Pseudopotential of an interaction with a power-law decay in two-dimensional systems

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We analytically derive the general pseudopotential operator of an arbitrary isotropic interaction for particles confined in two-dimensional (2D) systems using the frame work developed by Huang and Yang for three-dimensional scattering. We also analytically derive the low-energy dependence of the scattering phase shift for an arbitrary interaction with a power-law decaying tail, $V_{2D}(\rho)\propto\rho^{-\alpha}$ (for $\alpha>2$). We apply our results to the 2D dipolar gases ($\alpha=3$) as an example, calculating the momentum and dipole moment dependences of the pseudopotential for both *s*- and *p*-wave scattering channels if the two scattering particles are in the same 2D layer. Results for the *s*-wave scattering between particles in two different (parallel) layers are also investigated. Our results can be directly applied to the systems of dipolar atoms and/or polar molecules in a general 2D geometry.

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Low-dimensional strongly correlated systems have been one of the most important subjects in condensed-matter physics in the last few decades. From the many-body point of view, the standard mean-field approximation for the three-dimensional (3D) system is usually broken down by thermal fluctuation at finite temperature, while from the two-body point of view, the widely used first Born approximation for a 3D weak potential totally fails in lower-dimensional systems too [1]. As a result, a proper effective interaction (or called pseudopotential) becomes essential to go beyond the weak-interaction limit of 3D scattering or in the low-energy limit of two-dimensional (2D) and one-dimensional (1D) systems. For the 2D system that we want to concentrate in this Brief Report, an important progress was made by Schick [2] for the studying of 2D bosons with a hard-disk potential, and the relevant applications to cold atom systems are also investigated by several groups [3–5]. Recently Kanjilal and Blume [6] derived a general form of the pseudopotentials for all angular momentum channels of a short-ranged interaction. The pseudopotential for a long-ranged dipolar interaction in 2D systems was also studied in the *s*-wave channel by one of us [7], but its extension to higher angular momentum channels is still unexplored even though several important results have been carried out in 3D systems recently [8].

In this Brief Report, we systematically generalize earlier results and apply to the systems of 2D dipolar gases: (1) first, we apply Huang and Yang's theory [9,10] to derive a general form of the pseudopotential in 2D systems. Our results can be shown equivalent to Kanjilal and Blume's results [6,11], derived from another approach. (2) For a general power-law decaying interaction, $V_{2D}(\rho)\propto\rho^{-\alpha}(\alpha>2)$, we further analytically calculate the low-energy dependence of the scattering phase shift, up to a single nonuniversal parameter to be determined by the short-ranged details of V_{2D}. (3) Finally we numerically evaluate the nonuniversal parameter for a model interaction in the *s*- and *p*-wave scattering channels of dipolar interaction ($\alpha=3$). The *s*-wave scattering for the two scattering particles confined in two different (parallel) 2D layers are also investigated, showing a Feshbach-type resonance even at zero dipole moment limit. Our results can therefore be applied to the many-body physics of magnetic dipolar atoms [12], cold polar molecules [13], or indirect excitons in a semiconductor based double-well system [14].

We start from solving the following two-particle 2D Schrödinger equation with total energy E:

$$-\frac{\hbar^2}{2\mu}\nabla_\perp^2\psi(\mathbf{r}_\perp)+V_{2D}(\rho)\psi(\mathbf{r}_\perp)=E\psi(\mathbf{r}_\perp), \tag{1}$$

where $\nabla_\perp^2\equiv\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}$ in cylindrical coordinate, $\mu=M/2$ is the reduced mass, and $\psi(\mathbf{r}_\perp)$ is the scattered wave function in the relative coordinate, $\mathbf{r}_\perp\equiv(x,y)$. $V_{2D}(\rho)$ is the effective 2D interaction obtained by integrating out the transverse degree of freedom (z) and is assumed to be isotropic about the z axis here. Note that we also have assumed that the transverse confinement potential is so strong that no confinement-induced resonance [3] has to be considered here.

Since $V_{2D}(\rho)$ is assumed to be isotropic and decays faster than ρ^{-2} in large ρ, the wave function, $\psi(\mathbf{r})$, can be always expanded by noninteracting eigenstates in large distance: $\psi(\rho,\phi)=\Sigma_{m=0}^{\infty}u_m(k,\rho)\Sigma_{\sigma=\pm}C_m^\sigma(k)e^{i\sigma m\phi}$, where $k=\sqrt{2\mu E/\hbar^2}$, and $u_m(k,\rho)\equiv A_m(k)J_m(k\rho)+B_m(k)N_m(k\rho)$ is the radial wave function with $J_m(x)/N_m(x)$ being the Bessel function of the first or second kind. Here $A_m(k)$, $B_m(k)$, and $C_m^\pm(k)$ are the coefficients to be determined by boundary conditions. Similar to the 3D case [9], we first investigate the short-distance behavior in the leading-order terms:

$$u_0(k,\rho)\sim A_0(k)+\frac{2B_0(k)}{\pi}\ln\left(\frac{k\rho}{2\beta_0}\right), \tag{2}$$

$$u_m(k,\rho)\sim\frac{A_m(k)}{m!}\left(\frac{k\rho}{2}\right)^m-\frac{B_m(k)(m-1)!}{\pi}\left(\frac{2}{k\rho}\right)^m+\frac{2B_m(k)}{\pi m!}\left(\frac{k\rho}{2}\right)^m\ln\left(\frac{k\rho}{2\beta_m}\right),\quad(m\neq0). \tag{3}$$

Here we define $\beta_m\equiv e^{-\gamma+H_m/2}$, with $\gamma\approx0.57722$ being the Euler's constant and $H_m\equiv\Sigma_{k=1}^m k^{-1}$ being the Harmonic number [15] (here $H_0\equiv0$). We note that the third term in the right-hand side of Eq. (3), resulted from the irregular solu-

tion, $N_m(k\rho)$, is of the same order (up to a logarithmic function) as the first term if $A_m(k) \sim B_m(k)$. For a typical short-range interaction, however, this term can be neglected because $B(k)/A(k) \propto k^{2m}$ in the long-wavelength limit. Here, we still keep this term for the most general application. Such hybridization between the regular and irregular solutions of noninteracting partial waves does not exist in the 3D case [9]. All other terms can be shown irrelevant to the derivation of the pseudopotential below.

To derive the proper pseudopotential, we have to apply the noninteracting Hamiltonian on the asymptotic wave function above [9,10] and integrate over a small spherical area of radius ρ by using Green's theorem [10]. Separating contributions from the s-wave and the non-s-wave parts, we obtain

$$-\frac{\hbar^2}{2\mu}[\nabla^2 + k^2]\psi(\mathbf{r}_\perp) = -\frac{\hbar^2}{2\mu}\delta(\mathbf{r}_\perp)\left[4B_0(k) + \sum_{m=1}^{\infty}\frac{B_m(k)2^{m+2}m!}{(k\rho)^m}\sum_{\sigma=\pm}C_m^\sigma(k)e^{i\sigma m\phi}\right]. \tag{4}$$

The next step is to rewrite the right-hand side to be a function of $\mathcal{P}_m(k) \equiv B_m(k)/A_m(k)$, which is the only quantity related to the phase shift of the mth partial wave, $\delta_m(k)$. [In fact, $\mathcal{P}_m(k) = -\tan\delta_m(k)$.] In order to get an expression of $A_m(k)$, we have to take certain derivatives on the wave function and let $\rho \to 0$, as in the 3D case [9]. After some simple calculation we obtain

$$A_0(k) = \lim_{\rho\to 0} -\left(\ln\frac{k\rho}{2\beta_0}\right)^2 \rho\frac{\partial}{\partial\rho}\left[\frac{u_0(k,\rho)}{\ln(k\rho/2\beta_0)}\right], \tag{5}$$

$$A_m(k) = -\frac{2B_m(k)}{\pi}\left[H_{2m} + \ln\left(\frac{k\rho}{2\beta_m}\right)\right] + \lim_{\rho\to 0}\frac{m!}{(2m)!}\left(\frac{2}{k}\right)^m\frac{\partial}{\partial\rho^{2m}}[\rho^m u_m(k,\rho)], \tag{6}$$

where we have used the following identity: $\frac{\partial^{2m}}{\partial x^{2m}}[x^{2m}\ln(x/b)] = (2m)![H_{2m} + \ln(x/b)]$ [15]. As a result, by combining Eqs. (4)–(6), we find

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(\mathbf{r}_\perp) + \sum_{m=0}^{\infty}\hat{\mathcal{V}}_m\psi(\mathbf{r}_\perp) = E\psi(\mathbf{r}_\perp), \tag{7}$$

where the pseudopotential operator, $\hat{\mathcal{V}}_m$, is

$$\hat{\mathcal{V}}_0 \equiv \delta(\mathbf{r}_\perp)\frac{-4\hbar^2}{2\mu}\mathcal{P}_0(k)\left(\ln\frac{k\rho}{2\beta_0}\right)^2\rho\frac{\partial}{\partial\rho}\frac{1}{\ln(k\rho/2\beta_0)}, \tag{8}$$

$$\hat{\mathcal{V}}_m \equiv \delta(\mathbf{r}_\perp)\frac{\hbar^2}{2\mu}\frac{4(m!)^2/(2m)!}{\mathcal{P}_m(k)^{-1} + \frac{2}{\pi}[H_{2m} + \ln(k\rho/2\beta_m)]} \times\frac{2^{2m}}{k^{2m}\rho^m}\frac{\partial}{\partial\rho^{2m}}\rho^m. \tag{9}$$

Equations (7)–(9) can be interpreted as the effective interaction of Eq. (1) with the same boundary condition at origin ($\mathbf{r}_\perp = 0$) in the low-energy limit ($E, k\rho \to 0$), and hence is the 2D version of Huang and Yang's result in Ref. [9] [see Eq. (12) therein]. We note that the pseudopotentials derived above are equivalent to results of earlier work both in the s-wave channel [2–6] and in the higher angular momentum channels [6,11].

After deriving the most general form of pseudopotential for 2D scattering, we further derive an analytical closed form of the momentum dependence of $\mathcal{P}_m(k)$ for a power-law decaying potential: $V_{2D}(\rho) \approx U/\rho^\alpha$ as $\rho \to \infty$. Here U measures the strength of interaction, and $\alpha > 2$ is the decay exponent. We start from the zero energy scattering ($E = k = 0$) of Eq. (1), and the radial wave function, $u_m(0,\rho) = u_m(\rho)$, can be calculated analytically: $u_m(\rho) = \tilde{A}_m I_{\frac{m}{\xi}}(\frac{\Delta_\alpha^\xi}{\xi\rho^\xi}) + \tilde{B}_m K_{\frac{m}{\xi}}(\frac{\Delta_\alpha^\xi}{\xi\rho^\xi})$, with $\tilde{A}_m$ and $\tilde{B}_m$ being the coefficients to be determined by the short-distance behavior of $V_{2D}(\rho)$. Here $\xi \equiv \alpha/2 - 1$, $\Delta_\alpha \equiv (\frac{MU}{\hbar^2})^{1/2\xi}$, and $I_m(x)/K_m(x)$ is the modified Bessel function of the first or second kind. In the limit of long distance (or weak interaction, $\Delta_\alpha^\xi/\xi\rho^\xi \ll 1$), we have

$$u_0(\rho) \sim \tilde{A}_0 + \tilde{B}_0\left[\ln(2\beta_0\xi) + \xi\ln\left(\frac{\rho}{\Delta_\alpha}\right)\right],$$

$$u_m(\rho) \sim \frac{\tilde{A}_m(2\xi)^{-m/\xi}}{\Gamma\left(\frac{m}{\xi}+1\right)}\frac{\Delta_\alpha^m}{\rho^m} + \tilde{B}_m\frac{(2\xi)^{m/\xi}}{2}\Gamma\left(\frac{m}{\xi}\right)\frac{\rho^m}{\Delta_\alpha^m},$$

which should be also reproducible by taking the zero energy limit ($k \to 0$) of Eqs. (2) and (3) [the last term of Eq. (3) can be neglected in this limit]. Therefore the relationship between $\mathcal{P}_m(k)$ and $\tilde{P}_m \equiv \tilde{B}_m/\tilde{A}_m$ can be easily derived to be

$$\mathcal{P}_0(k) = \frac{\xi\pi/2}{\tilde{P}_0^{-1} + \ln(2\beta_0\xi) - \xi\ln(k\Delta_\alpha/2\beta_0)}, \tag{10}$$

$$\mathcal{P}_m(k) = \frac{-2\pi(2\xi)^{-2m/\xi}}{m!\,(m-1)!}\frac{(k\Delta_\alpha/2)^{2m}}{\Gamma\left(\frac{m}{\xi}+1\right)\Gamma\left(\frac{m}{\xi}\right)}\tilde{P}_m^{-1}, \tag{11}$$

where $\tilde{P}_m \equiv \tilde{B}_m/\tilde{A}_m$ is the only nonuniversal parameter, depending on the detailed shape of $V_{2D}(\rho)$ in the short-distance regime. Note that above results apply only in the low-energy and/or weak-interaction limits, i.e., $k \ll \rho^{-1} \ll \xi^{1/\xi}/\Delta_\alpha$.

For s-wave scattering channel, we can define an effective scattering length, $a_\alpha \equiv \Delta_\alpha(2\beta_0\xi)^{-1/\xi}e^{-1/\xi\tilde{P}_0}$ so that

$$\hat{\mathcal{V}}_0\psi(\mathbf{r}_\perp) = \frac{-2\pi\hbar^2}{2\mu\ln(ka_\alpha/2\beta_0)}\delta(\mathbf{r}_\perp)\psi(\mathbf{r}_\perp), \tag{12}$$

if we assume the scattered wave function can be approximated by a smooth function at origin after cross graining the short-ranged fluctuation (for example, the mean-field condensate wave function of bosonic particles). The resulting pseudopotential above becomes the same as a hard-disk potential [2,4,5] with an effective "radius," a_α. The justification of the 2D pseudopotential depends on the interaction strength, i.e., when $ka_\alpha \sim k\Delta_\alpha \ll 1$.

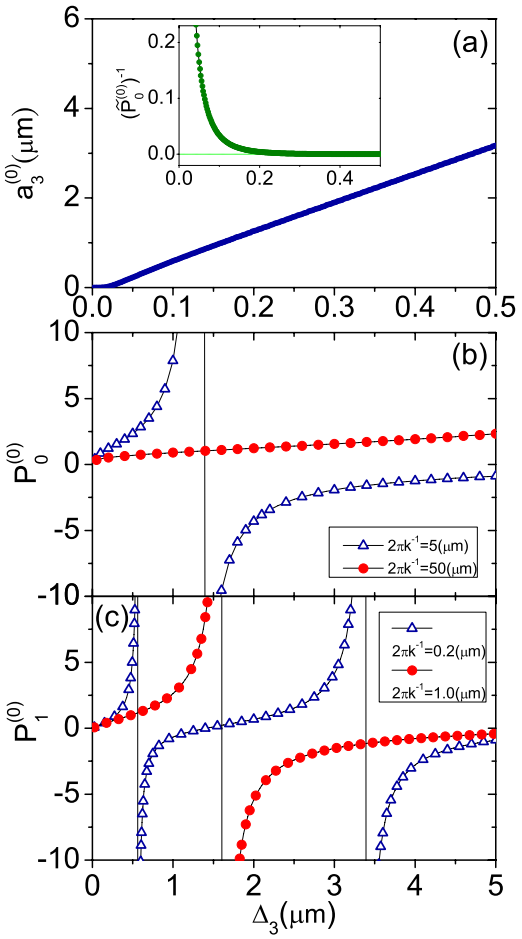

FIG. 1. (Color online) [(a) and (b)] Calculated s-wave scattering length and amplitude, $a_3^{(0)}$ and $\mathcal{P}_0^{(0)}(k)$, as a function of Δ_3 for case A. The inset shows results for $(\tilde{P}_0^{(0)})^{-1}$. Here we set $W=0.1$ μm (see the text). (c) shows the calculated $\mathcal{P}_1^{(0)}(k)$ for case B. Results for different values of incident wave vector, k, are also shown together.

In the rest of this Brief Report, we will concentrate on a physical example, say systems of polar molecules, for the results of dipolar interaction ($\alpha=3$). An external electric field is assumed to applied perpendicular to the layer plane, inducing a field-dependent dipole moment, D. We consider three cases of scattering here: case A: s-wave scattering between identical bosons in the same layer; case B: p-wave scattering between identical fermions in the same layer; and case C: s-wave scattering between identical bosons or fermions in two parallel layers with layer separation d. The last case can be directly applied to the systems of multilayer structure made by 1D optical lattice [16]. In the rest of the Brief Report, we will use $V_{2D}^{(0)/(1)}$ to denote the bare intralayer/interlayer interaction with the superscript $^{(0)/(1)}$ to identify all the quantities obtained by either of them. For the convenience of numerical calculation, we further approximate the effective 2D interaction by the following analytic form: for the intralayer interaction, we use $V_{2D}^{(0)}(\rho)=\frac{D^2}{\rho^3}$ for $\rho>W$ and $=\frac{D^2}{W^3}$ for $\rho\leq W$, where W should be about the same order of the layer width and is fixed to be 0.1 μm in the following calculation. We note that different choices of the cutoff, W, can bring only minor quantitative difference in the results of phase shift (not shown here) because the intralayer interaction, $V_{2D}^{(0)}(\rho)$, is assumed to be repulsive for all ρ, and hence no Feshbach-resonance-type resonance should be expected. For the interlayer interaction, we use $V_{2D}^{(1)}(\rho)=\frac{D^2(\rho^2-2d^2)}{(\rho^2+d^2)^{5/2}}$, where the effect of finite layer width is expected to be smaller since $W\ll d$ in a deep optical lattice. As a result, the only length scale associated with our present model interaction is $\Delta_3=MD^2/\hbar^2$ (also denoted to be a_d in the literature [12]). For a typical molecule, say SrO, the fully polarized dipole moment can be $D=8.9$ Debye, leading to Δ_3 as large as 123.2 μm. However, for magnetic atoms such as ^{52}Cr, the maximum value of Δ_3 is just about 1.03 nm.

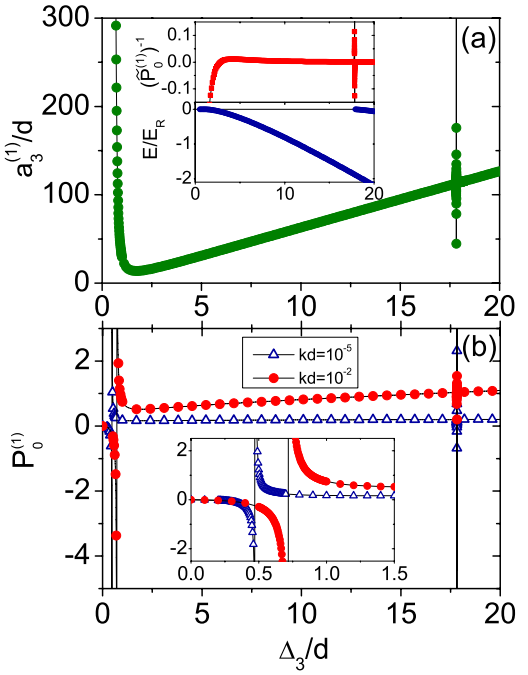

FIG. 2. (Color online) Results for case C: (a) is the value of $a_3^{(1)}/d$ as a function of Δ_3/d. In the inset: the upper one shows $(\tilde{P}_0^{(1)})^{-1}$ for zero energy scattering, and the lower one shows the bound-state energy in unit of recoil energy, $E_R\sim\hbar^2\rho^2/2Md^2$. (b) shows the value of $\mathcal{P}_0^{(1)}(k)$ for different incident wave vectors, k. Inset: the magnified plot for the first resonance.

In Fig. 1, we show the numerical results for case A and case B together by evaluating the original two-particle Schrödinger equation of Eq. (1): in (a), we show $\tilde{P}_0^{(0)}$ and $a_3^{(0)}$ as a function of dipolar strength, Δ_3. One can see that when Δ_3 is small, $(\tilde{P}_0^{(0)})^{-1}$ can be quiet large, leading to a very small scattering length, $a_3^{(0)}$ for $\Delta_3<0.05$ μm. However, for larger Δ_3, $a_3^{(0)}$ becomes proportional to Δ_3, which is the only relevant length scale in this regime (i.e., the short-ranged details of the dipolar interaction becomes negligible). In Fig. 1(b), we show the calculated strength of pseudopotential, $\mathcal{P}_0^{(0)}(k)$, for different values of incident wave vectors, k. One can see that for a given k, $\mathcal{P}_0^{(0)}(k)$ decreases to zero logarithmically as $\Delta_3\to 0$, while it has a resonancelike behavior at a certain value of Δ_3. Such "resonancelike" behavior occurs as $\delta_0(k)=\pi/2$, indicating that the interaction is so strong to push the wave front of the scattered wave function well

ahead of the noninteracting one. It is therefore nothing to do with the Feshbach resonance in 3D, and only results for $ka_3 \sim k\Delta_3 \ll 1$ are correct for true low-energy scattering. In (c) we show the results for case B: $\mathcal{P}_1^{(0)}(k)$ as a function of dipolar strength. However, unlike the boson case, where the typical incident wave vector is determined by the condensate (i.e., system) size at low temperature, the typical incident wave vector for fermions at low temperature should be about the Fermi wave vector (i.e., the inverse of interparticle distance) due to the Pauli exclusion principle. Therefore we calculate results for a much larger k in (c), but similar interaction dependence is still observed. Note that our numerical results are consistent with the analytic results derived in Eqs. (10) and (11) in the low-energy limit.

In Fig. 2, we show the results for case C: the s-wave scattering between particles in two different layers. In (a) and its inset, we show the calculated scattering length, $a_3^{(1)}$, and the associated $\tilde{P}_0^{(1)}$ as a function of Δ_3. It is interesting to see that, different from the intralayer case, $(\tilde{P}_0^{(1)})^{-1}$ diverges to negative infinity and $a_3^{(1)}$ also diverges in the regime of small Δ_3. Such divergence originates from the fact that our dipolar interaction can always sustain an interlayer bound state in 2D system even when the interaction strength is infinitely small. The calculated bound-state energy shows a logarithmically small binding energy for the first bound state, while the second bound state appears near $\Delta_3/d \sim 18$. When considering the finite-size effect, i.e., ka is bounded below, the first resonance will occur at a finite dipole moment as shown in (b) (also see Ref. [7]). The existence of an interlayer bound state can lead to a strong modification of the pseudopotential strength (similar to the Feshbach resonance), and some exotic many-body phases as predicted in Refs. [7,16].

In summary, we analytically derive the general form of the pseudopotential for an arbitrary short-ranged and isotropic interaction in a uniform 2D system. The analytic energy and interaction dependence of the pseudopotential is also derived for an arbitrary power-law interaction. Numerical results are provided for the dipolar interaction and therefore can be applied to the 2D quantum dipolar gases.

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