Tunable high-temperature thermodynamics of weakly-interacting dipolar gases

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We consider dilute gases of dipolar bosons or fermions in the high-temperature limit in a spherically symmetric harmonic trapping potential. We examine the system using a virial expansion up to second order in the fugacity. Using the Born approximation and assuming purely dipolar interactions, we find that the second-order virial coefficient for both bosons and fermions depends quadratically on the dipole length and is negative at high temperature, indicating that to lowest order in the dipole-dipole interactions the dipolar single-component quantum gases are repulsive. If the $s$-wave scattering length for the bosonic system is tunable and its absolute value is made small, then the $s$-wave interactions dominate and the dipolar gas behaves like a weakly-interacting Bose gas with isotropic $s$-wave interactions. If the generalized scattering lengths for the fermionic system are tunable, then the dipole length can enter linearly in the virial equation of state, enhancing the dipole-dipole effects in the thermodynamic observables.

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I. INTRODUCTION

There has been much interest in the past few years in ultracold systems of dipoles \[ \text{\textit{D}} \]. Anisotropic long-range interactions can arise due to the interactions between the magnetic moments of atoms or due to the interactions between heteronuclear diatomic molecules (in this case, each molecule is treated as an electric dipole). Experimentally, dipole-dipole interactions play a prominent role in the dynamics of ultracold atomic clouds consisting of Cr \[ \text{\textit{D}} \], Dy \[ \text{\textit{D}} \], and Er \[ \text{\textit{D}} \]. In these systems, the effects of the dipole-dipole interactions have been observed in the degenerate regime via expansion cloud imaging \[ \text{\textit{D}} \text{, \textit{D}} \text{, \textit{D}} \]. Additionally, polar molecules such as KRb \[ \text{\textit{D}} \], RbCs \[ \text{\textit{D}} \] and LiCs \[ \text{\textit{D}} \] have been created and the effects of the anisotropic interactions have been observed in KRb clouds with phase space densities just above degeneracy \[ \text{\textit{D}} \text{, \textit{D}} \].

It remains an open question whether the effects from the anisotropic and long-range dipole-dipole interactions can be observed in thermodynamic observables at high temperature, i.e., at temperatures above the degeneracy temperature. For isotropic short-range interactions, the high-temperature behavior of two-component Fermi gases is well described by the virial equation of state \[ \text{\textit{D}} \text{, \textit{D}} \]. At unitarity, i.e., for infinitely large interspecies $s$-wave scattering length, the virial equation of state has been validated through careful measurements \[ \text{\textit{D}} \text{, \textit{D}} \]. This paper derives the virial equation of state for dipolar gases and investigates the interplay between the short-range and long-range interactions. Specifically, we focus on the temperature regime above quantum degeneracy and show that signatures of the dipole-dipole interactions can be enhanced if one of the generalized scattering lengths in a low partial wave channel is tuned.

We consider a single-component gas of aligned dipolar bosons or fermions under spherically symmetric harmonic confinement and calculate the second-order virial coefficient for weak dipole-dipole interactions. If the dipole-dipole scattering properties are calculated in the first-order Born approximation and if the dipole length $D$ is small compared to the harmonic oscillator length $a_{ho}$, then the second-order virial coefficient $\Delta b_2$, which accounts for the two-body interactions, is negative at large $T$ for both identical bosons and identical fermions and depends quadratically (and not linearly) on $D$. This implies that the leading order effect of the two-body interactions for aligned dipolar gases under spherically symmetric harmonic confinement is repulsive at high temperature. Moreover, because $\Delta b_2$ depends quadratically on $D$, the effects of the dipole-dipole interactions will be hard to extract from thermodynamic observables. It is well known that the generalized scattering lengths, which characterize the scattering properties of the two dipole system, can be modified through the application of an external magnetic or electric field \[ \text{\textit{D}} \text{, \textit{D}} \]. For fermions, we show that by reducing one of the generalized scattering lengths, $\Delta b_2$ depends linearly (and not quadratically) on $D$. This implies that the effects of the dipole-dipole interactions can be enhanced by tuning one of the generalized scattering lengths to near zero.

The remainder of this paper is organized as follows. Section II introduces the virial equation of state for a single-component quantum gas, the two-body Hamiltonian for aligned dipoles, and the different models used to treat the interaction between the dipoles. Section III studies the low-energy dipole-dipole scattering properties and characterizes the behavior of the generalized scattering lengths. Special attention is paid to low-energy shape resonances. Our main results are presented in Secs. IV and V. Section IV determines the virial coefficient $\Delta b_2$ for dipolar Bose and Fermi gases under spherically symmetric confinement within various approximations. The resulting virial coefficients are used in Sec. V to determine thermodynamic observables such as the total energy and...
free energy. Finally, Sec. \( \text{VII} \) concludes.

## II. VIRIAL EQUATION OF STATE AND SYSTEM UNDER STUDY

For a single component gas, where the chemical potential \( \mu \) is held fixed, the thermodynamic potential \( \Omega \) in the grand canonical ensemble reads \([24, 25]\)

\[
\Omega = -\beta^{-1} \ln \text{Tr } e^{-\beta (H_n - \mu n)},
\]

where \( H_n \) is the Hamiltonian of the \( n \)-body system, \( \beta \) is \( (k_B T)^{-1} \), \( k_B \) is Boltzmann’s constant, \( T \) is the temperature, and \( \text{Tr} \) is the trace operator. In the high-temperature limit, the chemical potential becomes large and negative, such that the fugacity \( z = \exp(\mu \beta) \), is a small parameter. Taylor expanding Eq. (1) in the high-temperature limit, i.e., for \( z \ll 1 \), yields the thermodynamic potential in terms of the virial coefficients \( b_n \),

\[
\Omega \approx -\beta^{-1} Q_1 \sum_{n=1}^{\infty} b_n z^n.
\]

The \( b_n \)'s are determined by the canonical partition functions \( Q_n \),

\[
Q_n = \text{Tr } e^{-\beta H_n}.
\]

We evaluate the trace by inserting a complete set of eigenstates with eigenenergies \( E_n^{(j)} \), yielding

\[
Q_n = \sum_j e^{-E_n^{(j)} \beta},
\]

where the summation index \( j \) collectively denotes the complete set of quantum numbers allowed by symmetry.

To isolate the effect of the two-body interactions, we express the grand canonical potential \( \Omega \) in terms of the grand canonical potential \( \Omega^{\text{NI}} \) of the noninteracting system plus corrections \( \Delta \Omega \) \([17, 26]\),

\[
\Omega = \Omega^{\text{NI}} + \Delta \Omega.
\]

We are interested in accounting for the leading-order effect of the two-body interactions. Correspondingly, we truncate Eq. (2) at \( n = 2 \). Collecting terms of the same order in the fugacity, the second-order virial coefficient reads

\[
b_2 = b_2^{\text{NI}} + \Delta b_2,
\]

where \( b_2^{\text{NI}} \) characterizes the noninteracting two-body system and \( \Delta b_2 \),

\[
\Delta b_2 = \frac{Q_2 - Q_2^{\text{NI}}}{Q_1},
\]

contains the leading-order effect of the two-body interactions. In Eq. (7), \( Q_2 \) and \( Q_2^{\text{NI}} \) denote the canonical partition functions of the interacting and noninteracting two-body systems, respectively. For spherically symmetric harmonic confinement with angular trapping frequency \( \omega \), as considered throughout this paper, we find \([27]\)

\[
b_n^{\text{NI}} = \frac{(\pm 1)^{n-1}}{n} Q_1(n\beta),
\]

where

\[
Q_1(\beta) = \left( \frac{e^{E_{\text{ho}} \beta / 2} - 1}{e^{E_{\text{ho}} \beta / 2} + 1} \right)^3.
\]

In Eq. (8), the plus sign is for identical bosons while the minus sign is for identical fermions. We define the dimensionless quantity \( \tilde{\omega} \) as the ratio of the harmonic oscillator energy \( E_{\text{ho}} \), \( E_{\text{ho}} = \hbar \omega \) (i.e., the characteristic energy of the noninteracting system), and the thermal energy scale \( \beta^{-1} \), \( \tilde{\omega} = E_{\text{ho}} / \beta \).

To determine the second-order virial coefficient \( \Delta b_2 \) that accounts for the interactions between the dipoles [see Eq. (7)], we need to determine \( Q_2 \), i.e., we need to determine the eigenenergies \( E_2^{(j)} \) of the interacting two-body system [see Eq. (4)]. Since the two-body interaction depends only on the distance vector \( r \), the center of mass and relative motion separate, implying \( E_2 = E_2^{	ext{cm}} + E_2^\text{rel} \). The center of mass contribution has been determined in the literature \([17, 26]\) and we thus focus in the following on the relative contribution. The Schrödinger equation for the relative distance vector \( r \) reads

\[
\left[-\frac{\hbar^2}{2\mu_{\text{red}}} \nabla_r^2 + \frac{1}{2} \mu_{\text{red}} \omega^2 r^2 + V_{\text{int}}(r)\right] \Psi(r) = E_2^\text{rel} \Psi(r),
\]

where \( \mu_{\text{red}} \) denotes the reduced mass and \( V_{\text{int}}(r) \) the two-body interaction potential (see below for details). In what follows, we assume that the dipoles are aligned by an external field. This implies that \( V_{\text{int}} \) is azimuthally symmetric and that the projection quantum number \( m \) is a good quantum number. The relative orbital angular momentum \( l \), in contrast, is not a good quantum number. Specifically, the interaction potential couples angular momentum channels with the same parity. For identical bosons, the even relative angular momenta \( l \) are coupled. For identical fermions, in contrast, the odd relative angular momenta \( l \) are coupled.

We solve Eq. (10) using two different representations of the interaction potential. In the first approach, \( V_{\text{int}} \) is given by \([28]\)

\[
V_{\text{model}}(r) = \begin{cases} d^2 \frac{1 - 3 \cos^2 \theta}{r^3} & \text{if } r \geq r_c, \\ \infty & \text{if } r < r_c, \end{cases}
\]

where \( \theta \) denotes the angle between the distance vector \( r \) and the axis along which the dipoles are aligned. The model potential \( V_{\text{model}} \) is characterized by two length
scales, the hard wall radius (or short-range length) $r_c$ and the dipole length (or long-range length) $D$, $D = \mu \text{rel} \sqrt{D^2 / \hbar^2}$, where $d$ denotes the dipole moment. In the second approach, we use the regularized zero-range pseudopotential $V_{pp, reg}^{m}$.

$$V_{pp, reg}^{m}(r) = \sum_{l,l'} V_{l,l'}^{m}(r). \quad (12)$$

Equation (12) contains an infinite number of terms. The $V_{l,l'}^{m}(r)$ are defined by how they act on a wavefunction,

$$V_{l,l'}^{m}(r) \Phi(r) = \frac{\hbar^2 a_{l,l'}^{m} ((2l + 1)!)^2 (2l' + 1)! \delta(r)}{2\mu \text{rel} (l + 1)! r^{l+2}} \times \left[ \frac{\partial^{2l+1}}{\partial r^{2l+1}} r^{l+1} \int_{r \to 0} Y_{l,m}(r') \Phi(r') d(r') \right], \quad (13)$$

where the $Y_{l,m}$ denote the spherical harmonics and where $\hbar k$ is the relative scattering momentum. In the absence of the confinement, $k$ is given by the relative scattering energy $E_{\text{rel}}^{scatt}$, $\hbar^2 k^2 = 2\mu \text{rel} E_{\text{rel}}^{scatt}$. In the presence of the harmonic trap, $k$ is determined, in a self-consistent manner, by the eigenenergies $E_{l}^{rel}$ of Eq. (10) [31]. Since $m$ is a good quantum number, each $m$-channel is treated by a $m$-specific pseudopotential; for details on the $m = 0$ case, see Ref. [31]. The generalized scattering lengths $a_{l,l'}^{m}$ depend on the dipole moment $d$. To use $V_{pp, reg}^{m}$, the $a_{l,l'}^{m}$ have to be provided as input. The next section discusses how these input parameters are determined.

### III. TWO-DIPOLE SCATTERING

This section determines the generalized free-space scattering lengths $a_{l,l'}^{m}$ for the shape-dependent model potential $V_{\text{model}}$, Eq. (11). To determine the $a_{l,l'}^{m}$, we consider the relative free-space Schrödinger equation [Eq. (10) with $\omega = 0$] and propagate the logarithmic derivative matrix using Johnson's algorithm [32] with an adaptive step size. At large $r$, the logarithmic derivative matrix is matched to the asymptotic solution and the generalized scattering lengths are determined from the partial wave phase shifts $\delta_{l,l'}^{m}(k) = -\tan(\delta_{l,l'}^{m}(k)) / k$ [33].

Before presenting our numerical results, we briefly review the expected low-energy properties of the $a_{l,l'}^{m}$. Away from resonances, the generalized scattering lengths $a_{l,l'}^{m}$, $|l,l'| \neq (0,0)$ are, in general, well approximated by applying the first-order Born approximation to the dipole-dipole potential $V_{dd}$, $V_{dd} = d^2(1 - 3 \cos^2 \theta) / r^3$ [33]. The Born approximation yields

$$a_{l,l}^{m} = \frac{-2D[(l+1) - 3m^2]}{(2l - 1)(2l + 3)(l+1)} \quad (14)$$

and

$$a_{l,l-2}^{m} = \frac{-D \sqrt{(l^2 - m^2)[(l-1)^2 - m^2]}}{(2l - 1)(l-1)\sqrt{(2l+1)(2l-3)}} \quad (15)$$

All other $a_{m}^{m}$, with $(l,l') \neq (0,0)$ are zero. For $m = 0$, Eqs. (14) and (15) agree with Eqs. (9) and (10) of Ref. [31]. It is important to note that the scattering length $a_{0,0}^{0}$ cannot, in general, be determined reliably within the first-order Born approximation [25].

In the following, we focus on the scattering properties of two identical fermionic dipoles, implying that $l$ and $l'$ are odd, with $m = 0$. Solid lines in Fig. 1 show the numerically obtained generalized scattering lengths $a_{l,l'}^{m}$, with $l',l \leq 3$ for $V_{\text{model}}$ with $D = 10.5 r_c$ as a function of the scattering energy $E_{\text{rel}}^{scatt}$. The scattering energy has been scaled by the dipole energy $E_D$, $E_D = \hbar^2 / (\mu \text{rel} D^2)$. For comparison, dotted horizontal lines show the generalized scattering lengths predicted by the Born approximation. The numerically obtained scattering lengths $a_{1,3}^{0}$ and $a_{3,3}^{0}$ [see Figs. 1(b) and 1(c)] are well approximated by the Born approximation estimates over a wide range of scattering energies. Deviations occur in narrow en-
FIG. 2: (Color online) Adiabatic potential curves $U_\nu(r)$ for two aligned fermionic dipoles. Though the angular momentum $l$ is not a good quantum number, the curves can be approximately labeled by $l$. Solid, dash-dotted, and dash-dot-dotted lines are for $l \approx 1, 3,$ and $5,$ respectively. The hard wall is indicated by a hatched region extending from zero to $r_c = D/10.5$. The horizontal dashed line indicates the energy of the quasi-bound state.

Energy windows around $E_{\text{scatt}}^{\text{rel}}/E_D \approx 0.015$ and $5$. The deviations between the exact values and the corresponding Born approximation values are larger for $a_{1,1}^0$ [see Fig. 3(a)] than for $a_{3,1}^0$ and $a_{3,3}^0$. The deviations from the Born approximation values can be attributed to a quasi-bound state that is, approximately, tied to the $l = 1$ channel [see dashed line in Fig. 3(a)].

To understand the emergence of the quasi-bound state, we treat Eq. (10) using $V_{\text{model}}$ in the adiabatic representation [34, 35]. Figure 2 shows the lowest three adiabatic potential curves for two aligned fermionic dipoles with $r_c = D/10.5$ as a function of the distance coordinate $r$. Though the angular momentum $l$ is not a good quantum number, each curve can be labeled approximately by $l$. Solid, dash-dotted, and dash-dot-dotted lines are for $l \approx 1, 3,$ and $5,$ respectively. The $l \approx 1$ potential curve exhibits a barrier of height around $0.2E_D$, indicating that the true bound state—which is to a good approximation described by the lowest potential curve [34, 35]—turns into a quasi-bound state with positive energy after crossing the zero-energy threshold.

Figure 3 shows the energy dependence of $a_{1,1}^0$ for various ratios between the long-range and short-range length scales in the vicinity of a shape resonance. For $D/r_c$ values, for which no quasi- or shallowly-bound states exist, the Born approximation is valid for $E \lesssim E_D$ [see the solid and dotted lines in Fig. 3(a)]. As $D/r_c$ increases, $a_{1,1}^0$ develops a “dip” around $E_{\text{scatt}}^{\text{rel}} \approx 0.7E_D$ [see the dash-dotted line in Fig. 3(a)]. At yet larger $D/r_c$, the dip turns into two resonance-like features, i.e., $a_{1,1}^0$ diverges at energies above and below the barrier of the $l \approx 1$ adiabatic potential curve [see the dash-dot-dotted and solid lines in Figs. 3(a) and 3(b), respectively]. We associate the resonance features with the appearance of a quasi-bound state that “lives” to the left of the barrier of the adiabatic potential curve (see Fig. 2). As $D/r_c$ increases further, the energy of the quasi-bound state moves to smaller (positive) energies [see the solid line in Fig. 3(b)]. For $D/r_c = 10.55$, $a_{1,1}^0$ is nearly constant for $0.01E_D \lesssim E_{\text{scatt}}^{\text{rel}} \lesssim E_D$ [see the dotted line in Fig. 3(b)]. For larger $D/r_c$, the quasi-bound state turns into a true bound state and $a_{1,1}^0$ “returns”, in the low energy regime, to its Born approximation value [see dash-dotted line in Fig. 3(b)].

In the next section, we make two assumptions. (i) We assume that one of the generalized scattering lengths is tunable while the other generalized scattering lengths are well described by their Born approximation values. (ii) We assume that all generalized scattering lengths are, to a good approximation, independent of energy. To fulfill these assumptions approximately, the external field should be tuned to a value near resonance. Experiments on fermionic alkali atoms [36, 37] have demonstrated that the regime where only one of the scattering lengths differs notably from its Born approximation value can be reached. The requirement to sit near but not on resonance allows one to take advantage of the fact that the resonance feature of the tunable scattering length is much broader than that of the other scattering lengths; this implies that the energy-dependence of the scattering lengths approximated by their Born approximation values is weak. Lastly, as shown by the dotted line in Fig. 3(b) for $a_{1,1}^0$, the near-resonance regime also
allows one to realize a regime where the tunable scattering length is roughly independent of energy over a wide energy regime.

IV. SECOND-ORDER VIRIAL COEFFICIENT $\Delta b_2$

This section discusses the virial coefficient $\Delta b_2$ that accounts for the two-body interactions for two identical bosons and two identical fermions as a function of the temperature. To determine $\Delta b_2$, we take advantage of the fact that the relative eigenenergies $E_2^{rel}$ for the trapped two-dipole system interacting through $V_{pp,reg}$ can, provided the generalized scattering lengths $a_{pp}^{l,l'}$ are known, be obtained by solving a transcendental equation. As indicated in our discussion at the end of Sec. III we solve the transcendental equation assuming that the generalized scattering lengths are energy-independent. We have checked that the use of an energy-dependent pseudo-potential leaves our main conclusions unaltered. Combining $E_2^{rel}$ and $E_2^{pp}$, the canonical partition function $Q_2$ [see Eq. 1] and correspondingly the virial coefficient $\Delta b_2$ can be calculated. Since the relative two-body energy spectrum is, in practice, only known up to a maximum energy $E_2^{rel,max}$, $\Delta b_2$ is only accurate up to a maximum temperature or down to a minimum dimensionless inverse temperature $\tilde{\omega}$. To distinguish the second-order virial coefficient for two identical bosons and two identical fermions, we use the superscripts (B) and (F), respectively.

We start our discussion by considering two identical bosons. The solid lines in Figs. 4(a) and 4(b) show the virial coefficient $\Delta b_2^{(B)}$ for a relatively small dipole length $D$, $D = 0.1a_{ho}$ ($a_{ho}$ denotes the oscillator length, $a_{ho} = \sqrt{\hbar/(\mu \omega)}$). To determine the relative eigenenergies $E_2^{rel}$, the generalized scattering lengths $a_{pp}^{l,l'}$ with $(l,l') \neq (0,0)$ are approximated by the Born approximation values [see Eqs. (14) and (15)]. As discussed in Sec. III the s-wave scattering length $a_{0,0}^{(l,l')}$ cannot be determined within the Born approximation. Figure 4(a) assumes that $a_{0,0}^{(l,l')} = 0$. Correspondingly, the resulting virial coefficient is that for a “purely” dipolar system. Figure 4(b) assumes that $a_{0,0}^{(l,l')} = -0.1a_{ho}$. Thus, the virial coefficient shown in Fig. 4(b) reflects the combined effect of the long-range dipole-dipole interaction and the short-range s-wave interaction. For the $\tilde{\omega}$ values shown, the solid lines are converged to better than 1% and include all states with relative energy less than 51.5$\hbar\omega$, that is, $E_2^{rel,max} < 51.5\hbar\omega$.

For the Born approximation to be applicable, two conditions have to be met. First, the virial coefficient $\Delta b_2^{(B)}$ has to be converged for an energy cutoff $E_2^{rel,max}$ that is smaller than $E_D$. This condition comes from the fact that the Born approximation is only valid for $E_2^{rel,scatt} \ll E_D$. In Figs. 4(a) and 4(b), we have $E_D \approx 100\hbar\omega$ and thus $E_2^{rel,max} < E_D$. Second, the system has to be away from shape resonances that are associated with quasi-bound states whose energy lies below $E_2^{rel,max}$.

The second-order virial coefficient $\Delta b_2^{(B)}$ for the purely dipolar Bose gas under spherically symmetric harmonic confinement [Fig. 4(a)] is negative for all $\tilde{\omega}$ shown, indicating that the leading-order effect of the dipole-dipole interaction is repulsive for aligned Bose gases with $D/a_{ho}$ small compared to one. Figure 4(a) shows that the effect...
of the two-body interaction is very small. Specifically, the contribution \( \Delta b_2^{(B)} \) is about three orders of magnitude smaller than the noninteracting contribution \( b_{scatt}^{(B)} \) at \( \tilde{\omega} = 0 \) [see the right axis of Fig. 3(a)], suggesting that the effects of the dipole-dipole interactions would be hard to extract from thermodynamic observables for a purely dipolar gas with small \( D/\omega_h \). The virial coefficient for \( a_{0,0}^{(B)} = -0.1\omega_h \) [Fig. 3(b)] is about three orders of magnitude larger than that for \( a_{0,0}^{(F)} = 0 \) [Fig. 4(a)]. Moreover, the sign is reversed. Since the dipole length \( D \) is the same in Figs. 3(a) and 4(b), it is clear that the increase of \( \Delta b_2^{(B)} \) is due to the change in \( a_{0,0}^{(B)} \). The fact that \( \Delta b_2^{(B)} \) is positive for \( a_{0,0}^{(B)} = -0.1\omega_h \) makes sense intuitively since a positive \( \Delta b_2^{(B)} \) implies an effective attraction as would be naively expected for a negative \( a_{0,0}^{(B)} \).

We now consider two identical fermions. The solid lines in Figs. 4(c) and 4(d) show \( \Delta b_2^{(F)} \) for two identical dipolar fermions for \( D = 0.1\omega_h \). In Fig. 4(c), the energies \( E_k^{rel} \) are obtained by approximating all generalized scattering lengths by the Born approximation values. Thus, the virial coefficient shown in Fig. 4(c) is that for a purely dipolar gas under spherically symmetric external confinement with small \( D/\omega_h \). \( \Delta b_2^{(F)} \) is negative at high temperature, changes sign at \( k_BT \approx E_h/0.2 \), and is positive for smaller temperatures (larger \( \tilde{\omega} \)). In Fig. 4(d), in contrast, the energies \( E_k^{rel} \) are obtained by approximating all but one of the generalized scattering lengths by their Born approximation value. Specifically, we choose \( a_{1,1}^{(F)} = 0 \), i.e., we assume that this generalized scattering length is tuned away from its Born approximation value through the application of an external field. Figure 4(d) shows that \( \Delta b_2^{(F)} \) is negative for all temperatures and that \( |\Delta b_2^{(F)}| \) is between one and two orders of magnitude larger than the absolute value of the virial coefficient for the purely dipolar gas [see Fig. 4(c)]. Since the dipole length \( D \) is the same in Figs. 4(c) and 4(d), it is clear that the increase of \( \Delta b_2^{(F)} \) is due to the change in \( a_{1,1}^{(F)} \). Figure 4 shows that the scenario considered here can be realized, at least approximately, for the model potential \( V_{model} \). For the parameters considered in Fig. 4, the \( a_{n,l'}^{m} \), with \( (l, l') \neq (1, 1) \), are, except for a tiny energy window, well approximated by the Born approximation value for \( E_{scatt} \) up to \( E_{scatt} \approx E_D \). Moreover, the discussion around Fig. 4 shows that \( a_{1,1}^{(F)} \) can, at least approximately, be tuned to a value different from the Born approximation value while all other \( a_{n,l'}^{m} \) are quite well described by their Born approximation value.

We now develop a perturbative approach that (i) shows analytically that the second-order virial coefficients \( \Delta b_2^{(B)} \) and \( \Delta b_2^{(F)} \) for the purely dipolar gases do not contain terms linear in \( D \), thereby explaining the small values of \( \Delta b_2^{(B)} \) and \( \Delta b_2^{(F)} \) in Figs. 4(a) and 4(c), and (ii) yields analytic expressions in the case where one or more of the generalized scattering lengths are assumed to be tunable [see dashed lines in Figs. 4(b) and 4(d)]. The idea is to calculate the relative energies \( E_k^{rel} \) perturbatively and to then use the perturbative energy expressions to calculate \( \Delta b_2 \) analytically to linear order in \( D/\omega_h \).

We assume that \( D/\omega_h \) is small and employ first-order degenerate perturbation theory. Specifically, we treat the noninteracting harmonic oscillator Hamiltonian in the relative degrees of freedom as the unperturbed Hamiltonian and the regularized pseudopotential \( V_{pp,reg} \) as a perturbation. We label the unperturbed states \( \psi_{nl,m}^{(0)} \) by the principal quantum number \( n \), the orbital angular momentum quantum number \( l \), and the projection quantum number \( m \), and find compact analytic expressions for the matrix elements \( \langle V_{nl,n'l'}^{m} \rangle = \langle \psi_{nl,m}^{(0)} | V_{l,l'}^{(0)} | \psi_{n'l',m}^{(0)} \rangle \),

\[
\langle V_{nl,n'l'}^{m} \rangle = \delta_{m,m} \delta_{m,m} \delta_{l,l} \delta_{l,l} \frac{2^{l+l'+1}}{\pi} \frac{a_{n,l}^{m}}{k^{l+l'+1+1} a_{ho}^{m}} \times \sqrt{\frac{\Gamma(n+l+3/2)}{n!}} \sqrt{\frac{\Gamma(n'+l'+3/2)}{n'!}} \frac{\omega_h}{E_h}.
\]

Diagonalizing the perturbation matrix spanned by the matrix elements \( \langle V_{nl,n'l'}^{m} \rangle \) for each noninteracting energy manifold, i.e., for the manifolds with unperturbed energies \( 3E_h/2, 5E_h/2 \), and so on, we find the first-order energy shifts \( \Delta E^{(1)}_{n,l,m}, \Delta E^{(1)}_{n,l,m} = c_{n,l,m} E_h \). Using these energy shifts in Eqs. 14 and 17, the second-order virial coefficient in the weakly-interacting regime can be written as

\[
\Delta b_2 \approx \tilde{\omega} \sum_{nlm} c_{n,l,m} e^{-(2n+l+3/2)\omega}.
\]

So far, the discussion is general, i.e., we have not yet specified whether we are dealing with bosons or fermions. Correspondingly, Eq. 17 writes \( \Delta b_2 \) without the \((B)/(F)\) superscript. Inspection of Eq. 19 shows that the matrix elements \( \langle V_{nl,n'l'}^{m} \rangle \) depend on \( m \) only through the generalized scattering lengths. Using this and rewriting the sum of eigenvalues for each energy manifold in terms of the trace of the corresponding perturbation matrix, we find

\[
\Delta b_2 \approx \tilde{\omega} \sum_{nl} e^{-(2n+l+3/2)\omega} \times \frac{2^{l+2} \Gamma(n+l+3/2)}{(2n+l+3/2)! \pi n!} \left( \sum_{m=-l}^{l} a_{n,l}^{m} \right),
\]

where we have replaced the scattering momentum \( \hbar k \) by the unperturbed energies, that is, we used \( k^2 = 2(2n+l+3/2)/\omega_h^2 \). In Eq. 18, the sum over \( l \) is restricted to even or odd \( l \) for bosons or fermions, respectively.

We now apply Eq. 19 to the purely dipolar Bose and Fermi gases. Using the Born approximation values [see Eq. 13], we find

\[
\sum_{m=-l}^{l} a_{n,l}^{m} = 0.
\]
This shows that $\Delta b_2^{(B)}$ and $\Delta b_2^{(F)}$ do not, in the small $D/a_{ho}$ regime, contain terms that are linear in the dipole length $D$, in agreement with the fact that the virial coefficients shown in Figs. 3(a) and 3(c) are very small.

To determine the leading-order dependence of $\Delta b_2$ on $D$ for purely dipolar gases, our treatment would have to be modified in two places. First, the generalized scattering lengths would have to be known to second order in $D$ and, second, the perturbation treatment would have to be pushed to second order. These generalizations are not pursued in this work.

Next, we focus on the scenario where one or more of the generalized scattering lengths are tunable [see Figs. 3(b) and 3(d)]. For identical bosons, we assume that the $a_{l,m}^{(0,0)}$ with $(l,l') \neq (0,0)$ are given by the Born approximation values and that $a_{0,0}^{(0,0)}$ takes a small but finite value ($|a_{0,0}^{(0,0)}/a_{ho}$ much smaller than one). Under these assumptions, the perturbative treatment yields

$$\Delta b_2^{(B)} \approx -\tilde{\omega} \frac{2}{\sqrt{\pi}} \left( \frac{e^{-3\tilde{\omega}/2}}{(1 - e^{-2\tilde{\omega}})^{3/2}} \frac{a_{0,0}^{(0,0)}}{a_{ho}} \right) + O((D/a_{ho})^2).$$

Equation (20) breaks down in the $\tilde{\omega} \to 0$ limit but is expected to be valid in the $\tilde{\omega}$ regime considered in this paper. The dashed line in Fig. 3(b) shows Eq. (20). The agreement with the solid line is excellent, indicating that the virial coefficient $\Delta b_2^{(B)}$ is, to a very good approximation, determined by $a_{0,0}^{(0,0)}$ alone and independent of $D$.

For identical fermions, we assume that the scattering lengths with $l = 1$ are tunable and that all other generalized scattering lengths are approximated by the Born approximation values. Using the perturbative energies (i.e., assuming $|a_{1,1}^{(0,1)}| \ll a_{ho}$) and evaluating the sums in Eq. (19), we find

$$\Delta b_2^{(F)} \approx -\tilde{\omega} \frac{12e^{-5\tilde{\omega}/2}}{5\sqrt{\pi}} \left( \frac{a_{1,1}^{(0,1)}}{a_{ho}} + \frac{a_{1,1}^{(0)}}{a_{ho}} \right) \times _2F_1 \left( \frac{5}{4}, \frac{9}{4}, -2\tilde{\omega} \right) + O((D/a_{ho})^2),$$

where $_2F_1$ is the hypergeometric function. Equation (21) breaks down in the $\tilde{\omega} \to 0$ limit but is expected to be valid in the $\tilde{\omega}$ regime considered in this paper. The dashed line in Fig. 3(d) shows Eq. (21) with $a_{1,1}^{(0,1)} = 0$ and $a_{1,1}^{(0)}$ given by their Born approximation value. The agreement with the solid line is excellent. Our analysis shows that the virial coefficient $\Delta b_2^{(F)}$ depends linearly on $D$ if one of the $a_{l,m}^{(0,0)}$ is tuned away from its Born approximation value. Perturbative expressions analogous to Eqs. (20) and (21) can be derived if other low partial-wave scattering lengths are assumed to be tunable.

V. THERMODYNAMICS

This section examines the thermodynamics of aligned dipolar gases under spherically symmetric harmonic confinement using the virial equation of state up to second order in the fugacity. Figures 5 and 6 show the total energy per particle $U/N$ for $N = 100$ identical fermions under spherically symmetric confinement as a function of the temperature $T$. The solid line shows $U/N$ for the non-interacting Fermi gas. Dashed and dotted lines show $U/N$ for the interacting Fermi gas with $D = 0.1 a_{ho}$ obtained using the virial equation of state to second order in the fugacity. The dashed line shows results for the purely dipolar Fermi gas. The dotted line shows results for $a_{1,1}^{(0)} = 0$ while other $a_{l,m}^{(0,0)}$ are approximated by their Born-approximation value.

![Graph](image)

FIG. 5: (Color online) Total energy per particle $U/N$ for $N = 100$ identical fermions under spherically symmetric confinement as a function of the temperature $T$. The solid line shows $U/N$ for the non-interacting Fermi gas. Dashed and dotted lines show $U/N$ for the interacting Fermi gas with $D = 0.1 a_{ho}$ obtained using the virial equation of state to second order in the fugacity. The dashed line shows results for the purely dipolar Fermi gas. The dotted line shows results for $a_{1,1}^{(0)} = 0$ while other $a_{l,m}^{(0,0)}$ are approximated by their Born-approximation value.
The dashed and solid lines are indistinguishable on the scale shown.

The dependence of the thermodynamic observables on the dipolar interactions is enhanced. The difference between the thermodynamic observables for the interacting and non-interacting systems is of the order of 3\% for \( k_B T \approx 0.8 E_F \). This suggests that dedicated cold atom experiments on erbium or dysprosium might be able to detect the effects of the dipolar interactions in thermodynamic measurements at temperatures around the Fermi temperature. As discussed above, the tunability of one of the scattering lengths is possible if the system under study exhibits non-overlapping resonances. In practice, a given scattering length may change a fair amount in the relevant energy range or overlapping resonances may lead to deviations in more than one scattering length. While an exhaustive study of all possible non-universal parameter combinations is beyond the scope of this work, our key point, namely, the fact that tuning one of the scattering lengths away from its Born approximation value (and possibly to zero) can enhance the signatures of the dipole-dipole interactions of weakly-interacting gases in thermodynamic observables, should apply also in more complicated situations.

**VI. CONCLUSION**

This paper considered the high-temperature virial equation of state of weakly-interacting single-component dipolar quantum gases under spherically symmetric harmonic confinement. For purely bosonic and fermionic dipoles, we found that the lowest-order correction to the ideal gas is repulsive in the high-temperature limit. Compared to the non-interacting gases, the modifications of the thermodynamic observables are very small. Using a perturbative approach, we showed that the corrections are small since the second order virial coefficient depends quadratically on the dipole length \( D \); terms linear in \( D \) average to zero within the Born approximation. We argued that the effects of the dipole-dipole interactions can be enhanced if one or more generalized scattering lengths can be tuned away from their Born approximation value. For the fermionic gas, we showed explicitly that the generalized scattering length \( a_{11}^0 \) can be tuned in the vicinity of a low-energy shape resonance, leading to a second order virial coefficient that depends linearly on the dipole length. Correspondingly, the effects of the dipolar interaction are, compared to the purely dipolar case, greatly enhanced.

Throughout, we considered single-component Bose and Fermi gases. If we considered two-component dipolar gases, then the thermodynamic properties would depend on the interspecies and intraspecies virial coefficients. For a two-component Fermi gas, e.g., the intraspecies virial coefficients would be given by \( \Delta b_{2}^{(F)} \) while the interspecies virial coefficient would be given by a combination of the even and odd \( l \) virial coefficients, i.e., \( \Delta b_{2}^{(B)} \) and \( \Delta b_{2}^{(F)} \). While the thermodynamic observables would differ from those considered in this paper, our perturbative analysis of the virial coefficients carries over unchanged.

The present work presents a first step toward understanding the thermodynamic properties of dipolar systems. While the present work provides some insights into weakly-interacting dipolar gases at finite temperature, many questions remain unanswered. What happens if the dipolar interactions are of intermediate strength or strong? Do these systems exhibit universal thermodynamic properties? What are the effects of the third- and higher-body virial coefficients? What are the effects of anisotropic confinement geometries?

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