm$ ) and ( $l'm'$ ) via off-diagonal elements of the  $K$  matrix. From examining Eq. (A2) in the Appendix, one may determine that angular selection rules lead to coupling of  $s$  and  $d$  waves for dipolar interactions and  $s$  and  $g$  waves for quadrupolar interactions. In the following we assume that the dominant anisotropic effect on condensate properties arises due to these particular couplings. Therefore,

$$\hat{V}_{\text{anis}}^{\text{DD}} \approx -\frac{\hbar^2}{M} \frac{\mathcal{K}_{00}^{20}}{k^3} (\hat{v}_{00}^{20} + \hat{v}_{20}^{00}),$$

$$\hat{V}_{\text{anis}}^{\text{QQ}} \approx -\frac{\hbar^2}{M} \frac{\mathcal{K}_{00}^{40}}{k^5} (\hat{v}_{00}^{40} + \hat{v}_{40}^{00}).$$

For dipolar interactions it may be shown (Refs. [22,23] and the Appendix of this paper) that the following low-energy limit is finite:

$$a_{sd}^{\text{DD}} = -\lim_{k \rightarrow 0} \frac{\mathcal{K}_{00}^{20}(k)}{k}. \quad (23)$$

We will call this quantity off-diagonal scattering length. Similarly, for quadrupolar interactions we may introduce off-diagonal scattering volume

$$a_{sg}^{\text{QQ}} = -\lim_{k \rightarrow 0} \frac{\mathcal{K}_{00}^{40}(k)}{k^3}. \quad (24)$$

In the Appendix we employ the Born approximation and find

$$a_{sd}^{\text{DD}} \approx \frac{1}{12\sqrt{5}} \frac{M}{\hbar^2} C_3,$$

$$a_{sg}^{\text{QQ}} \approx \frac{2}{7!} \frac{M}{\hbar^2} C_5.$$

It is worth noting that the above results are valid only away from resonances. In a general case one has to find off-diagonal scattering length or volume by solving corresponding scattering problem.

Finally the total truncated pseudopotential is given by

$$\hat{V} \approx 4\pi \frac{\hbar^2}{M} a_{ss} \delta(\mathbf{r}) + \hat{V}_{\text{anis}}^{\text{DD,QQ}}, \quad (25)$$

with

$$\hat{V}_{\text{anis}}^{\text{DD}} \Phi(\mathbf{r}) \approx \frac{\hbar^2}{M} \frac{a_{sd}^{\text{DD}}}{k^2} \sqrt{5} \times \left\{ \frac{1}{8} \delta(\mathbf{r}) \left[ \left( \frac{\partial}{\partial r} \right)^5 r^3 \int P_2(\cos \theta) \Phi(\mathbf{r}) d\Omega \right] + 9 \frac{\delta(r)}{r^4} P_2(\cos \theta) \left[ \frac{\partial}{\partial r} [r \Phi(\mathbf{r})] \right]_{r \rightarrow 0} \right\} \quad (26)$$

for dipolar interactions and

$$\hat{V}_{\text{anis}}^{\text{QQ}} \Phi(\mathbf{r}) \approx \frac{1}{2^7} \frac{\hbar^2}{M} \frac{a_{sg}^{\text{QQ}}}{k^2} \times \left\{ \delta(\mathbf{r}) \left[ \left( \frac{\partial}{\partial r} \right)^9 r^5 \int P_4(\cos \theta) \Phi(\mathbf{r}) d\Omega \right] + 5(8!) \frac{\delta(r)}{r^6} P_4(\cos \theta) \left[ \frac{\partial}{\partial r} [r \Phi(\mathbf{r})] \right]_{r \rightarrow 0} \right\} \quad (27)$$

for quadrupolar interactions. Quantities  $\delta(r)/r^n$  may be recognized as the  $n^{\text{th}}$  derivatives of the Dirac delta-function.

The constructed pseudopotential depends on the relative momentum  $k$ , i.e., the potential is velocity dependent. In practice, the velocity dependence is most easily treated in the momentum representation and in the following section we evaluate the matrix element of the derived pseudopotential in the basis of plane waves.

#### V. MATRIX ELEMENT OF ANISOTROPIC PSEUDOPOTENTIAL IN FREE-PARTICLE BASIS

While considering effects of two-particle interactions on properties of a quantum many-body system, one may require a matrix element of the derived pseudopotential in free-particle (plane-wave) basis. We define this matrix element as

$$\bar{V}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}'_1, \mathbf{k}'_2) \equiv \frac{1}{(2\pi)^6} \int d\mathbf{r} d\mathbf{r}' e^{-i\mathbf{k}_1 \cdot \mathbf{r}} e^{-i\mathbf{k}_2 \cdot \mathbf{r}'} \times \hat{Y}(\mathbf{r} - \mathbf{r}') e^{i\mathbf{k}'_1 \cdot \mathbf{r}} e^{i\mathbf{k}'_2 \cdot \mathbf{r}'}. \quad (28)$$

The pseudopotential  $\hat{Y}$ , Eq. (13), depends on the momentum of relative motion of the interacting pair  $\mathbf{k} = \frac{1}{2}(\hat{\mathbf{p}} - \hat{\mathbf{p}}')$ , where  $\hat{\mathbf{p}}$  and  $\hat{\mathbf{p}}'$  are momenta conjugated to  $\mathbf{r}$  and  $\mathbf{r}'$ , respectively. To separate center of mass and relative motions, we change the variables to  $\mathbf{R} = (\mathbf{r} + \mathbf{r}')/2$  and  $\mathbf{r}_{12} = \mathbf{r} - \mathbf{r}'$ . With such a substitution

$$\bar{V}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}'_1, \mathbf{k}'_2) = \frac{1}{(2\pi)^3} \delta_{\mathbf{k}'_1 + \mathbf{k}'_2, \mathbf{k}_1 + \mathbf{k}_2} \left( -\frac{\hbar^2}{M} \right) \times \sum_{l'l'mm'} \xi_{lm}^{l'm'}(k') \int d\mathbf{r}_{12} \times \exp[-i\mathbf{k} \cdot \mathbf{r}_{12}] \hat{v}_{lm}^{l'm'} \exp[i\mathbf{k}' \cdot \mathbf{r}_{12}].$$

Here we introduced two relative momenta

$$\mathbf{k} = \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2) \quad \text{and} \quad \mathbf{k}' = \frac{1}{2}(\mathbf{k}'_1 - \mathbf{k}'_2). \quad (29)$$

The delta function  $\delta_{\mathbf{k}'_1 + \mathbf{k}'_2, \mathbf{k}_1 + \mathbf{k}_2}$  ensures conservation of the total linear momentum. Further we use partial-wave expansion

$$\exp[i\mathbf{k}' \cdot \mathbf{r}_{12}] = 4\pi \sum_{l'm_1} i^{l_1} j_{l_1}(k' r_{12}) Y_{l_1 m_1}^*(\hat{k}') Y_{l_1 m_1}(\hat{r}_{12})$$

and arrive at

$$\int d\mathbf{r}_{12} \exp[-i\mathbf{k} \cdot \mathbf{r}_{12}] \hat{v}_{lm}^{l'm'}(\mathbf{r}_{12}) \exp[i\mathbf{k}' \cdot \mathbf{r}_{12}] = (4\pi)^2 i^{l'-l} \frac{l+1}{2l+1} (k')^{l'} k^l Y_{l'm'}^*(\hat{k}') Y_{lm}(\hat{k}).$$

Finally, the matrix element of the anisotropic pseudopotential may be expressed in terms of relative momenta as

$$\bar{V}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}'_1, \mathbf{k}'_2) = \delta_{\mathbf{k}'_1 + \mathbf{k}'_2, \mathbf{k}_1 + \mathbf{k}_2} \times \bar{v} \left( \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2), \frac{1}{2}(\mathbf{k}'_1 - \mathbf{k}'_2) \right),$$

with

$$\bar{v}(\mathbf{k}, \mathbf{k}') = -\frac{\hbar^2}{M} \frac{1}{\pi} \sum_{l'l'mm'} i^{l'-l} \frac{\mathcal{K}_{lm}^{l'm'}(k')}{k'} \times \left( \frac{k}{k'} \right)^l \frac{2l+2}{2l+1} Y_{l'm'}^*(\hat{k}') Y_{lm}(\hat{k}). \quad (30)$$

Let us once again specialize the discussion to dipolar and quadrupolar interactions. As in Sec. IV we assume that the dominant anisotropic effect arises due to couplings of  $s$  and  $d$

partial waves for dipolar interactions and due to mixing of  $s$  and  $g$  waves for quadrupolar interactions. The corresponding truncated matrix element (30) may be represented as

$$\bar{v}(\mathbf{k}, \mathbf{k}') \approx \frac{1}{2\pi^2} \frac{\hbar^2}{M} \{a_{ss} + \mathcal{F}(\mathbf{k}, \mathbf{k}')\} \quad (31)$$

with  $\mathcal{F}$  replaced by

$$\mathcal{F}^{\text{DD}}(\mathbf{k}, \mathbf{k}') = -a_{sd}^{\text{DD}} \left\{ \sqrt{5} P_2(\cos \theta_{k'}) + \frac{3}{\sqrt{5}} \left( \frac{k}{k'} \right)^2 P_2(\cos \theta_k) \right\}$$

for dipolar interactions and by

$$\mathcal{F}^{\text{QQ}}(\mathbf{k}, \mathbf{k}') = a_{sg}^{\text{QQ}} \left\{ 3(k')^2 P_4(\cos \theta_{k'}) + \frac{10}{3} k^2 \left( \frac{k}{k'} \right)^2 P_4(\cos \theta_k) \right\}$$

for quadrupolar interactions. In these expressions  $a_{ss}$  is a generalized scattering length (19) and  $a_{sd}^{\text{DD}}$  and  $a_{sg}^{\text{QQ}}$  are off-diagonal scattering length and volume defined by Eq. (23) and Eq. (24), respectively.

## VI. CONCLUSION

I rigorously derived the anisotropic pseudopotential arising in the context of adiabatic collisions of two particles polarized by an external field. Such a low-energy pseudopotential may be useful in describing collective properties of dilute quantum gases, such as molecules polarized by an external electric field or metastable  $^3P_2$  atoms polarized by magnetic field. The pseudopotential is given by Eq. (13). It is naturally expressed in terms of the reactance ( $K$ ) matrix. The potential is non-Hermitian and velocity dependent. It is worth noting that in the derivation I did not require the validity of the Born approximation as in Ref. [5]. Rather I followed the method of Huang and Yang [4] and at large separations demanded the equality of solutions of the two-body Schrödinger equation with a full original potential and with a pseudopotential. Thus, compared to Eq. (5) by Yi and You [5], the derived two-body pseudopotential is expected to be also valid in the vicinity of scattering resonances.

I argued that in most applications the pseudopotential may be represented as a sum of the traditional spherically symmetric contact term and the anisotropic part, Eq. (25). The former contribution may be parametrized by a generalized scattering length (19). We specialized discussion of the anisotropic part of the pseudopotential to dipolar and quadrupolar interactions and found that it can be characterized by off-diagonal scattering length  $a_{sd}^{\text{DD}}$ , Eq. (23), for dipolar interactions and off-diagonal scattering volume  $a_{sg}^{\text{QQ}}$ , Eq. (24), for quadrupolar interactions. Although in a particular application these parameters should be determined from a solu-

tion of a multichannel scattering problem, I have derived  $a_{sd}^{\text{DD}}$  and  $a_{sg}^{\text{QQ}}$  in the Born approximations. Keeping in mind many-body applications, I have also derived a two-body matrix-element in the plane-wave basis, Eq. (30). Thus in this work I have rigorously derived an anisotropic pseudopotential for polarized dilute quantum gases and investigated its properties.

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### APPENDIX: OFF-DIAGONAL SCATTERING LENGTH $a_{sd}^{\text{DD}}$ AND SCATTERING VOLUME $a_{sg}^{\text{QQ}}$ IN THE BORN APPROXIMATION

Here we obtain expressions for the reactance ( $K$ ) matrix in the Born approximation. Using the derived  $K$  matrix we estimate off-diagonal scattering length  $a_{sd}^{\text{DD}}$  and scattering volume  $a_{sg}^{\text{QQ}}$  for dipolar (DD) and quadrupolar (QQ) interactions.

The full solution of the Schrödinger equation (6) may be represented as

$$\Phi(\mathbf{r}) = \sum_{lm} Y_{lm}(\theta, \phi) \frac{u_{lm}(r)}{kr}. \quad (\text{A1})$$

It can be shown that the radial functions  $u_{lm}(r)$  satisfy the following system of coupled differential equations:

$$\left\{ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2 \right\} u_{lm}(r) = 2\mu \sum_{l'm'} \langle lm|V|l'm' \rangle u_{l'm'}(r), \quad (\text{A2})$$

with

$$\langle lm|V|l'm' \rangle(r) = \int d\Omega Y_{lm}^*(\Omega) V(\mathbf{r}) Y_{l'm'}(\Omega). \quad (\text{A3})$$

It is convenient to introduce regular and irregular solutions of homogeneous radial equations

$$F_l(kr) = kr j_l(kr),$$

$$G_l(kr) = -kr n_l(kr)$$

and corresponding standing-wave Green's function

$$g_l(r, r') = -\frac{1}{k} \begin{cases} G_l(kr') F_l(kr), & r < r' \\ G_l(kr) F_l(kr'), & r > r'. \end{cases}$$

Using these definitions, solutions to the system of inhomogeneous equations (A2) regular at  $r=0$  may be represented as

$$u_{lm}(r) = \alpha_{lm} F_l(kr) + \int_0^\infty dr' g_l(r, r') \times \left[ 2\mu \sum_{l'm'} \langle lm|V|l'm' \rangle u_{l'm'}(r') \right], \quad (\text{A4})$$

where constants  $\alpha_{lm}$  are chosen to satisfy some boundary conditions. In the spirit of the Born approximation we may find the solution of integral equations (A4) iteratively starting from

$$u_{lm}(r) \approx \alpha_{lm} F_l(kr).$$

In the lowest order in  $V$  at large  $r$  one obtains

$$u_{lm}(r) \rightarrow \alpha_{lm} F_l(kr) + G_l(kr) \alpha_{lm} \times \sum_{l'm'} \left[ -\frac{2\mu}{k} \int_0^\infty dr' F_l(kr') \times \langle lm|V|l'm' \rangle F_l(kr') \right].$$

By comparing with Eqs. (7) and (9), we arrive at an expression for elements of the  $K$  matrix in the Born approximation,

$$\mathcal{K}_{lm}^{l'm'} \approx -\frac{2\mu k}{\hbar^2} \int_0^\infty r^2 j_l(kr) j_{l'}(kr) \langle lm|V|l'm' \rangle dr. \quad (\text{A5})$$

The Born approximation generally does not hold for low-energy atomic collisions, since realistic interactions are singular at small  $r$ . However, for dipolar interactions You and co-workers [22,23] found numerically that away from resonances Born approximation works well for off-diagonal matrix elements. Keeping this observation in mind, below we derive off-diagonal scattering length and volume introduced in the main body of the paper. These parameters were defined as low-energy limits

$$a_{sd}^{\text{DD}} = -\lim_{k \rightarrow 0} \frac{[\mathcal{K}^{\text{DD}}]_{00}^{20}(k)}{k},$$

$$a_{sg}^{\text{QQ}} = -\lim_{k \rightarrow 0} \frac{[\mathcal{K}^{\text{QQ}}]_{00}^{40}(k)}{k^3}$$

for DD and quadrupolar QQ interactions. In Sec. I the DD and QQ interactions were parametrized as

$$V_{\text{DD}} = \frac{C_3}{r^3} P_2(\cos \theta),$$

$$V_{\text{QQ}} = \frac{C_5}{r^5} P_4(\cos \theta).$$

$$a_{sg}^{\text{QQ}} = \frac{1}{1260} \frac{\mu}{\hbar^2} C_5. \quad (\text{A7})$$

Using these definitions and Eq. (A5), we arrive at

$$a_{sd}^{\text{DD}} = \frac{1}{6\sqrt{5}} \frac{\mu}{\hbar^2} C_3, \quad (\text{A6})$$

It is worth emphasizing that these results were derived in the Born approximation. In a general case, to obtain parameters entering anisotropic pseudopotential (13), one has to numerically solve the system of equations (A2), especially in the vicinity of resonances.

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## Erratum: Anisotropic pseudopotential for polarized dilute quantum gases [Phys. Rev. A 67, 033607 (2003)]

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The presented derivation has made use of certain intermediate results by Huang and Yang [1,2]. These Huang-Yang formulas contained an algebraic mistake which was recently rectified by me in Ref. [3]. Taking into account the corrected Huang-Yang construction, here I present the revised versions of the affected expressions for anisotropic pseudo-potential.

Reference [3] corrects the erroneous Huang-Yang prefactor in Eq. (8). The revised Eq. (8) reads

$$\hat{V}\Phi_{\infty}(\mathbf{r}) = -\frac{\hbar^2}{2\mu} \sum_{lm} \beta_{lm} Y_{lm}(\theta, \varphi) \frac{(2l+1)!! \delta(r)}{k^{l+1} r^{l+2}}, \quad (1)$$

where  $(2l-1)!!(l+1)$  is replaced by  $(2l+1)!!$ .

In Eq. (14) the prefactor  $(2l)!(l+1)$  is replaced by  $(2l+1)!$ . The revised Eq. (14) is

$$\hat{v}_{lm}^{l'm'} \Phi(\mathbf{r}) = \frac{1}{2^{l+l'} l' ! l !} (2l+1)! Y_{lm}(\theta, \varphi) \frac{\delta(r)}{r^{l+2}} \left[ \left( \frac{d}{dr} \right)^{2l'+1} \left( r^{l'+1} \int Y_{l'm'}^*(\Omega) \Phi(r, \Omega) d\Omega \right) \right]_{r=0}. \quad (2)$$

The anisotropic parts of truncated pseudopotential for dipolar interaction, Eq. (26) Sec. IV, is changed to (in the second term the prefactor of 9 is replaced by 15).

$$\hat{V}_{\text{anis}}^{\text{DD}} \Phi(\mathbf{r}) \approx \frac{\hbar^2 a_{sd}^{\text{DD}}}{M k^2} \sqrt{5} \left\{ \frac{1}{8} \delta(\mathbf{r}) \left[ \left( \frac{\partial}{\partial r} \right)^5 r^3 \int P_2(\cos \theta) \Phi(\mathbf{r}) d\Omega \right] + 15 \frac{\delta(r)}{r^4} P_2(\cos \theta) \left[ \frac{\partial}{\partial r} [r \Phi(\mathbf{r})] \right]_{r=0} \right\}.$$

Similar modifications are introduced in the pseudopotential for quadrupolar interactions, Eq. (27),

$$\hat{V}_{\text{anis}}^{\text{QQ}} \Phi(\mathbf{r}) \approx \frac{1}{2^7} \frac{\hbar^2 a_{sg}^{\text{QQ}}}{M k^2} \left\{ \delta(\mathbf{r}) \left[ \left( \frac{\partial}{\partial r} \right)^9 r^5 \int P_4(\cos \theta) \Phi(\mathbf{r}) d\Omega \right] + 9! \frac{\delta(r)}{r^6} P_4(\cos \theta) \left[ \frac{\partial}{\partial r} [r \Phi(\mathbf{r})] \right]_{r=0} \right\},$$

where in the second contribution a prefactor of  $5(8!)$  is replaced by  $9!$ .

The matrix element of an anisotropic pseudopotential in free-particle basis (Sec. V) is modified to read

$$\int d\mathbf{r}_{12} \exp[-i\mathbf{k} \cdot \mathbf{r}_{12}] \hat{v}_{lm}^{l'm'}(\mathbf{r}_{12}) \exp[i\mathbf{k}' \cdot \mathbf{r}_{12}] = (4\pi)^2 i^{l'-l} (k')^{l'} k^l Y_{l'm'}^*(\hat{k}') Y_{lm}(\hat{k}),$$

where the prefactor of  $(l+1)/(2l+1)$  has been removed. Equation (30) becomes

$$\bar{v}(\mathbf{k}, \mathbf{k}') = -\frac{\hbar^2}{M \pi} \frac{2}{\pi^{l'mm'}} \sum_{l'l'mm'} i^{l'-l} \frac{\mathcal{K}_{lm}^{l'm'}(k')}{k'} \left( \frac{k}{k'} \right)^l Y_{l'm'}^*(\hat{k}') Y_{lm}(\hat{k}),$$

with  $(2l+2)/(2l+1)$  replaced by 2.

Finally, the corrected kernel  $\mathcal{F}$  in Eq. (30) specialized for dipolar interaction is (the prefactor  $3/\sqrt{5}$  in front of the second term of the original equation is replaced with prefactor  $\sqrt{5}$ ; the resulting equation is simplified)

$$\mathcal{F}^{\text{DD}}(\mathbf{k}, \mathbf{k}') = -a_{sd}^{\text{DD}} \sqrt{5} \left\{ P_2(\cos \theta_{k'}) + \left( \frac{k}{k'} \right)^2 P_2(\cos \theta_k) \right\}.$$

For quadrupolar interactions, the corrected kernel reads (the prefactor  $10/3$  in front of the second term of the original equation is replaced with a value of 3)

$$\mathcal{F}^{\text{QQ}}(\mathbf{k}, \mathbf{k}') = a_{sg}^{\text{QQ}} 3 \left\{ (k')^2 P_4(\cos \theta_{k'}) + k^2 \left( \frac{k}{k'} \right)^2 P_4(\cos \theta_k) \right\}.$$

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