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An effective many-body theory for strongly interacting polar molecules

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Abstract. We derive a general, effective many-body theory for bosonic polar molecules in the strong interaction regime, which cannot be correctly described by previous theories within the first Born approximation. The effective Hamiltonian has additional interaction terms, which surprisingly reduce the anisotropic features of the condensate profile near the shape resonance regime. In a two-dimensional (2D) system with the dipole moment perpendicular to the plane, we find that the phonon dispersion scales as $\sqrt{|\mathbf{p}|}$ in the low-momentum (\mathbf{p}) limit, showing the same low energy properties as a 2D charged Bose gas with Coulomb ($1/r$) interactions.

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1. Introduction

Recent developments in the trapping and cooling of chromium atoms [1] and polar molecules [2] provide a new direction for investigating quantum states resulting from the anisotropic dipole interaction. Dipolar effects on the condensate profile [3] and elementary excitations [4] have been extensively studied both theoretically and experimentally. Several exotic many-body states resulting from dipolar interactions are also proposed [5]. However, so far, most theoretical works are based on the pseudo-potential developed by Yi and You [6] within the first Born approximation (FBA). As a result, these results do not become justified when applied to systems of polar molecules, which can have large electric dipole moments and hence renormalize the scattering amplitude beyond the FBA.

In [7], Derevianko extended Huang and Yang's approach [8] to the anisotropic dipolar interaction, and showed how it is possible to go beyond the Born approximation in a dipolar gas system. The derived pseudo-potential, however, is non-Hermitian in the low-energy limit, and therefore cannot be easily used for constructing the effective theory of strongly interacting dipolar gases. In [9], the authors studied the systems of bosonic dipoles via Monte Carlo calculations, and found that the ground-state energy can be well explained by Yi and You's pseudo-potential within FBA if one uses a dipole-dependent s-wave scattering. But the validity of applying it to polar molecules with large dipole moment in a strong field is still questionable, because the higher-order renormalization (FBA is the first-order perturbation) to the scattering amplitude of the *non-s-wave* channels is not included at all. For example, in [10]¹, Deb and You found that the scattering matrix element between s-wave and d-wave channels also has strong deviation from the FBA result when near the shape resonance. It is therefore reasonable to believe that such a kind of deviation should also occur in other channels in the stronger dipole moment regime, which can be easily achieved by applying a strong electric field in a polar molecule system. As a result, developing a correct and widely applicable pseudo-potential and the associated many-body theory for systems of dipolar atoms/molecules is a very important and crucial step for future theoretical and experimental studies.

In this paper, we derive a complete, effective many-body theory that can correctly describe bosonic polar molecules both in the weak and strong interaction regimes and/or near the shape resonance. The resulting effective Hamiltonian is modified by additional three-point and four-point interactions, which may significantly change the nature of condensate profile/dynamics. For example, when the dipole moment is near the first s-wave shape resonance regime, we find that the additional interaction (new terms beyond the FBA) can reduce the anisotropy of the condensate profile. In a two dimensional (2D) uniform system with the dipole moment perpendicular to the plane, we find that the phonon dispersion scales as $\sqrt{|\mathbf{q}|}$ (instead of $|\mathbf{q}|$ in the typical Bogoliubov mode) in the long-wavelength limit, showing the same low-energy physics as 2D charged bosons with Coulomb ($1/r$) interactions [11]. As a result, our theory is important not only in the study of strongly interacting polar molecules, but also in the possible application of simulating the liquid phase of 2D charged bosons by neutral particles. Such a simulation cannot be done in ion traps because of the strong Coulomb interaction energy compared to the kinetic energy. These results may also be useful in studying the properties of a high T_c superconducting thin film, where the coherent lengths of Cooper pairs are known to be very small as a composite charged boson [12].

¹ To extract the value of $\Delta a_{ll'}^{(m)}$, we use the results shown in figure 2 of [10] for the scattering matrix elements of different channels.

The paper is organized as follows: in section 2, we first discuss the general scattering theory of dipolar interaction and briefly review theories used in previous works. In section 3, we used an exactly solvable model to examine the validity of the FBA of dipole interaction. In section 4, we derive the correct effective theory and the associated Gross–Pitaivskii equation for bosonic polar molecules in a 3D system. We then discuss in section 5, the condensate wavefunction by using the variational method. Finally, in section 6, we extend the 3D results to develop an effective theory in the quasi-2D system and calculate the phonon mode dispersion as well as the Kosterlitz–Thouless transition temperature. We then summarize our work in section 7.

2. Low-energy scattering theory of dipoles

For the convenience of later discussions, we first briefly review recent progress in the scattering problem of dipolar gas, where the electric/magnetic dipole moment is polarized by the external electric/magnetic field along the z -direction. The most general form of the scattering amplitude between two identical particles in such a situation can be expressed as

$$f(\mathbf{k}, \mathbf{k}') = 4\pi \sum_{lm} \sum_{l'm'} t_{lm}^{l'm'}(k) Y_{lm}^*(\hat{k}) Y_{l'm'}(\hat{k}'), \quad (1)$$

where the scattering matrix element, $t_{lm}^{l'm'}(k)$, depends on the relative incident momentum, k , and the summation is over even l for bosons and odd l for fermions. $Y_{lm}(\hat{k})$ is the spherical harmonic function of unit vector \hat{k} . At large distances, the inter-particle potential is dominated by the dipolar term, $V_d(\mathbf{r}) = D^2(1 - 3\cos^2\theta)/|\mathbf{r}|^3$, where D is the electric dipole moment in cgs units (for simplicity, here we use electric dipoles to formulate the theory for polar molecules, while a similar version for magnetic dipolar gases can also be obtained easily); θ is the angle between the distance \mathbf{r} and the dipole direction (polarized in the z -direction). However, at short distances the potential becomes much more complicated due to the Coulomb and spin exchange interactions between electrons. Deb and You [10] first calculated the scattering matrix elements between two electronically polarized atoms within a model potential and studied how they change as a function of the external electric field. Based on the numerical results, Yi and You [6] then proposed a pseudo-potential:

$$V_{ps}(\mathbf{r}) \equiv \frac{4\pi a_s \hbar^2}{M} \delta(\mathbf{r}) + V_d(\mathbf{r}), \quad (2)$$

to calculate the *low-energy* scattering matrix element within the FBA in the limit of weak external field. Here $a_s = -t_{00}^{00}(0)$ is the s -wave scattering length in the zero field limit. Within the FBA [3, 4],

$$f_B(\mathbf{k}, \mathbf{k}') = \frac{-M}{4\pi \hbar^2} \int d\mathbf{r} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} V_{ps}(\mathbf{r}) = -a_s - \frac{2}{3} a_d P_2(\cos \theta_{\mathbf{k}-\mathbf{k}'}),$$

where $a_d \equiv MD^2/\hbar^2$ is a length scale and $P_2(x)$ is the Legendre polynomial. $\theta_{\mathbf{k}}$ is the angle between the momentum \mathbf{k} and the z -axis. As a result, the associated matrix elements become:

$$t_{B lm}^{l'm'}(k) = 4\sqrt{\frac{\pi}{5}} a_d i^{l-l'} \int d\Omega_r Y_{lm}(\hat{r}) Y_{l'm'}^*(\hat{r}) Y_{20}(\hat{r}) \int_{kr_c}^{\infty} \frac{dr}{r} j_l(r) j_{l'}(r)$$

with $j_l(r)$ being the spherical Bessel function. Here r_c is a cut-off in the atomic length scale and therefore we can always take $kr_c \rightarrow 0$ in the low-energy limit. In the above FBA result, all the short-ranged effects are included in the s-wave part (a_s) only, while all other matrix elements, $t_{B_{lm}}^{l'm'}(0)$, are proportional to the same length scale, $a_d \propto D^2$. Therefore, it is easy to see why such results cannot be valid when the dipole moment (or external field) is sufficiently strong as higher-order renormalization becomes important.

In [7], Derevianko developed a different pseudo-potential for dipolar interaction to go beyond the FBA. Although the most general expression of the pseudo-potential is derived for each scattering channel and the results are in principle applicable to the strong interaction regime, only one term (the scattering between the s-wave and the d-wave, i.e. the $t_{00}^{20}(0) = t_{20}^{00}(0)$ term in equation (1)) is evaluated within the leading order perturbative method (equivalent to the FBA level). In fact, we observe that Derevianko's result for the on-shell scattering channel ($|\mathbf{k}| = |\mathbf{k}'|$) is equivalent to the first two terms of the FBA result (i.e. the full $f_B(\mathbf{k}, \mathbf{k}')$ is replaced by $-a_s - \frac{a_d}{6} [P_2(\cos \theta_{\mathbf{k}}) + P_2(\cos \theta_{\mathbf{k}'})]$, using $Y_{20}(\hat{k}) = \sqrt{5/4\pi} P_2(\cos \theta_{\mathbf{k}})$). This explains why the meanfield calculation by Yi and You ([13], which included only the s-wave and s-d scattering channel of the pseudo-potential of [7]) is not consistent with the previous FBA result even in the weak dipole moment regime, where the FBA is supposed to be valid. (We note that this inconsistency will exist even if Yi and You had used the corrected coefficient derived in the erratum of [7]. The key point is that contributions from all other scattering channels are all proportional to D^2 within the FBA and hence cannot be neglected compared to $t_{00}^{20}(0)$.) In [9], Bortolotti *et al* claimed that $V_{ps}(\mathbf{r})$ in equation (2) can be a good pseudo-potential if only one uses a dipole-dependent s-wave scattering length (i.e. $a_s(D)$). However, their results cannot apply to the strong dipole moment regime when the higher-order renormalization of the scattering matrix element in other channels (different from s-wave, t_{00}^{00}) in realistic polar molecule systems of high polarization. Therefore, a general and useful approach to study the low-energy many-body physics of strongly interacting polar molecules is still needed.

3. Criterion for the first Born approximation

For completeness, we now explicitly examine the criterion for justifying the FBA in the low-energy limit. We consider the following model potential: $V_{\text{mdl}}(\mathbf{r}) = V_d(\mathbf{r})$ for $|\mathbf{r}| > r_c$, and $V_{\text{mdl}}(\mathbf{r}) = \infty$ for $|\mathbf{r}| \leq r_c$. Although this model potential is over-simplified compared to the realistic interaction potential between polar molecules, it still catches the most important feature, anisotropic dipolar interaction, and hence should be useful in studying the validity of the Born approximation in the low-energy limit. The full scattering wavefunction $\psi(\mathbf{r})$ can be solved by:

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) - \frac{M}{\hbar^2} \int' \frac{d\mathbf{r}'}{4\pi} G(\mathbf{r}, \mathbf{r}') V_{\text{mdl}}(\mathbf{r}') \psi(\mathbf{r}'), \quad (3)$$

where $\int' d\mathbf{r}'$ is for $|\mathbf{r}'| > r_c$ only, and

$$\psi_0(\mathbf{r}) = 4\pi \sum_{lm} i^l e^{i\delta_l(k)} \cos \delta_l(k) j_{n_l}(k, r) Y_{lm}^*(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}}) \quad (4)$$

is the *exact* scattered wavefunction for the hard core potential of radius r_c *without* dipole moment. Here, we have defined $j_{n_l}(k, r) = j_l(kr) - \tan \delta_l(k) n_l(kr)$ with $\delta_l(k) \equiv \tan^{-1}(j_l(kr_c)/n_l(kr_c))$ being the scattering phase shift. $j_l(x)$ and $n_l(x)$ are the conventional

spherical Bessel functions. Green's function, $G(\mathbf{r}, \mathbf{r}')$, satisfies $\nabla^2 G(\mathbf{r}, \mathbf{r}') + k^2 G(\mathbf{r}, \mathbf{r}') = -4\pi\delta(\mathbf{r} - \mathbf{r}')$ with the boundary condition $G(r_c \hat{r}, \mathbf{r}') = 0$, and therefore can be evaluated by using separation of variables. After some straightforward calculation, Green's function can be expressed as

$$G(\mathbf{r}, \mathbf{r}') = \sum_{lm} Y_{lm}^*(\theta', \phi') Y_{lm}(\theta, \phi) \frac{-4\pi k}{i + \tan \delta_l} j_{n_l}(k, r_{<}) h_l^{(1)}(kr_{>}), \quad (5)$$

where $r_{>(<)}$ is the larger (smaller) one of r and r' , and $h_l^{(1)}(x) \equiv j_l(x) + in_l(x)$.

Within the FBA, the scattered wavefunction is given by the first-order iteration: $\psi_B(\mathbf{r}) = \psi_0(\mathbf{r}) - \frac{M}{\hbar^2} \int' \frac{d\mathbf{r}'}{4\pi} G(\mathbf{r}, \mathbf{r}') V_{\text{mdl}}(\mathbf{r}') \psi_0(\mathbf{r}')$. Therefore, its validity relies on the assumption that the change of the wavefunction is much smaller than $\psi_0(r)$ in the *whole* range of space [14]. We can therefore define a parameter, ξ , to measure the deviation of $\psi_B(\mathbf{r})$: $\xi \equiv \lim_{k \rightarrow 0} \lim_{|\mathbf{r}| \rightarrow r_c} |\psi_B(\mathbf{r}) - \psi_0(\mathbf{r})| / |\psi_0(\mathbf{r})|$. In such a limit, we have $\psi_0(\mathbf{r}) \sim \frac{\Delta r}{r_c} + \mathcal{O}(kr_c)$, where $\Delta r = |\mathbf{r}| - r_c \ll r_c$. Expanding Green's function, $G(\mathbf{r}, \mathbf{r}')$, in the small \mathbf{r} regime, we obtain $\psi_B(\mathbf{r}) - \psi_0(\mathbf{r}) = \frac{\Delta r}{r_c} \cdot \frac{\pi^{3/2}}{3\sqrt{5}} \cdot \frac{MD^2}{\hbar^2 r_c} + \mathcal{O}(kr_c)$. As a result, the condition to justify the FBA is $\xi = \frac{\pi^{3/2} a_d}{3\sqrt{5} r_c} \ll 1^2$. For example, we consider the magnetic dipolar atom, ^{52}Cr , with $r_c \sim 100a_0$ as the typical length scale of van der Waals interaction. We find $\xi_{\text{Cr}} \sim 0.4 < 1$ and this explains why results obtained in the FBA for ^{52}Cr are comparable to experiments [3, 4]. However, for polar molecules with electric dipole moment of the order of a few Debyes, the value of ξ can easily be several hundred or more, where a shape resonance can occur in different channels to break down the FBA. Therefore, in order to correctly describe the effective many-body physics of polar molecules, one needs a self-consistent theory beyond the pseudo-potential, $V_{\text{ps}}(\mathbf{r})$, and the FBA.

4. Effective Hamiltonian in 3D space

To study the low-energy physics of a general dipole interaction in the many-body medium, one has to use an *effective* two-particle interaction, Γ , which is just the vertex function integrating out all the contributions of virtual scattering in the high-energy limit [15]. A complete calculation of the vertex function is usually not available (except in some special models of 1D systems), but can be well approximated by using the standard ladder approximation (see figure 1). It is well known that such a ladder approximation is correct in the low-density limit, and is therefore a very suitable approximation for systems of dilute cold atoms/molecules. Following the standard approach for evaluating the Bethe–Salpeter equation of bosonic particles [15], we can calculate the effective two-particle interaction (i.e. vertex function) within the ladder approximation by using the two-particle scattering amplitude, $f(\mathbf{p}, \mathbf{p}')$:

$$\begin{aligned} \frac{M}{4\pi\hbar^2} \Gamma(\mathbf{p}, \mathbf{p}', \mathbf{P}, P_0) &= -f(\mathbf{p}, \mathbf{p}') + \frac{4\pi}{\Omega} \sum_{\mathbf{k}} f(\mathbf{p}, \mathbf{k}) f(\mathbf{p}', \mathbf{k})^* \\ &\times \left(\frac{1}{\epsilon + 2M\mu/\hbar^2 - k^2 + i0^+} + \frac{1}{k^2 - p'^2 - i0^+} \right), \end{aligned} \quad (6)$$

² The above result is also supported by the numerical calculation in [9], where the dipole moment-*independent* s-wave scattering length, $a_s = r_c$, becomes invalid when dipole moment is large but still away from the shape resonance regime.

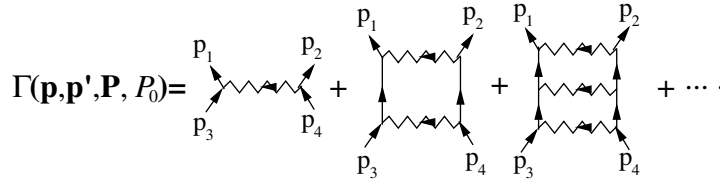


Figure 1. Series expansion for effective interaction in the ladder approximation. The solid line represents Green's function of bosonic particles and the zigzag line is for bare interaction. Here $\mathbf{p} \equiv \frac{1}{2}(\mathbf{p}_1 - \mathbf{p}_2)$ and $\mathbf{p}' \equiv \frac{1}{2}(\mathbf{p}_3 - \mathbf{p}_4)$ are half of the relative momentum, and $\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2 = \mathbf{p}_3 + \mathbf{p}_4$ is the total momentum of the two scattering particles with frequency P_0 (see also [15]).

where $\epsilon = \frac{M}{\hbar^2} (\hbar P_0 - \hbar^2 \mathbf{P}^2 / 4M)$ is the total kinetic energy in the center-of-mass frame; μ is the chemical potential and Ω is the system volume.

Using the fact, $f(\mathbf{p}', \mathbf{k})^* = f(\mathbf{k}, \mathbf{p}')$, the final term of equation (6) can be evaluated explicitly by integrating over the solid angle of momentum \mathbf{k} in the scattering amplitude, equation (1). Furthermore, since the partial wave scattering matrix element, $t_{lm}^{l'm'}(k)$, is known to be insensitive to the incident momentum, k , in the low-energy limit, we can also neglect their momentum dependence and replace their value by a constant, $t_{lm}^{l'm'}(0)$. As a result, the last term of equation (6) can be calculated to be

$$(4\pi)^3 \int_0^\infty \frac{k^2 dk}{(2\pi)^3} \left(\frac{1}{\epsilon + 2M\mu/\hbar^2 - k^2 + i\eta} + \frac{1}{k^2 - p'^2 - i\eta} \right) \times \left[\sum_{l,l',m} \sum_{l''} t_{lm}^{l''m}(0) t_{l''m}^{l'm}(0) Y_{lm}^*(\hat{p}) Y_{l'm}(\hat{p}') \right], \quad (7)$$

where we have set $m = m'$ due to the rotational symmetry about the polarization axis (z). It is easy to see that the real part of the integration cancels out, and the imaginary part is proportional to $\sqrt{2M\mu/\hbar^2}$ in the limit of low-energy scattering ($|p'|, \epsilon \rightarrow 0$). Therefore, the last term of equation (6) can be shown to be negligible when compared with the second term, $f(\mathbf{p}, \mathbf{p}')$, in the low-density limit, i.e. $|t_{lm}^{l'm'}(0) n_{3D}^{1/3}| \ll 1$. (Here, n_{3D} is the 3D particle density.) As a result, in the low-energy and dilute limit, one can use $\Gamma(\mathbf{p}, \mathbf{p}') = \frac{-4\pi\hbar^2}{M} f(\mathbf{p}, \mathbf{p}')$ as an effective 'pseudo-potential' in momentum space (there is no dependence on total momentum and energy in such a limit and we could omit them in Γ). Note that, different from the FBA used in the literature, we do not have to assume weak bare interaction in the above derivation (strong interaction may still give a small value of the scattering matrix element, $|t_{lm}^{l'm'}(0)|$, in the low-energy limit, just as in the usual s-wave scattering of cold atoms). Complicated electronic structure and shape resonance effects are all included in the full calculation (or experimental measurement) of the matrix elements, $t_{lm}^{l'm'}(0)$, in all channels. In the rest of this paper, we will study the general effective theory and possible new many-body physics beyond the FBA *without* directly evaluating the scattering matrix elements.

Using the derived pseudo-potential (or effective interaction), $\Gamma(\mathbf{p}, \mathbf{p}') = \frac{-4\pi\hbar^2}{M} f(\mathbf{p}, \mathbf{p}')$, we can write down the interacting Hamiltonian in momentum space by using the second

quantization formalism:

$$H_I = \frac{1}{2\Omega} \sum_{\mathbf{p}, \mathbf{p}', \mathbf{P}} \hat{a}_{\mathbf{P}/2+\mathbf{p}}^\dagger \hat{a}_{\mathbf{P}/2-\mathbf{p}}^\dagger \hat{a}_{\mathbf{P}/2-\mathbf{p}'} \hat{a}_{\mathbf{P}/2+\mathbf{p}'} \Gamma(\mathbf{p}, \mathbf{p}'), \quad (8)$$

where $\hat{a}_{\mathbf{p}}$ and $\hat{a}_{\mathbf{p}}^\dagger$ are field operators for bosonic polar molecules at momentum \mathbf{p} . The momentum summation from now on is restricted to the low-momentum regime as implied by the effective interaction, $\Gamma(\mathbf{p}, \mathbf{p}')$. In order to address the effect of pseudo-potential beyond the FBA (equation (2)), we can divide the contribution of the pseudo-potential, $\Gamma(\mathbf{p}, \mathbf{p}')$, into three parts:

$$\Gamma(\mathbf{p}, \mathbf{p}') = \frac{4\pi\hbar^2 a_s}{M} + V_d(\mathbf{p} - \mathbf{p}') - \frac{4\pi\hbar^2}{M} f_\Delta(\mathbf{p}, \mathbf{p}'), \quad (9)$$

where the first term is from the known (dipole moment-dependent) isotropic s-wave scattering, the second term is the usual FBA result for anisotropic dipolar interaction, the third term, f_Δ , is the scattering amplitude deviating from the known FBA results. It can be denoted as

$$f_\Delta(\mathbf{p}_1, \mathbf{p}_2) \equiv -4\pi \sum_{l'l'} i^{l'-l} \sum_m \Delta a_{ll'}^{(m)} Y_{lm}^*(\hat{p}_1) Y_{l'm}(\hat{p}_2), \quad (10)$$

with $\Delta a_{ll'}^{(m)} \equiv -i^{l'-l} (t_{lm}^{l'm}(0) - t_{B_{lm}}^{l'm}(0))$ being the *difference* between a full matrix element and its FBA result. Here, $\sum_{l'l'}$ has excluded the $l = l' = 0$ term. Note that in the limit of a weak external field, we have the following orders of magnitude: $a_s = \mathcal{O}(1)$, $V_d = \mathcal{O}(D^2)$ and $\Delta a_{ll'}^{(m)} = \mathcal{O}(D^4)$. Therefore, it is easy to see that the pseudo-potential, Γ , shown in equation (9) has a very smooth connection with the known FBA results [3, 4, 6, 9] in the limit of small dipole moment. From equations (8) and (9), it is straightforward to write down the full effective Hamiltonian to describe the low-energy many-body physics of polar molecules:

$$\begin{aligned} H = & \sum_{\mathbf{p}} (\epsilon_{\mathbf{p}} - \mu) \hat{a}_{\mathbf{p}}^\dagger \hat{a}_{\mathbf{p}} + \frac{1}{\Omega} \sum_{\mathbf{p}_1, \mathbf{p}_2} \hat{a}_{\mathbf{p}_1}^\dagger \hat{a}_{\mathbf{p}_2} V_{\text{ext}}(\mathbf{p}_1 - \mathbf{p}_2) \\ & + \frac{1}{2\Omega} \left(\sum_{\mathbf{p}_1, \mathbf{p}_2, \mathbf{P}} \hat{a}_{\mathbf{P}/2+\mathbf{p}_1}^\dagger \hat{a}_{\mathbf{P}/2-\mathbf{p}_1}^\dagger \hat{a}_{\mathbf{P}/2-\mathbf{p}_2} \hat{a}_{\mathbf{P}/2+\mathbf{p}_2} \right) \\ & \times \left[\frac{4\pi\hbar^2 a_s}{M} + V_d(\mathbf{p}_1 - \mathbf{p}_2) - \frac{4\pi\hbar^2 a_s}{M} f_\Delta(\mathbf{p}_1, \mathbf{p}_2) \right], \quad (11) \end{aligned}$$

where $V_{\text{ext}}(\mathbf{p})$ is the external trapping potential in momentum space. Note that equation (11) has included scattering from all channels and is also consistent with the FBA results in the weak dipole limit ($|f_\Delta| \propto \mathcal{O}(D^4)$ as $D \rightarrow 0$). When the external electric field is strong enough, there will be some modification of the scattering amplitude to be beyond the results of FBA even in channels different from the s-wave, i.e. $\Delta a_{ll'}^{(m)} \neq 0$ for $l, l' \neq 0$. Calculating the magnitude of such a modification beyond the FBA has to be based on the first principle calculation of two scattering molecules, and is beyond the scope of this work. Our interest in the present paper, is in studying the effective Hamiltonian and the possible many-body physics when f_Δ is known.

In order to compare with the existing theory of weakly interacting dipoles [3, 4, 6, 9], it is instructive to express equation (11) in real space. Details of the transformation are shown in the

appendix. The final result is

$$\begin{aligned}
H = & \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) \left[\frac{-\hbar^2 \nabla^2}{2m} - \mu + V_{\text{ext}}(\mathbf{r}) \right] \hat{\psi}(\mathbf{r}) \\
& + \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' V_{\text{ps}}(\mathbf{r} - \mathbf{r}') \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) \\
& + \frac{2\sqrt{\pi}\hbar^2}{M} \int d\mathbf{R} \left[\hat{\psi}^\dagger\left(\mathbf{R} + \frac{\mathbf{r}}{2}\right) \hat{\psi}^\dagger\left(\mathbf{R} - \frac{\mathbf{r}}{2}\right) \sum_l \Delta a_{0l}^{(0)} \hat{\phi}_{l0}(\mathbf{R}) + \text{h.c.} \right] \\
& + \frac{2\hbar^2}{M} \sum_{l,l'}'' \sum_m \Delta a_{ll'}^{(m)} \int d\mathbf{R} \hat{\phi}_{lm}^\dagger(\mathbf{R}) \hat{\phi}_{l'm}(\mathbf{R}), \tag{12}
\end{aligned}$$

where $\hat{\psi}(\mathbf{r})$ is the bosonic field operator in space. Here $\sum''_{ll'}$ is defined to exclude any term with $l = 0$ or $l' = 0$, and we have used the fact that $\Delta a_{ll'}^{(m)} \neq 0$ only for $|l - l'| = 0, 2, 4, \dots$ due to the anisotropic nature of dipole potential, $V_d(\mathbf{r}) \propto Y_{20}(\hat{r})$, and its higher-order effect. As shown in the appendix, we have defined $\hat{\phi}_{lm}(\mathbf{R}) \equiv \frac{(l+1)!!}{2^{l/2}} \int d\mathbf{r} \frac{Y_{lm}(\hat{r})}{r^3} \hat{\psi}\left(\mathbf{R} + \frac{\mathbf{r}}{2}\right) \hat{\psi}\left(\mathbf{R} - \frac{\mathbf{r}}{2}\right)$ as a ‘pairing’ operator in the angular momentum (l, m) channel with a spatial ‘wavefunction’ $Y_{lm}(\hat{r})/r^3$. Although such pairing operators do not represent true composite particles, they can be used to describe the relative motion of two dipoles before and after scattering: the first term of the last line indicates an association–dissociation process between a pair and two dipoles, while the last term describes a transition between ‘pairs’ of different angular momentum channels. These two novel interaction terms may bring completely new physics in strongly interacting polar molecules, and are worthy of further investigation in the future.

Starting from the effective Hamiltonian, equation (12), we can also derive the associated Gross–Pitaevskii-type meanfield equation for condensate dynamics by using $i\hbar \partial \hat{\psi} / \partial t = [\hat{\psi}, H]$ and approximating the bosonic field operator, $\hat{\psi}(\mathbf{r})$, to be a c -number, $\Psi(\mathbf{r})$. The resulting equation can be written in the following form:

$$\begin{aligned}
i\hbar \frac{\partial \Psi(\mathbf{r})}{\partial t} = & \left[\frac{-\hbar^2 \nabla^2}{2m} - \mu + V_{\text{ext}}(\mathbf{r}) + \int d\mathbf{r}' V_{\text{ps}}(\mathbf{r} - \mathbf{r}') |\Psi(\mathbf{r}')|^2 \right] \Psi(\mathbf{r}) \\
& + \frac{2\sqrt{\pi}\hbar^2}{M} \int \frac{d\mathbf{r}'}{|\mathbf{r}'|^3} \left[\sum_l \frac{(l+1)!!}{2^{l/2}} Y_{l0}(\hat{r}') \right] \\
& \times \left[\Psi(\mathbf{r})^* \Psi\left(\mathbf{r} - \frac{\mathbf{r}'}{2}\right) \Psi\left(\mathbf{r} + \frac{\mathbf{r}'}{2}\right) + \Psi(\mathbf{r} - \mathbf{r}')^* \Psi\left(\mathbf{r} - \frac{\mathbf{r}'}{2}\right)^2 \right] \\
& + \frac{2(4\pi)^2 \hbar^2}{M} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \Psi^*(\mathbf{r} - \mathbf{r}_1) \Psi\left(\mathbf{r} - \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}\right) \Psi\left(\mathbf{r} - \frac{\mathbf{r}_1 - \mathbf{r}_2}{2}\right) \\
& \times \frac{1}{2} \sum_{ll'm}'' \Delta a_{ll'}^{(m)} \left[\frac{4\pi}{(2\pi)^3} Y_{lm}^*(\hat{r}_1) \frac{(l+1)!!}{2^{l/2}} \frac{\pi}{r_1^3} \right] \left[\frac{4\pi}{(2\pi)^3} Y_{l'm}(\hat{r}_2) \frac{(l'+1)!!}{2^{l'/2}} \frac{\pi}{r_2^3} \right], \tag{13}
\end{aligned}$$

where $\Psi(\mathbf{r}) = \langle \hat{\psi}(\mathbf{r}) \rangle$ is the condensate wavefunction. Similarly, one can also derive the associated Bogoliubov–de Gennes equations for the elementary excitations. Note that the effective Hamiltonian, equations (11) and (12), and the meanfield equation, equation (13), contain all the effects beyond the simple FBA results, and they will reproduce the known FBA results when taking $\Delta a_{ll'}^{(m)} = 0$.

5. 3D condensate profile

5.1. Gaussian variational wavefunction

To study the aspect ratio and the stability regime of the condensate profile, it is convenient to use the variational approach [16]. Here we use a Gaussian-type trial wavefunction,

$$\Psi(\mathbf{r}) = \frac{\sqrt{N} \exp(-\rho^2/2R_0^2 - z^2/2R_z^2)}{\pi^{3/4} R_0 R_z^{1/2}} \quad (14)$$

for the condensate wavefunction in harmonic trapping potential: $V_{\text{ext}}(\mathbf{r}) = \frac{1}{2}M\omega_0^2(x^2 + y^2) + \frac{1}{2}M\omega_z^2z^2$, where ω_0 and ω_z are the associated trapping frequencies. Here N is the total number of dipoles, and R_0 and R_z are the Gaussian radii of the condensate in the x - y plane and along the z -axis, respectively. The variational energy can be obtained easily from the effective Hamiltonian in the momentum space, equation (11), by replacing $\hat{a}_{\mathbf{k}}$ by $\Psi_{\mathbf{k}} \equiv \langle \hat{a}_{\mathbf{k}} \rangle = \frac{1}{\sqrt{\Omega}} \int d\mathbf{r} \Psi(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}$. We therefore obtain

$$\frac{E(R_0, \beta)}{E_0} = \frac{1 + 2\beta^2}{2\beta^2 \tilde{R}_0^2} + \frac{\tilde{R}^2(2\kappa^2 + \beta^2)}{2\kappa^2} + \frac{2N\tilde{a}_s}{\sqrt{2\pi} \tilde{R}_0^3 \beta} + \frac{16A_2(\beta) N\tilde{a}_d}{3\sqrt{10\pi} \tilde{R}_0^3} + \frac{32\beta N}{\sqrt{2\pi} \tilde{R}_0^3} \left[\sum_{l=2}^{\infty} \Delta\tilde{a}_{l,l}^{(0)} A_l(\beta)^2 - 2 \sum_{l \neq l'}^{\infty} \Delta\tilde{a}_{l,l'}^{(0)} A_l(\beta) A_{l'}(\beta) \right], \quad (15)$$

where $A_l(\beta) \equiv \frac{\sqrt{2l+1}}{8} \int_{-1}^1 dx \frac{P_l(x)}{(1+(\beta^2-1)x^2)^{3/2}}$. $\beta \equiv R_z/R_0$ and $\kappa \equiv \omega_0/\omega_z$ are the condensate and trapping aspect ratios. We have also scaled all the length scales (a_s , a_d , $\Delta\tilde{a}_{l,l'}^{(0)}$ and R_0) by the horizontal oscillator length, $a_{\text{osc},0} \equiv \sqrt{\hbar/M\omega_0}$ (i.e. $\tilde{R}_0 = R_0/a_{\text{osc},0}$, 0, etc), and used $E_0 \equiv N\hbar^2/2ma_{\text{osc},0}^2$ as the energy scale.

The first two terms in the right-hand side of equation (15) are from the kinetic and potential energies, respectively, and the third is from the s-wave scattering channel. The fourth term is from the contribution within the FBA and the second line is from the effects beyond the FBA. Again we find that the whole meanfield energy of equation (15) will become the same as calculated within the FBA by taking $\Delta\tilde{a}_{l,l+2}^{(0)} = 0$. Using the fact that $A_0(\beta) = (4\beta)^{-1}$, we find that the contribution of the FBA is of the same form as the term with $\Delta\tilde{a}_{0,2}^{(0)}$ (both of them are proportional to $A_2(\beta)$). However, such a coincidence is simply due to the special form Gaussian trial wavefunction. Using other trial wavefunctions can easily give different aspect ratio dependences of these two effects. Besides, we also note that $A_l(\beta = 1) = 0$ for $l \neq 0$, showing that for a spherically symmetric condensate ($\beta = 1$), only s-wave scattering channels is relevant: scattering in finite angular momentum channels is cancelled out due to spherical symmetry of the condensate profile. When the condensate profile is highly anisotropic due to external confinement (say in cigar shape, $\beta \gg 1$, or in pancake shape, $\beta \ll 1$), the effects beyond the FBA will become very crucial.

5.2. Example: near shape resonance

For the general form of the effective Hamiltonian of equations (11) and (12), values of $a_{l,l'}^{(m)}$ have to be obtained from first principle calculations [9, 10], which is however beyond the scope

of this paper. In fact, due to the highly nontrivial inter-molecule interaction at short distances, the low-energy scattering matrix element, $t_{lm}''(0)$, can be very different from the results of the Born approximation in the strong dipole regime. Here, we consider the simplest case to study the effect beyond the FBA: we assume the external electric field is still weak but near the first shape resonance regime, where the shape resonance occurs in the s-wave channel so that both $t_{00}^{00}(0)$ and $t_{00}^{20}(0)$ strongly deviate from the results in the weak interaction limit. Scattering matrix elements in other channels are less affected because of the centrifugal potential for $l \neq 0$. This picture is also consistent with the numerical results shown in [10], where their numerical results of $t_{20}^{40}(0)$ are almost unaffected by the shape resonance in the s-wave channel. (But it does not exclude the possibility of having a significant deviation in other channels in the regime of much stronger dipolar interaction.)

Under such an assumption, we may consider $\Delta a_{0,2}^{(0)} \neq 0$, and $\Delta a_{l,l'}^{(0)} = 0$ for all $(l, l') \neq (0, 2), (2, 0)$ or $(0, 0)$. As a result, the variational energy of equation (4) becomes (using $A_0(\beta) = 1/4\beta$):

$$\frac{E(R_0, \beta)}{E_0} = \frac{1 + 2\beta^2}{2\beta^2 \tilde{R}_0^2} + \frac{\tilde{R}^2(2\kappa^2 + \beta^2)}{2\kappa^2} + \frac{2N}{\sqrt{2\pi} \tilde{R}_0^3} \left[\frac{\tilde{a}_s}{\beta} + 8 \left(\frac{\tilde{a}_d}{3\sqrt{5}} - \Delta \tilde{a}_{0,2}^{(0)} \right) A_2(\beta) \right]. \quad (16)$$

From the above result, we find that the contribution of the $\Delta a_{0,2}^{(0)}$ term can reduce (since $\Delta a_{0,2}^{(0)} > 0$ near the first shape resonance, see [10]) the effect of the anisotropic feature of dipole interaction. Although this result is derived from the Gaussian trial wavefunction, such a reduction of anisotropy of the condensate wavefunction should still be qualitatively correct for a more accurate condensate profile.

We note that the ground-state energy and the pseudo-potential study have also been discussed in [9], where they include the dipole dependence in the s-wave scattering length (i.e. $a_s(D)$) and use the FBA results (equation (2)) for the dipole interaction near the first few shape resonances. In other words, they did not consider the effect of strong deviation of $t_{00}^{20}(0)$ from the FBA, which is a very significant result as shown in [10]. If considering an even stronger dipole moment (larger than the value for the first few shape resonances), where the scattering amplitudes may deviate from the FBA result in *all* channels, one has to solve equations (11)–(13) with finite values of $\Delta a_{l,l'}^{(m)}$ for the correct many-body physics of polar molecules.

6. The effective Hamiltonian and excitations in 2D

In a 2D homogeneous system, we can assume that the wavefunction in the z -axis is of Gaussian type: $\phi(z) = \frac{1}{\pi^{1/4} R_z^{1/2}} e^{-z^2/2R_z^2}$, where R_z is the width of such a quasi-2D potential layer. After integrating out the degree of freedom in the z -direction (i.e. along the direction of the external electric field) of the 3D effective Hamiltonian, equation (11), we obtain

$$H_{2D} = \sum_{\mathbf{p}} \left(\frac{\mathbf{p}^2}{2M} - \mu \right) \hat{b}_{\mathbf{p}}^\dagger \hat{b}_{\mathbf{p}} + \frac{1}{2\Omega_{\perp}} \sum_{\mathbf{p}_1, \mathbf{p}_2, \mathbf{q}} [V_s + V_B(\mathbf{q})] \hat{b}_{\mathbf{p}_1 + \frac{\mathbf{q}}{2}}^\dagger \hat{b}_{\mathbf{p}_2 - \frac{\mathbf{q}}{2}}^\dagger \hat{b}_{\mathbf{p}_2 + \frac{\mathbf{q}}{2}} \hat{b}_{\mathbf{p}_1 - \frac{\mathbf{q}}{2}} + \frac{1}{2\Omega_{\perp}} \sum_{\mathbf{p}_1, \mathbf{p}_2, \mathbf{P}} V_{\Delta}(\mathbf{p}_1, \mathbf{p}_2) \hat{b}_{\mathbf{P}/2 + \mathbf{p}_1}^\dagger \hat{b}_{\mathbf{P}/2 - \mathbf{p}_1}^\dagger \hat{b}_{\mathbf{P}/2 - \mathbf{p}_2} \hat{b}_{\mathbf{P}/2 + \mathbf{p}_2}, \quad (17)$$

where we define $\hat{b}_{\mathbf{p}}$ and $\hat{b}_{\mathbf{p}}^\dagger$ as the field operators in the 2D system with \mathbf{p} being the *in-plane* momentum vector from now on. Ω_\perp is the 2D area, and

$$V_s \equiv \frac{4\pi\hbar^2 a_s}{\sqrt{2\pi} M R_z}$$

is the contribution of s-wave scattering.

$$V_B(\mathbf{q}) \equiv \frac{\hbar^2 a_d}{M R_z} \frac{4\sqrt{2\pi}}{3} g\left(\frac{|\mathbf{q}| R_z}{\sqrt{2}}\right),$$

where $g(x) = 1 - (3\sqrt{\pi}/2)x e^{x^2} \text{Erfc}(x)$ with $\text{Erfc}(x)$ being the complementary error function. We also have

$$V_\Delta(\mathbf{p}_1, \mathbf{p}_2) \equiv \frac{8\sqrt{2\pi}\hbar^2}{M R_z} \sum_{l,l'} \sum_m \Delta a_{l,l'}^{(m)} i^{l-l'} F_{lm}^*(\mathbf{p}_1) F_{l'm}(\mathbf{p}_2) \quad (18)$$

to account for the contribution beyond FBA, where

$$\begin{aligned} F_{lm}(\mathbf{p}) &\equiv R_z \int d p_z e^{-p_z^2 R_z^2} Y_{lm}(\hat{p}) \\ &= \int_{-\infty}^{\infty} dx e^{-x^2} \sqrt{\frac{2l+1}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}} P_l\left(\sqrt{\frac{x^2}{x^2 + p^2 R_z^2}}\right) e^{im\phi_p}, \end{aligned} \quad (19)$$

with $\phi_p \equiv \tan^{-1}(p_y/p_x)$ being the angle in the 2D plane.

At zero temperature, the dipolar atoms/molecules condense at $\mathbf{p} = 0$, so that the total energy is $E_{2D} = \frac{N^2}{2\Omega_\perp} [V_s + V_B(0) + V_\Delta(0, 0)]$, with the chemical potential being $\mu = n_{2D}[V_s + V_B(0) + V_\Delta(0, 0)]$, where $n_{2D} = N/\Omega_\perp$ is the particle density in the 2D plane. Keeping only the condensate part ($\hat{b}_0 = \hat{b}_0^\dagger = \sqrt{n_{2D}}$) and the quadratic order of fluctuations ($\mathbf{p} \neq 0$), the effective Hamiltonian becomes:

$$\begin{aligned} H_{\text{eff}} &= \sum_{\mathbf{p}} \left(\frac{\mathbf{p}^2}{2m} - \mu \right) a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + \frac{N}{2\Omega_\perp} \sum_{\mathbf{p}} [V_s + V_B(\mathbf{p}) + V_{2D}(\mathbf{p}, 0)] (a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger + a_{-\mathbf{p}} a_{\mathbf{p}}) \\ &\quad + \frac{N}{2\Omega_\perp} \sum_{\mathbf{p}} \left[4V_s + 2V_B(0) + 2V_B(\mathbf{p}) + 2V_\Delta\left(\frac{\mathbf{p}}{2}, \frac{\mathbf{p}}{2}\right) + 2V_\Delta\left(\frac{\mathbf{p}}{2}, -\frac{\mathbf{p}}{2}\right) \right] a_{\mathbf{p}}^\dagger a_{\mathbf{p}}, \end{aligned} \quad (20)$$

where we have used the fact that $V_\Delta(\mathbf{p}_1, \mathbf{p}_2) = V_\Delta(-\mathbf{p}_1, -\mathbf{p}_2) = V_\Delta(\mathbf{p}_2, \mathbf{p}_1)$. Finally, we could use the Bogoliubov transformation to diagonalize the above Hamiltonian and obtain the following phonon excitation spectrum:

$$\omega_{\mathbf{p}}^2 = \left[\frac{\mathbf{p}^2}{2M} + n_{2D} W_-(\mathbf{p}) \right] \left[\frac{\mathbf{p}^2}{2m} + 2n_{2D} (V_s + V_B(\mathbf{p}) + W_+(\mathbf{p})) \right], \quad (21)$$

where $W_\pm(\mathbf{p}) \equiv V_\Delta(\frac{\mathbf{p}}{2}, \frac{\mathbf{p}}{2}) + V_\Delta(\frac{\mathbf{p}}{2}, -\frac{\mathbf{p}}{2}) - V_\Delta(0, 0) \pm V_\Delta(\mathbf{p}, 0)$ accounts for the effects beyond the FBA results.

Similar to the 3D case, we now study the situation when only $\Delta a_{0,2}^{(0)} \neq 0$ in $V_\Delta(\mathbf{p}_1, \mathbf{p}_2)$, and obtain

$$V_\Delta(\mathbf{p}_1, \mathbf{p}_2) = \frac{-2\sqrt{10\pi}\hbar^2}{M R_z} \Delta a_{0,2}^{(0)} [g(|\mathbf{p}_1| R_z) + g(|\mathbf{p}_2| R_z)].$$

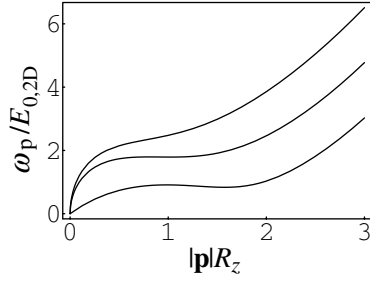


Figure 2. Phonon dispersion, $\omega_{\mathbf{p}}$, as a function of $|\mathbf{p}|R_z$ in the 2D system. $n_{2D}\Delta a_{0,2}^{(0)}R_z = 0, 0.05$ and 0.1 , for curves from the bottom to top. The other parameters are: $n_{2D}a_sR_z = 0.5$, $n_{2D}a_dR_z = 1.4$ and $E_{0,2D} = \hbar^2/MR_z^2$ is the energy scale.

The calculated dispersion, $\omega_{\mathbf{p}}$, for different values of $\Delta a_{0,2}^{(0)} > 0$ are shown in figure 2. There are two significant effects to be noted: Firstly, in the short-wavelength regime, the roton minimum, predicted [4] as a feature of dipolar interaction for the 2D bosonic polar molecules, becomes weaker as $a_{0,2}^{(0)}$ becomes stronger. Secondly, in the long-wavelength limit, instead of the typical linear dispersion [4], we find $\omega_{\mathbf{p}} = C\sqrt{|\mathbf{p}|R_z}(1 + \mathcal{O}(|\mathbf{p}|R_z))$ with the prefactor

$$C = 2\sqrt{6}(5\pi^3)^{1/4} \sqrt{\Delta a_{0,2}^{(0)} \left(a_s + \frac{2}{3}a_d - 2\sqrt{5}\Delta a_{0,2}^{(0)} \right)} \times \frac{\hbar^2 n_{2D}}{MR_z}.$$

As a result, the phase fluctuation becomes much stiffer than predicted in the FBA, showing an enhancement of the condensate/superfluid density at zero temperature. More precisely, we can calculate the normal fluid density, ρ_n , according to the transverse current correlation function [17]. The sublinear dispersion of $\omega_{\mathbf{p}}$ gives $\rho_n(T) = \frac{7! \zeta(7) \hbar^2 (k_B T)^7}{2\pi M C^8 R_z^4}$, which shows a much smaller temperature (T) dependence than the result obtained for linear dispersion ($\rho_n = \frac{3\zeta(3)(k_B T)^3}{2\pi M \hbar^2 c_1^4}$ if $\omega_{\mathbf{p}} = c_1 \hbar |\mathbf{p}|$ [17]). According to Landau's two-fluid model and the universal relation between the 2D superfluid density and the Kosterlitz–Thouless transition temperature, the superfluid transition temperature (T_c) of the 2D dipolar system is then determined by $k_B T_c = \pi \hbar^2 \rho_s(T_c)/2M = \pi \hbar^2 (n_{2D} - \rho_n(T_c))/2M$. At temperatures below T_c , the single-particle correlation function has a power-law decay with zero condensate density. These results are also equivalent to a 2D charged Bose gas ($V(r) = Q^2/r$) [11] with an effective charge, $Q = C\sqrt{R_z M/n_{2D}\hbar^2}$. Such an interesting equivalence implies the possibility to use neutral polar molecules to simulate a 2D charged boson system in liquid phase (not dopable for ion traps due to the strong Coulomb interaction and a large atom mass), which may be important for understanding the superconducting Cooper pairs in a high T_c thin film [12].

7. Summary

In summary, we have developed a complete effective many-body theory for 3D and 2D dipolar Bose gases beyond the simple FBA. One of the significant consequences is that the dipolar interaction effect in the 3D condensate can be reduced near the shape resonance regime. For the 2D system (highly anisotropic regime), such an effect brings a significant change of the

low-energy excitation spectrum. We believe that there should be more interesting results for a polar molecule system in the strong external field regime, where all scattering channels (besides the t_{00}^{20} channel) can deviate significantly from the FBA. Therefore our results are especially important for future studies of the many-body properties of strongly interacting polar molecules.

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Appendix A. The effective Hamiltonian in real space

We note that the single-particle part, s-wave scattering, and the FBA part of interaction can be transformed easily into real space as shown in the literature; therefore here, we just show the results for the interaction part beyond the FBA, i.e. the last term of equation (11). To Fourier-transform the effective Hamiltonian, we use $\hat{a}_{\mathbf{p}} = \int \frac{d\mathbf{r}}{\sqrt{\Omega}} \hat{\psi}(\mathbf{r}) e^{-i\mathbf{p}\cdot\mathbf{r}}$ and the interaction part beyond FBA (denoted by H'_I) becomes:

$$\begin{aligned}
 H'_I &= \frac{-4\pi\hbar^2}{M} \frac{1}{2\Omega} \sum_{\mathbf{p}_1, \mathbf{p}_2, \mathbf{P}} \hat{a}_{\mathbf{P}/2+\mathbf{p}_1}^* \hat{a}_{\mathbf{P}/2-\mathbf{p}_1}^* \hat{a}_{\mathbf{P}/2-\mathbf{p}_2} \hat{a}_{\mathbf{P}/2+\mathbf{p}_2} f_{\Delta}(\mathbf{p}_1, \mathbf{p}_2) \\
 &= \frac{(4\pi)^2\hbar^2}{M} \frac{1}{2\Omega^3} \sum_{\mathbf{p}_1, \mathbf{p}_2, \mathbf{P}} \sum_{l'l'm} \Delta a_{l'l'}^{(m)} i^{l'-l} Y_{l'm}^*(\hat{p}_1) Y_{lm}(\hat{p}_2) \int d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 d\mathbf{r}_4 \\
 &\quad \times e^{i(\mathbf{P}/2+\mathbf{p}_1)\cdot\mathbf{r}_1} e^{i(\mathbf{P}/2-\mathbf{p}_1)\cdot\mathbf{r}_2} e^{-i(\mathbf{P}/2-\mathbf{p}_2)\cdot\mathbf{r}_3} e^{-i(\mathbf{P}/2+\mathbf{p}_2)\cdot\mathbf{r}_4} \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_3) \hat{\psi}(\mathbf{r}_4) \\
 &= \frac{(4\pi)^2\hbar^2}{M} \frac{1}{2\Omega^2} \sum_{\mathbf{p}_1, \mathbf{p}_2} \sum_{l'l'm} \Delta a_{l'l'}^{(m)} i^{l'-l} Y_{l'm}^*(\hat{p}_1) Y_{lm}(\hat{p}_2) \\
 &\quad \times \int d\mathbf{R} d\mathbf{r}_1 d\mathbf{r}_2 e^{i\mathbf{p}_1\cdot\mathbf{r}_1} e^{-i\mathbf{p}_2\cdot\mathbf{r}_2} \hat{\psi}^\dagger\left(\mathbf{R} + \frac{\mathbf{r}_1}{2}\right) \hat{\psi}^\dagger\left(\mathbf{R} - \frac{\mathbf{r}_1}{2}\right) \hat{\psi}\left(\mathbf{R} - \frac{\mathbf{r}_2}{2}\right) \hat{\psi}\left(\mathbf{R} + \frac{\mathbf{r}_2}{2}\right), \quad (\text{A.1})
 \end{aligned}$$

where we have integrated out the total momentum, \mathbf{P} , and the center of mass position before scattering, $\mathbf{R}' \equiv (\mathbf{r}_3 + \mathbf{r}_4)/2$. Note that the summation of angular momentum quantum number, $\sum_{l'l'm}$, has excluded the pure s-wave scattering channel, $l = l' = m = 0$.

Now, we consider the expansion of a plane wave in spherical harmonic functions:

$$e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{lm} i^l j_l(kr) Y_{lm}^*(\hat{r}) Y_{lm}(\hat{k}) \quad (\text{A.2})$$

or equivalently

$$\int d\Omega_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} Y_{lm}^*(\hat{k}) = \begin{cases} 4\pi i^l j_l(kr) Y_{lm}^*(\hat{r}), & \text{for } r \neq 0, \\ \sqrt{4\pi} \delta_{l,0}, & \text{for } r = 0. \end{cases} \quad (\text{A.3})$$

Equation (A.3) suggests that it is more convenient to separate terms with zero angular momentum quantum number, $\Delta a_{0l}^{(0)} = \Delta a_{l0}^{(0)}$, from the others in equation (A.1) before carrying out the momentum integral. (We note that the higher-order correction of dipolar

interaction, $V_d(\mathbf{r}) \propto Y_{20}(\hat{r})$, can couple s-wave to higher-momentum channels in the strong dipole momentum limit.) As a result, equation (A.1) can be rewritten as follows:

$$H'_1 = H'_{11} + H'_{12},$$

$$\begin{aligned} H'_{11} &= \frac{(4\pi)^2 \hbar^2}{M} \int d\mathbf{R} d\mathbf{r}_1 d\mathbf{r}_2 \hat{\psi}^\dagger \left(\mathbf{R} + \frac{\mathbf{r}_1}{2} \right) \hat{\psi}^\dagger \left(\mathbf{R} - \frac{\mathbf{r}_1}{2} \right) \hat{\psi} \left(\mathbf{R} - \frac{\mathbf{r}_2}{2} \right) \hat{\psi} \left(\mathbf{R} + \frac{\mathbf{r}_2}{2} \right) \\ &\quad \times \sum_l \frac{(-1)^{l/2} \Delta a_{0l}^{(0)}}{2\Omega^2} \sum_{\mathbf{p}_1, \mathbf{p}_2} e^{i\mathbf{p}_1 \cdot \mathbf{r}_1} e^{-i\mathbf{p}_2 \cdot \mathbf{r}_2} (Y_{l0}^*(\hat{p}_1) Y_{00}(\hat{p}_2) + Y_{00}^*(\hat{p}_1) Y_{l0}(\hat{p}_2)) \\ &= \frac{(4\pi)^2 \hbar^2}{M} \int d\mathbf{R} d\mathbf{r}_1 \hat{\psi}^\dagger \left(\mathbf{R} + \frac{\mathbf{r}_1}{2} \right) \hat{\psi}^\dagger \left(\mathbf{R} - \frac{\mathbf{r}_1}{2} \right) \hat{\psi}(\mathbf{R}) \hat{\psi}(\mathbf{R}) \\ &\quad \times \sum_l \frac{(-1)^{l/2} \Delta a_{0l}^{(0)}}{2\sqrt{4\pi}} \left[\frac{1}{\Omega} \sum_{\mathbf{p}_1} e^{i\mathbf{p}_1 \cdot \mathbf{r}_1} Y_{l0}^*(\hat{p}_1) \right] \\ &\quad + \frac{(4\pi)^2 \hbar^2}{M} \int d\mathbf{R} d\mathbf{r}_2 \hat{\psi}^\dagger(\mathbf{R}) \hat{\psi}^\dagger(\mathbf{R}) \hat{\psi} \left(\mathbf{R} - \frac{\mathbf{r}_2}{2} \right) \hat{\psi} \left(\mathbf{R} + \frac{\mathbf{r}_2}{2} \right) \\ &\quad \times \sum_l \frac{(-1)^{l/2} \Delta a_{0l}^{(0)}}{2\sqrt{4\pi}} \left[\frac{1}{\Omega} \sum_{\mathbf{p}_2} e^{-i\mathbf{p}_2 \cdot \mathbf{r}_2} Y_{l0}(\hat{p}_2) \right], \end{aligned} \quad (\text{A.4})$$

$$\begin{aligned} H'_{12} &= \frac{(4\pi)^2 \hbar^2}{M} \int d\mathbf{R} d\mathbf{r}_1 d\mathbf{r}_2 \hat{\psi}^\dagger \left(\mathbf{R} + \frac{\mathbf{r}_1}{2} \right) \hat{\psi}^\dagger \left(\mathbf{R} - \frac{\mathbf{r}_1}{2} \right) \hat{\psi} \left(\mathbf{R} - \frac{\mathbf{r}_2}{2} \right) \hat{\psi} \left(\mathbf{R} + \frac{\mathbf{r}_2}{2} \right) \\ &\quad \times \frac{1}{2} \sum_{l'l''}'' \Delta a_{l'l''}^{(m)l'-l} \left[\frac{1}{\Omega} \sum_{\mathbf{p}_1} e^{i\mathbf{p}_1 \cdot \mathbf{r}_1} Y_{l'm}^*(\hat{p}_1) \right] \left[\frac{1}{\Omega} \sum_{\mathbf{p}_2} e^{-i\mathbf{p}_2 \cdot \mathbf{r}_2} Y_{l'm}(\hat{p}_2) \right], \end{aligned} \quad (\text{A.5})$$

where $\sum_{l'l''}''$ in the last line is a summation excluding any terms with l or $l' = 0$. To get equation (A.4), we have used the fact that $\Omega^{-1} \sum_{\mathbf{p}} e^{i\mathbf{p} \cdot \mathbf{r}} = \delta(\mathbf{r})$ and have integrated out one of the relative coordinates. Now we can integrate out the solid angle of momentum variables (\mathbf{p}_1 and \mathbf{p}_2) by using equation (A.3) for $l \neq 0$:

$$\frac{1}{\Omega} \sum_{\mathbf{p}} e^{i\mathbf{p} \cdot \mathbf{r}} Y_{lm}^*(\hat{p}) = \int_0^\Lambda \frac{p^2 dp}{(2\pi)^3} \int d\Omega_{\mathbf{p}} e^{i\mathbf{p} \cdot \mathbf{r}} Y_{lm}^*(\hat{p}) = 4\pi i^l Y_{lm}^*(\hat{r}) \int_0^\Lambda \frac{p^2 dp}{(2\pi)^3} j_l(pr), \quad (\text{A.6})$$

where Λ is the momentum cut-off in the atomic length scale ($\sim r_c^{-1}$), due to the nature of the effective Hamiltonian obtained by integrating out the high-momentum/energy contribution within the ladder approximation of equation (6). In order to regularize it to get a universal expression, we can introduce another high-momentum cut-off, $e^{-\alpha p}$, inside the integrand and taking α to zero ($\alpha \rightarrow 0^+$) in the final results. Using the fact that only even angular quantum numbers ($l = 2m'$) are relevant for the scattering between bosonic polar molecules, and applying the following identity:

$$\lim_{\alpha \rightarrow 0^+} \int_0^\infty p^2 j_{2m'}(pr) e^{-\alpha p} dp = \frac{(2m' + 1)!!}{2^{m'}} \frac{\pi}{r^3} \quad (\text{A.7})$$

for $m' \neq 0$, we can simplify equation (A.6) further and rewrite the effective Hamiltonian (H'_{11} and H'_{12}) as follows:

$$\begin{aligned} H'_{11} &= \frac{(4\pi)^2 \hbar^2}{M} \int d\mathbf{R} d\mathbf{r} \left[\hat{\psi}^\dagger \left(\mathbf{R} + \frac{\mathbf{r}}{2} \right) \hat{\psi}^\dagger \left(\mathbf{R} - \frac{\mathbf{r}}{2} \right) \hat{\psi}(\mathbf{R}) \hat{\psi}(\mathbf{R}) \right. \\ &\quad \left. \times \sum_l \frac{\Delta a_{0l}^{(0)}}{2\sqrt{4\pi}} \frac{4\pi}{(2\pi)^3} Y_{l0}^*(\hat{r}) \frac{(l+1)!!}{2^{l/2}} \frac{\pi}{r^3} + \text{h.c.} \right] \\ &= \frac{2\sqrt{\pi} \hbar^2}{M} \int d\mathbf{R} \left[\hat{\psi}^\dagger \left(\mathbf{R} + \frac{\mathbf{r}}{2} \right) \hat{\psi}^\dagger \left(\mathbf{R} - \frac{\mathbf{r}}{2} \right) \sum_l \Delta a_{0l}^{(0)} \hat{\phi}_{l0}(\mathbf{R}) + \text{h.c.} \right], \end{aligned} \quad (\text{A.8})$$

$$\begin{aligned} H'_{12} &= \frac{(4\pi)^2 \hbar^2}{M} \int d\mathbf{R} d\mathbf{r}_1 d\mathbf{r}_2 \hat{\psi}^\dagger \left(\mathbf{R} + \frac{\mathbf{r}_1}{2} \right) \hat{\psi}^\dagger \left(\mathbf{R} - \frac{\mathbf{r}_1}{2} \right) \hat{\psi} \left(\mathbf{R} - \frac{\mathbf{r}_2}{2} \right) \hat{\psi} \left(\mathbf{R} + \frac{\mathbf{r}_2}{2} \right) \\ &\quad \times \frac{1}{2} \sum_{l'l'm} \Delta a_{l'l'}^{(m)} \left[\frac{4\pi}{(2\pi)^3} Y_{lm}^*(\hat{r}_1) \frac{(l+1)!!}{2^{l/2}} \frac{\pi}{r_1^3} \right] \left[\frac{4\pi}{(2\pi)^3} Y_{l'm}(\hat{r}_2) \frac{(l'+1)!!}{2^{l'/2}} \frac{\pi}{r_2^3} \right] \\ &= \frac{2\hbar^2}{M} \sum_{l,l'} \sum_m \Delta a_{l'l'}^{(m)} \int d\mathbf{R} \hat{\phi}_{lm}^\dagger(\mathbf{R}) \hat{\phi}_{l'm}(\mathbf{R}), \end{aligned} \quad (\text{A.9})$$

where we have defined an effective pairing operator:

$$\hat{\phi}_{lm}(\mathbf{R}) \equiv \frac{(l+1)!!}{2^{l/2}} \int \frac{d\mathbf{r}}{|\mathbf{r}|^3} Y_{lm}(\hat{r}) \hat{\psi} \left(\mathbf{R} + \frac{\mathbf{r}}{2} \right) \hat{\psi} \left(\mathbf{R} - \frac{\mathbf{r}}{2} \right), \quad (\text{A.10})$$

in the angular momentum (l, m) channel to simplify the notation. Therefore, after adding back the known single-particle Hamiltonian and the FBA results together, we can obtain the final total effective Hamiltonian in real space as shown in equation (12).

References

- [1] Stuhler J *et al* 2005 *Phys. Rev. Lett.* **95** 150406
Hensler S *et al* 2003 *Appl. Phys. B* **77** 765
- [2] Doyle J 2004 *Eur. Phys. J. D* **31** 149
Bethlem H L *et al* 2000 *Nature* **406** 491
Kerman A J *et al* 2004 *Phys. Rev. Lett.* **92** 033004
- [3] Goral K, Rzazewski K and Pfau T 2000 *Phys. Rev. A* **61** 051601
Goral K and Santos L 2002 *Phys. Rev. A* **66** 023613
Ronen S, Bortolotti D C E and Bohn J L 2007 *Phys. Rev. Lett.* **98** 030406
- [4] Santos L *et al* 2000 *Phys. Rev. Lett.* **85** 1791
Santos L *et al* 2003 *Phys. Rev. Lett.* **90** 250403
O'Dell D H J *et al* 2004 *Phys. Rev. Lett.* **92** 250401
Giovanazzi S, Santos L and Pfau T 2007 *Phys. Rev. A* **75** 015604
Fischer U R 2006 *Phys. Rev. A* **73** 031602
- [5] Barnett R *et al* 2006 *Phys. Rev. Lett.* **96** 190401
Diener R B and Ho T-L 2006 *Phys. Rev. Lett.* **96** 190405
Wang D-W *et al* 2006 *Phys. Rev. Lett.* **97** 180413
Wang D-W 2007 *Phys. Rev. Lett.* **98** 060403
Arguelles A and Santos L *Preprint cond-mat/0612522*

- [6] Yi S and You L 2000 *Phys. Rev. A* **61** 041604
- [7] Derevianko A 2003 *Phys. Rev. A* **67** 033607
Derevianko A 2005 *Phys. Rev. A* **72** 039901
- [8] Huang K and Yang C N 1957 *Phys. Rev. A* **105** 767
- [9] Bortolotti D C E *et al* 2006 *Phys. Rev. Lett.* **97** 160402
Ronen S *et al* 2006 *Phys. Rev. A* **74** 033611
Kanjilal K, Bohn J L and Blume D 2007 *Phys. Rev. A* **75** 052703
- [10] Deb B and You L 2001 *Phys. Rev. A* **64** 022717
- [11] Strepparola E, Minguzzi A and Tosi M P 2001 *Phys. Rev. B* **63** 104509
De Palo S, Conti S and Moroni S 2004 *Phys. Rev. B* **69** 035109
- [12] Wen X-G and Kan R 1988 *Phys. Rev. B* **37** 595
Fisher M P A 1990 *Phys. Rev. Lett.* **65** 923
Tanda S, Ohzeki S and Nakayama T 1992 *Phys. Rev. Lett.* **69** 530
Nakielski G *et al* 1996 *Phys. Rev. Lett.* **76** 2567
Kim S-H, Kim C K and Nahm K 2003 *Phys. Status Solidi b* **236** 129
- [13] Yi S and You L 2004 *Phys. Rev. Lett.* **92** 193201
- [14] Landau L D and Lifshitz E M 1977 *Quantum Mechanics* (New York: Pergamon)
- [15] Fetter A L and Walecka J D 1971 *Quantum Theory of Many-Particle Systems* (New York: McGraw-Hill)
- [16] Penthick C J and Smith H 2002 *Bose-Einstein Condensation in Dilute Gases* (Cambridge: Cambridge University Press)
- [17] Tauber U C and Nelson D R 1997 *Phys. Rep.* **289** 157