

Density functional of a two-dimensional gas of dipolar atoms: Thomas-Fermi-Dirac treatment

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We derive the density functional for the ground-state energy of a two-dimensional, spin-polarized gas of neutral fermionic atoms with magnetic-dipole interaction, in the Thomas-Fermi-Dirac approximation. For many atoms in a harmonic trap, we give analytical solutions for the single-particle spatial density and the ground-state energy, in dependence on the interaction strength, and we discuss the weak-interaction limit that is relevant for experiments. We then lift the restriction of full spin polarization and account for a time-independent inhomogeneous external magnetic field. The field strength necessary to ensure full spin polarization is derived.

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I. INTRODUCTION

Ultracold atomic gases provide highly controllable systems for the study of condensed-matter phenomena [1]. With the ongoing experimental efforts in ultracold gases of neutral Fermi atoms [2] and the possibility of a genuinely two-dimensional (2D) confinement [3–7], it is now possible to acquire data about dilute 2D degenerate Fermi gases of neutral atoms under adjustable laboratory conditions [8]. It is hoped that this will advance our understanding of various 2D phenomena, such as high- T_c superconduction [9,10], effective massless Dirac fermions [11,12], the Bose-Einstein condensate (BEC)–Berezinsky-Kosterlitz-Thouless crossover [13,14], and others.

While experiments of this kind will involve periodic potentials of various geometries, all experiments with ultracold atoms in a 2D configuration will make use of a confining potential. Before investigating aspects of specific periodic potentials, one can examine the behavior of the degenerate gas in the 2D trapping potential. We study this situation with the help of density functionals, and arrive at detailed predictions for the case of an isotropic harmonic trapping potential.

Density functional theory (DFT), which has its historical roots in the Thomas-Fermi model for atoms [15,16], was first formulated for the inhomogeneous electron gas [17], with immediate applications to atoms, molecules, and solids; see Ref. [18], for example. DFT can equally well be used for studying other physical systems, such as dilute gases of neutral fermionic atoms under the influence of a confining external potential. While the DFT formalism can be based on both the spatial [17] and the momental density [19], the spatial-density version gives a more natural description in the case of a position-dependent interaction, such as the magnetic-dipole interaction. We derive the density functionals for spin-polarized fermions with magnetic-dipole interaction, confined in a 2D harmonic potential, and investigate the ground-state density and energy of the system.

The article is organized as follows. Section II summarizes earlier investigations in three dimensions (3D). In Sec. III, we discuss how to appropriately reduce the dimensionality. Various 2D density functionals are derived in Sec. IV. A discussion about the scaling behavior of these functionals is then given in Sec. V. Section VI presents the analytic

results of the ground-state density and energy, and discusses the weak-interaction limit. Section VII extends the formalism to accommodate the spin dependence in an inhomogeneous magnetic field. We conclude with a summary and a brief outline of prospective work.

II. THE 3D CASE

It is expedient to recall some basic relations that were earlier established in 3D, mainly collected from Refs. [20–23].

A. Single-particle density and density matrix

The spatial one-particle density matrix $n^{(1)}(\mathbf{r}'; \mathbf{r}'')$ and the associated one-particle Wigner function $\nu(\mathbf{r}, \mathbf{p})$ are related by

$$n^{(1)}(\mathbf{r}'; \mathbf{r}'') = \int \frac{(d\mathbf{p})}{(2\pi\hbar)^3} \nu\left(\frac{1}{2}(\mathbf{r}' + \mathbf{r}''), \mathbf{p}\right) e^{i\mathbf{p}\cdot(\mathbf{r}' - \mathbf{r}'')/\hbar}, \quad (1)$$

with $(d\mathbf{p}) \equiv dp_x dp_y dp_z$ denoting the volume element in the momentum space. The spatial and momental one-particle densities are obtained by integrating $\nu(\mathbf{r}, \mathbf{p})$ over the other variable,

$$\begin{aligned} n(\mathbf{r}) &\equiv n^{(1)}(\mathbf{r}; \mathbf{r}) = \int \frac{(d\mathbf{p})}{(2\pi\hbar)^3} \nu(\mathbf{r}, \mathbf{p}), \\ \rho(\mathbf{p}) &= \int \frac{(d\mathbf{r})}{(2\pi\hbar)^3} \nu(\mathbf{r}, \mathbf{p}). \end{aligned} \quad (2)$$

Note that both densities are normalized to the total number of particles N ,

$$N = \int (d\mathbf{r}) n(\mathbf{r}) = \int (d\mathbf{p}) \rho(\mathbf{p}). \quad (3)$$

B. Density functionals for energy

For a system of spin-polarized fermions in an isotropic harmonic trap, the potential energy is given by

$$E_{\text{trap}}[n] = \int (d\mathbf{r}) \frac{1}{2} M \omega^2 r^2 n(\mathbf{r}), \quad (4)$$

where M and ω are the mass of an individual atom and the trap frequency, respectively, $r = |\mathbf{r}|$ is the length of the position vector \mathbf{r} , and the kinetic energy is

$$E_{\text{kin}} = \int (d\mathbf{p}) \frac{p^2}{2M} \rho(\mathbf{p}). \quad (5)$$

Both E_{trap} and E_{kin} are sums over single-particle contributions.

The interaction energy, E_{dd} , which is a sum over particle-pair contributions, is evaluated using the diagonal part of the two-particle density matrix $n^{(2)}(\mathbf{r}'_1, \mathbf{r}'_2; \mathbf{r}''_1, \mathbf{r}''_2)$,

$$E_{\text{dd}} = \frac{1}{2} \int (d\mathbf{r}') (d\mathbf{r}'') V_{\text{dd}}(\mathbf{r}' - \mathbf{r}'') n^{(2)}(\mathbf{r}', \mathbf{r}''; \mathbf{r}', \mathbf{r}'') \quad (6)$$

with the magnetic dipolar interaction potential

$$V_{\text{dd}}(\mathbf{r}) = \frac{\mu_0}{4\pi} \left[\frac{\mu^2}{r^3} - 3 \frac{(\boldsymbol{\mu} \cdot \mathbf{r})^2}{r^5} - \frac{8\pi}{3} \mu^2 \delta(\mathbf{r}) \right], \quad (7)$$

where $\boldsymbol{\mu}$ and μ are the magnetic-dipole moment and its magnitude of an individual atom. The contact term in $V_{\text{dd}}(\mathbf{r})$ is necessary to ensure that the magnetic field generated by the point dipole is divergence free.

C. TFD approximation

In the spirit of the approach that was pioneered by Thomas, Fermi, and Dirac (TFD), a twofold semiclassical approximation is employed here. First, $n^{(2)}$ is replaced by products of $n^{(1)}$ factors (due to Dirac [24]) according to

$$n^{(2)}(\mathbf{r}'_1, \mathbf{r}'_2; \mathbf{r}''_1, \mathbf{r}''_2) = n^{(1)}(\mathbf{r}'_1; \mathbf{r}''_1) n^{(1)}(\mathbf{r}'_2; \mathbf{r}''_2) - n^{(1)}(\mathbf{r}'_1; \mathbf{r}'_2) n^{(1)}(\mathbf{r}''_2; \mathbf{r}''_1). \quad (8)$$

This splitting corresponds to the direct and exchange terms when evaluating the interaction energy, E_{dd} . Note that this expression is only valid if the system is spin polarized. Otherwise, a multiplicative constant preceding the second term is needed to account for the spin multiplicity.

Second, the Wigner function is a uniform sphere of a finite size (due to Thomas [15] and Fermi [16])

$$v(\mathbf{r}, \mathbf{p}) = \eta(\hbar[6\pi^2 n(\mathbf{r})]^{1/3} - p), \quad (9)$$

where $\eta(\cdot)$ is the Heaviside unit step function. This applies when functionals of the spatial density $n(\mathbf{r})$ are considered. For functionals of the momental density $\rho(\mathbf{p})$, one has to use $v(\mathbf{r}, \mathbf{p}) = \eta(t(\mathbf{p}) - V(\mathbf{r}))$, where $V(\mathbf{r})$ is the external potential and $t(\mathbf{p})$ is determined by $\rho(\mathbf{p})$ through Eq. (2). In the case of an isotropic harmonic potential, $V(\mathbf{r}) \propto r^2$, this is

$$v(\mathbf{r}, \mathbf{p}) = \eta(\hbar[6\pi^2 \rho(\mathbf{p})]^{1/3} - r), \quad (10)$$

visibly the analog of Eq. (9).

This yields the familiar density functional of the kinetic energy,

$$E_{\text{kin}}[n] = \int (d\mathbf{r}) \frac{\hbar^2}{M} \frac{1}{20\pi^2} [6\pi^2 n(\mathbf{r})]^{5/3}. \quad (11)$$

Since the contributions of the contact term to the direct and to the exchange energy cancel each other in the fully spin-polarized situation under consideration, and the remaining exchange energy vanishes under the average over the

solid angle associated with the relative distance, the density functional of the interaction energy,

$$E_{\text{dd}}[n] = \frac{1}{2} \int (d\mathbf{r})(d\mathbf{r}') n(\mathbf{r}) \bar{V}_{\text{dd}}(\mathbf{r} - \mathbf{r}') n(\mathbf{r}'), \quad (12)$$

is characterized by an effective potential \bar{V}_{dd} ,

$$\bar{V}_{\text{dd}}(\mathbf{r}) = \frac{\mu_0}{4\pi} \left[\frac{\mu^2}{r^3} - 3 \frac{(\boldsymbol{\mu} \cdot \mathbf{r})^2}{r^5} \right]. \quad (13)$$

D. Ground-state energy and density

Thus, the functional for the total energy of the ground state in the TFD approximation is given by the sum of the three terms in Eqs. (4), (11), and (12),

$$E_{\text{TFD}}[n] = \int (d\mathbf{r}) \frac{\hbar^2}{M} \frac{1}{20\pi^2} [6\pi^2 n(\mathbf{r})]^{5/3} + \int (d\mathbf{r}) \frac{1}{2} M \omega^2 r^2 n(\mathbf{r}) + \frac{1}{2} \int (d\mathbf{r})(d\mathbf{r}') n(\mathbf{r}) \bar{V}_{\text{dd}}(\mathbf{r} - \mathbf{r}') n(\mathbf{r}'). \quad (14)$$

Upon applying the variational principle, we find that the density that minimizes E_{TFD} must obey the integral equation

$$\frac{\hbar^2}{2M} [6\pi^2 n(\mathbf{r})]^{2/3} + \frac{1}{2} M \omega^2 r^2 + \int (d\mathbf{r}') \bar{V}_{\text{dd}}(\mathbf{r} - \mathbf{r}') n(\mathbf{r}') = \frac{1}{2} M \omega^2 R^2, \quad (15)$$

where $\frac{1}{2} M \omega^2 R^2$ is a convenient way of parametrizing the Lagrange multiplier for the normalization constraint of Eq. (3).

III. FROM 3D TO 2D

The form of the density functional in Eq. (14) gives no explicit indication of its dependence on the spatial dimension. It is thus necessary to rederive the density functionals in 2D, with some suitable assumptions about the Wigner function.

A. A possible Wigner function

When the trapping potential in the z direction is harmonic and sufficiently stiff, as is the typical situation in an actual experiment, the system will remain in the ground state in this direction, and this gives rise to a factorizable Gaussian dependence in z and p_z in the Wigner function,

$$v(\mathbf{r}, \mathbf{p}) = v_{\perp}(\mathbf{r}_{\perp}, \mathbf{p}_{\perp}) 2 \exp\left(-\frac{z^2}{l_z^2} - \frac{p_z^2 l_z^2}{\hbar^2}\right), \quad (16)$$

where $l_z = \sqrt{\hbar/(M\omega_z)}$ is the harmonic oscillator length scale in the z direction, and the subscript \perp indicates that these various quantities live in the transverse xy plane. Here, ω_z is a finite but large frequency and, in order to achieve a 2D geometry, we require that $\hbar\omega_z \gg k_B T$ for the situation of ultracold atoms that we have in mind, although we take the limit $\omega_z \rightarrow \infty$ for mathematical convenience whenever possible.

B. Densities in 2D

In analogy with the densities defined in 3D, Eqs. (1) and (2), the densities in 2D are given by

$$\begin{aligned} n_{\perp}^{(1)}(\mathbf{r}'_{\perp}; \mathbf{r}''_{\perp}) &= \int \frac{(d\mathbf{p}_{\perp})}{(2\pi\hbar)^2} v_{\perp}\left(\frac{\mathbf{r}'_{\perp} + \mathbf{r}''_{\perp}}{2}, \mathbf{p}_{\perp}\right) e^{i\mathbf{p}_{\perp} \cdot (\mathbf{r}'_{\perp} - \mathbf{r}''_{\perp})/\hbar}, \\ n_{\perp}(\mathbf{r}_{\perp}) &= \int \frac{(d\mathbf{p}_{\perp})}{(2\pi\hbar)^2} v_{\perp}(\mathbf{r}_{\perp}, \mathbf{p}_{\perp}), \\ \rho_{\perp}(\mathbf{p}_{\perp}) &= \int \frac{(d\mathbf{r}_{\perp})}{(2\pi\hbar)^2} v_{\perp}(\mathbf{r}_{\perp}, \mathbf{p}_{\perp}). \end{aligned} \quad (17)$$

With the decomposition of the Wigner function in Eq. (16), we find that the densities in 2D and those in 3D are related in the following manner:

$$\begin{aligned} n^{(1)}(\mathbf{r}'; \mathbf{r}'') &= n_{\perp}^{(1)}(\mathbf{r}'_{\perp}; \mathbf{r}''_{\perp}) \frac{1}{l_z \sqrt{\pi}} \exp\left(-\frac{4z_+^2 + z_-^2}{4l_z^2}\right), \\ n(\mathbf{r}) &= n_{\perp}(\mathbf{r}_{\perp}) \frac{1}{l_z \sqrt{\pi}} \exp\left(-\frac{z^2}{l_z^2}\right), \\ \rho(\mathbf{p}) &= \rho_{\perp}(\mathbf{p}_{\perp}) \frac{l_z}{\hbar \sqrt{\pi}} \exp\left(-\frac{p_z^2 l_z^2}{\hbar^2}\right), \end{aligned} \quad (18)$$

where $z_+ = \frac{1}{2}(z' + z'')$, and $z_- = z' - z''$, such that the 2D densities are now normalized to the number of particles,

$$N = \int (d\mathbf{r}_{\perp}) n_{\perp}(\mathbf{r}_{\perp}) = \int (d\mathbf{p}_{\perp}) \rho_{\perp}(\mathbf{p}_{\perp}). \quad (19)$$

C. Various energy terms

By integrating over z and p_z , we immediately find the trap energy and the kinetic energy in terms of the 2D densities,

$$\begin{aligned} E_{\text{trap}} &= \int (d\mathbf{r}_{\perp}) n_{\perp}(\mathbf{r}_{\perp}) \frac{1}{2} M \omega_{\perp}^2 r_{\perp}^2 + \frac{N}{4} \hbar \omega_z, \\ E_{\text{kin}} &= \int (d\mathbf{p}_{\perp}) \rho_{\perp}(\mathbf{p}_{\perp}) \frac{p_{\perp}^2}{2M} + \frac{N}{4} \hbar \omega_z, \end{aligned} \quad (20)$$

where ω_{\perp} is the radial trap frequency in the xy plane, assuming isotropy. Note that both expressions contain parts analogous to the corresponding expressions in 3D and additive constants, which are the sum of single-particle energies in the ground state of the harmonic trap of the z confinement. Since these constants play no role in the dynamics of the system, we renormalize the expressions, such that

$$\begin{aligned} E_{\text{trap}} &= \int (d\mathbf{r}_{\perp}) n_{\perp}(\mathbf{r}_{\perp}) \frac{1}{2} M \omega_{\perp}^2 r_{\perp}^2, \\ E_{\text{kin}} &= \int (d\mathbf{p}_{\perp}) \rho_{\perp}(\mathbf{p}_{\perp}) \frac{p_{\perp}^2}{2M}, \end{aligned} \quad (21)$$

which are now independent of ω_z and unaffected when the limit $\omega_z \rightarrow \infty$ is taken.

To investigate the interaction energy, we employ the $(2+1)$ D version of Eq. (8),

$$\begin{aligned} n^{(2)}(\mathbf{r}', \mathbf{r}''; \mathbf{r}', \mathbf{r}'') &= n(\mathbf{r}') n(\mathbf{r}'') - n^{(1)}(\mathbf{r}'; \mathbf{r}'') n^{(1)}(\mathbf{r}'', \mathbf{r}') \\ &= \frac{e^{-(4z_+^2 + z_-^2)/(2l_z^2)}}{l_z^2 \pi} [n_{\perp}(\mathbf{r}'_{\perp}) n_{\perp}(\mathbf{r}''_{\perp}) \\ &\quad - n_{\perp}^{(1)}(\mathbf{r}'_{\perp}; \mathbf{r}''_{\perp}) n_{\perp}^{(1)}(\mathbf{r}''_{\perp}; \mathbf{r}'_{\perp})], \end{aligned} \quad (22)$$

which corresponds to the splitting of the direct and exchange energies. It is clear from Eq. (22) that the contact term in the interaction potential, Eq. (7), enforces $\mathbf{r}' = \mathbf{r}''$ and thus equal and opposite contributions from the direct and exchange energies, the familiar situation when the system is spin polarized. It is then permissible to drop the contact term, which amounts to replacing the original interaction potential by the effective potential of Eq. (13), i.e.,

$$\begin{aligned} E_{\text{dd}} &= \frac{1}{2} \int (d\mathbf{r}') (d\mathbf{r}'') \bar{V}_{\text{dd}}(\mathbf{r}' - \mathbf{r}'') \\ &\quad \times [n(\mathbf{r}') n(\mathbf{r}'') - n^{(1)}(\mathbf{r}'; \mathbf{r}'') n^{(1)}(\mathbf{r}'', \mathbf{r}')]. \end{aligned} \quad (23)$$

Since $\bar{V}_{\text{dd}}(\mathbf{r}' - \mathbf{r}'')$ depends only on the difference in the positions, we isolate the z direction by identifying $\boldsymbol{\rho} = (\mathbf{r}' - \mathbf{r}'')_{\perp}$,

$$\bar{V}_{\text{dd}}(\mathbf{r}' - \mathbf{r}'') = \frac{\mu_0 \mu^2}{4\pi} \left[\frac{1}{(\rho^2 + z_-^2)^{3/2}} - \frac{3z_-^2}{(\rho^2 + z_-^2)^{5/2}} \right], \quad (24)$$

where we assume that the magnetic-dipole moments of all fermions are polarized in the z direction, i.e., $\boldsymbol{\mu} = \mu \hat{\mathbf{e}}_z$.

It should be noted that the replacement of $V_{\text{dd}}(\mathbf{r})$ by $\bar{V}_{\text{dd}}(\mathbf{r})$ only takes place after the approximation in Eq. (22) is made. It may not be correct for a different approximation scheme, that is, when going beyond Dirac's approximation in Eq. (8).

In the limit of $\omega_z \rightarrow \infty$, the Gaussians of z_{\pm} become Dirac delta functions, yielding

$$\begin{aligned} E_{\text{dd}} &= \frac{1}{2} \int (d\mathbf{r}'_{\perp}) (d\mathbf{r}''_{\perp}) \frac{\mu_0 \mu^2}{4\pi} \frac{1}{|\mathbf{r}'_{\perp} - \mathbf{r}''_{\perp}|^3} \\ &\quad \times [n_{\perp}(\mathbf{r}'_{\perp}) n_{\perp}(\mathbf{r}''_{\perp}) - n_{\perp}^{(1)}(\mathbf{r}'_{\perp}; \mathbf{r}''_{\perp}) n_{\perp}^{(1)}(\mathbf{r}''_{\perp}; \mathbf{r}'_{\perp})]. \end{aligned} \quad (25)$$

In hindsight, we recognize the result above as an immediate consequence of having $\boldsymbol{\mu} \perp \mathbf{r}$, which forces their scalar product in Eq. (13) to vanish, while the contact term does not contribute for the reason discussed earlier.

IV. 2D FUNCTIONALS

From this section onward, for notational convenience, we leave out all the subscripts \perp . It is understood that all the densities refer to the 2D definition specified in Eqs. (17), and all the vectors reside in the xy plane.

A. TFD: A brutally simple Wigner function

In order to derive the density functionals in 2D, one first needs to complete the TFD approximation started in the previous section and assume a "brutally simple Wigner function" [23] analogous to Eq. (9), i.e.,

$$v(\mathbf{r}, \mathbf{p}) = \eta (\hbar [4\pi n(\mathbf{r})]^{1/2} - p), \quad (26)$$

where the power and prefactor of the density are determined by normalization.

B. Density functionals

Not surprisingly, the potential energy reads

$$E_{\text{trap}}[n] = \int (d\mathbf{r}) \frac{1}{2} M \omega^2 r^2 n(\mathbf{r}), \quad (27)$$

where we emphasize that ω is the radial trap frequency in the xy plane, assuming isotropy. Upon using Eqs. (17), (21), and (26), we find that

$$E_{\text{kin}}[n] = \int (d\mathbf{r}) \frac{\hbar^2}{M} \pi n(\mathbf{r})^2. \quad (28)$$

The $n(\mathbf{r})^2$ dependence of this 2D functional can also be obtained from dimensional analysis; similarly, dimensional analysis confirms the $n(\mathbf{r})^{5/3}$ dependence of the 3D functional in Eq. (11), and the 1D functional for the kinetic energy has the cube of the density; see Table I below.

The interaction energy, in particular, turns out to consist of two pieces with different dependence on the one-particle density, namely,

$$\begin{aligned} E_{\text{dd}} &= E_{\text{dd}}^{(1)} + E_{\text{dd}}^{(2)}, \\ E_{\text{dd}}^{(1)}[n] &= \frac{\mu_0 \mu^2}{4\pi} \int (d\mathbf{r}) \frac{256}{45} \sqrt{\pi} n(\mathbf{r})^{5/2}, \\ E_{\text{dd}}^{(2)}[n] &= -\frac{\mu_0 \mu^2}{4\pi} \pi \int (d\mathbf{r}) n(\mathbf{r}) \sqrt{-\nabla^2} n(\mathbf{r}), \end{aligned} \quad (29)$$

where $\sqrt{-\nabla^2}$ is an integral operator that is given by

$$\sqrt{-\nabla^2} n(\mathbf{r}) = \int \frac{(d\mathbf{r}')}{(2\pi)^2} (d\mathbf{k}) k e^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} n(\mathbf{r}'). \quad (30)$$

We report the details of deriving Eqs. (29) in the Appendix.

Note that the splitting of the interaction energy in Eqs. (29) does not correspond to the direct and exchange energies as in the 3D case, where, as we recall, the exchange energy exactly compensates for the contribution of the contact term to the direct energy. In 2D, both the direct and exchange energies are infinite individually, and they can only be considered together so that the total interaction energy is finite. Both contributions in Eqs. (29) stem from the sum of the direct and the exchange energy.

C. Ground-state energy and density

The total energy of the system in the TFD approximation is now given by the sum of the various energy terms derived above,

$$\begin{aligned} E_{\text{TFD}}^{(2D)}[n] &= \int (d\mathbf{r}) \frac{\hbar^2}{M} \pi n(\mathbf{r})^2 + \int (d\mathbf{r}) \frac{1}{2} M \omega^2 r^2 n(\mathbf{r}) \\ &+ \frac{\mu_0 \mu^2}{4\pi} \int (d\mathbf{r}) \left[\frac{256}{45} \sqrt{\pi} n(\mathbf{r})^{5/2} \right. \\ &\left. - \pi n(\mathbf{r}) \sqrt{-\nabla^2} n(\mathbf{r}) \right]. \end{aligned} \quad (31)$$

The density that minimizes the energy, constrained by the normalization condition (19), must then obey

$$\begin{aligned} \frac{2\hbar^2}{M} \pi n(\mathbf{r}) + \frac{1}{2} M \omega^2 r^2 \\ + \frac{\mu_0 \mu^2}{4\pi} \left[\frac{128}{9} \sqrt{\pi} n(\mathbf{r})^{3/2} - 2\pi \sqrt{-\nabla^2} n(\mathbf{r}) \right] &= \frac{1}{2} M \omega^2 R^2, \end{aligned} \quad (32)$$

where, as in Eq. (15), $\frac{1}{2} M \omega^2 R^2$ is the chemical potential.

A comparison between Eqs. (32) and (15) shows that the reduction of dimension does not yet provide any operational simplification when it comes to solving for the spacial density, because of the occurrence of the integral operator $\sqrt{-\nabla^2}$. But one should not fail to notice that the interaction is now made up of two contributions with different dependence on the density. As we will see in the next section, the integral term is rather unimportant in certain parameter regimes of interest and can then be neglected.

V. VIRIAL THEOREM AND SCALING

A. Scaling transformation

Let us consider scaling transformations that change both the length scale and the number of particles,

$$n(\mathbf{r}) \rightarrow \lambda^{2+\alpha} n(\lambda\mathbf{r}), \quad N \rightarrow \lambda^\alpha N. \quad (33)$$

They are consistent with the normalization constraint, Eq. (19), and affect the various terms of $E_{\text{TFD}}^{(2D)}$ in the following manner:

$$\begin{aligned} E_{\text{kin}} &\rightarrow \lambda^{2+2\alpha} E_{\text{kin}}, \\ E_{\text{trap}} &\rightarrow \lambda^{-2+\alpha} E_{\text{trap}}, \\ E_{\text{dd}}^{(1)} &\rightarrow \lambda^{3+5\alpha/2} E_{\text{dd}}^{(1)}, \\ E_{\text{dd}}^{(2)} &\rightarrow \lambda^{3+2\alpha} E_{\text{dd}}^{(2)}, \end{aligned} \quad (34)$$

so that the total energy $E \equiv E_{\text{TFD}}^{(2D)}$ transforms in accordance with

$$\begin{aligned} E &= E_{\text{kin}} + E_{\text{trap}} + E_{\text{dd}}^{(1)} + E_{\text{dd}}^{(2)} \\ &\rightarrow \lambda^{2+2\alpha} E_{\text{kin}} + \lambda^{-2+\alpha} E_{\text{trap}} \\ &\quad + \lambda^{3+5\alpha/2} E_{\text{dd}}^{(1)} + \lambda^{3+2\alpha} E_{\text{dd}}^{(2)}. \end{aligned} \quad (35)$$

B. Virial theorem

Since the minimum of E is achieved by the true ground-state density, all first-order changes of E in the vicinity of $\lambda = 1$ must be generated by the explicit change in N , $\delta N = \delta\lambda\alpha N$, so that

$$\begin{aligned} \alpha N \frac{\partial E}{\partial N} &= (2 + 2\alpha) E_{\text{kin}} + (-2 + \alpha) E_{\text{trap}} \\ &\quad + \left(3 + \frac{5}{2}\alpha \right) E_{\text{dd}}^{(1)} + (3 + 2\alpha) E_{\text{dd}}^{(2)} \end{aligned} \quad (36)$$

is true for all values of α . Choosing two values of α for independent statements, we have

$$2E_{\text{kin}} - 2E_{\text{trap}} + 3(E_{\text{dd}}^{(1)} + E_{\text{dd}}^{(2)}) = 0 \quad (37)$$

for $\alpha = 0$, and

$$2E_{\text{kin}} + 10E_{\text{trap}} + (E_{\text{dd}}^{(1)} - E_{\text{dd}}^{(2)}) = 4N \frac{\partial E}{\partial N} \quad (38)$$

for $\alpha = -\frac{4}{3}$, which are supplemented by the first line of Eq. (35). Further, we note the parametric dependence on μ , ω ,

and M ,

$$\begin{aligned}\mu \frac{\partial}{\partial \mu} E &= 2E_{\text{dd}} = 2(E_{\text{dd}}^{(1)} + E_{\text{dd}}^{(2)}), \\ \omega \frac{\partial}{\partial \omega} E &= 2E_{\text{trap}}, \\ M \frac{\partial}{\partial M} E &= E_{\text{trap}} - E_{\text{kin}}.\end{aligned}\quad (39)$$

Now, owing to the scaling argument, which will be presented next, we find that $E_{\text{dd}}^{(1)}/E_{\text{dd}}^{(2)} \sim \sqrt{N}$, which allows us to neglect $E_{\text{dd}}^{(2)}$ for large N . Applying $E_{\text{dd}}^{(1)} \pm E_{\text{dd}}^{(2)} \approx E_{\text{dd}}^{(1)}$ to the first line of Eqs. (35) and (37)–(39) then yields

$$E(\mu, \omega, M, N) \approx \hbar \omega N^{3/2} \mathcal{E}(\epsilon N^{1/4}), \quad (40)$$

where

$$\epsilon = \frac{\mu_0 \mu^2}{4\pi l_0^3} / (\hbar \omega) \quad (41)$$

is a dimensionless interaction strength that can be understood as the ratio between the interaction energy of two magnetic dipoles separated by $l_0 = \sqrt{\hbar/(M\omega)}$ and the transverse harmonic oscillator energy scale, and $\mathcal{E}(\cdot)$ is a dimensionless function of $\epsilon N^{1/4}$. We remark that the $N^{3/2}$ dependence in the prefactor results from the degeneracy of the harmonic confinement in 2D.

C. Dimensionless variables

We define the natural length scale of the system, a , the dimensionless position, \mathbf{x} , and the dimensionless density, $g(\mathbf{x})$, in accordance with

$$a = l_0 N^{1/4}, \quad \mathbf{x} = \frac{\mathbf{r}}{a}, \quad g(\mathbf{x}) = \frac{a^2}{N} n(\mathbf{r}), \quad (42)$$

so that the scaled density is normalized to unity. Choosing $\hbar \omega N^{3/2}$ as the energy unit, we have

$$\begin{aligned}\frac{E_{\text{TFD}}^{(2D)}[g]}{\hbar \omega N^{3/2}} &= \pi \int (d\mathbf{x}) g(\mathbf{x})^2 + \frac{1}{2} \int (d\mathbf{x}) x^2 g(\mathbf{x}) \\ &+ \epsilon N^{1/4} \left[\frac{256}{45} \sqrt{\pi} \int (d\mathbf{x}) g(\mathbf{x})^{5/2} \right. \\ &\left. - N^{-1/2} \pi \int (d\mathbf{x}) g(\mathbf{x}) \sqrt{-\nabla^2} g(\mathbf{x}) \right], \quad (43)\end{aligned}$$

where $-\nabla^2$ now differentiates with respect to position \mathbf{x} , and the scaled density that minimizes $E_{\text{TFD}}^{(2D)}$ must obey

$$\begin{aligned}2\pi g(\mathbf{x}) + \frac{1}{2} x^2 \\ + \epsilon N^{1/4} \left[\frac{128}{9} \sqrt{\pi} g(\mathbf{x})^{3/2} - N^{-1/2} 2\pi \sqrt{-\nabla^2} g(\mathbf{x}) \right] = \frac{1}{2} X^2,\end{aligned}\quad (44)$$

where $\frac{1}{2} X^2$ is the scaled chemical potential. The term preceded by $N^{-1/2}$ originates in $E_{\text{dd}}^{(2)}$, which was neglected for large N on the way to Eq. (40).

VI. DENSITY AND ENERGY OF THE GROUND STATE

For $N \sim 10^4$, which is a modest value for typical experiments with ultracold atoms, the $N^{-1/2}$ term is a correction in the 1% regime. Given that the TFD approximation is generally introducing errors of the order of a few percent, this term is of a negligible size. Therefore, we shall consistently discard it and all other $N^{-1/2}$ terms. Equation (44) then reduces to

$$\epsilon N^{1/4} \frac{128}{9} \sqrt{\pi} \sqrt{g(\mathbf{x})}^3 + 2\pi \sqrt{g(\mathbf{x})}^2 = \frac{1}{2} (X^2 - x^2), \quad (45)$$

which does not single out any spatial direction and thus implies an isotropic ground-state density, $g(\mathbf{x}) = g(x)$. We also recognize that Eq. (45) is a cubic equation for $\sqrt{g(x)}$ and can be solved analytically.

In Fig. 1, we plot the dimensionless density $g(x)$ for different values of $\epsilon N^{1/4}$. We observe that the stronger the dipole repulsion (larger ϵ), the lower the central density and the larger the radius of the cloud. This feature is reminiscent of the condensate wave function of bosonic atoms when a repulsive contact interaction is taken into account in the mean-field formalism [25]. In contrast to that exhibited by a 3D spin-polarized BEC [26], the simple symmetry of the isotropic harmonic confinement is *preserved* in the ground-state density in 2D. We remark that this is partially a consequence of choosing the direction of spin polarization along the z axis. The situation is markedly different, and more interesting, when the polarization direction breaks the axial symmetry. This will be discussed in Sec. VII.

On the other hand, the dipole interaction for alkali metals are typically small. In the limit of $\epsilon \rightarrow 0^+$, we recover the well-known Thomas-Fermi (TF) profile of noninteracting fermions in a 2D harmonic trap,

$$n(\mathbf{r}) = \frac{1}{4\pi} l_0^{-4} (R_{\text{TF}}^2 - r^2) \quad \text{for } 0 \leq r \leq R_{\text{TF}}, \quad (46)$$

where $R_{\text{TF}} = \sqrt{2}(2N)^{1/4} l_0$ is the Thomas-Fermi radius in 2D.

To evaluate the ground-state energy, we recognize that Eq. (45) provides a natural way of changing the integration

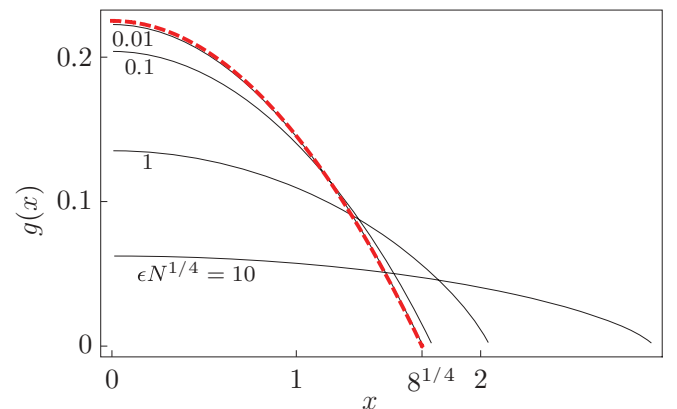


FIG. 1. (Color online) The dimensionless spatial density $g(x)$ at various values of $\epsilon N^{1/4} = 0.01, 0.1, 1, 10$ (thin lines). The TF profile (thick dashed line) is included as a reference. Note that there is an insignificant difference from the TF profile for $\epsilon N^{1/4} < 10^{-2}$.

variable,

$$-x dx = (\kappa g^{1/2} + 2\pi)dg \quad \text{with} \quad \kappa \equiv \epsilon N^{1/4} \frac{64}{3} \sqrt{\pi}, \quad (47)$$

where the position dependence of g is left implicit, such that all terms except $E_{\text{dd}}^{(2)}$ can be analytically expressed in terms of κ and the central density $G \equiv g(x=0)$,

$$\begin{aligned} \frac{E_{\text{kin}}}{\hbar\omega N^{3/2}} &= \frac{4\pi^2}{21}(3\kappa G^{7/2} + 7\pi G^3), \\ \frac{E_{\text{trap}}}{\hbar\omega N^{3/2}} &= \frac{1}{2}X^2 - \frac{\pi}{21}(7\kappa^2 G^4 + 40\pi\kappa G^{7/2} + 56\pi^2 G^3), \\ \frac{E_{\text{dd}}^{(1)}}{\hbar\omega N^{3/2}} &= \frac{2\pi}{105}(7\kappa^2 G^4 + 16\pi\kappa G^{7/2}). \end{aligned} \quad (48)$$

The values of G and X are in turn determined by

$$\begin{aligned} \kappa G^{3/2} + 3\pi G &= \frac{3}{4}X^2, \\ 2\kappa G^{5/2} + 5\pi G^2 &= \frac{5}{2\pi}, \end{aligned} \quad (49)$$

of which the top equation is Eq. (45) for $x=0$, and the bottom equation states the normalization of $g(\mathbf{x})$ to the unit integral. The analytic solutions for E_{kin} , E_{trap} , and $E_{\text{dd}}^{(1)}$ as functions of $\epsilon N^{1/4} = 3\kappa/(64\sqrt{\pi})$ are plotted in Fig. 2. On the far left-hand side in the figure, we observe the equipartition of kinetic and trap energies at vanishing interaction, as one expects in the case of a harmonic trapping potential.

For weakly interacting atoms, i.e., $\epsilon N^{1/4} \ll 1$, we obtain the various contributions to the energy up to the first order in $\epsilon N^{1/4}$,

$$\begin{aligned} \frac{E_{\text{kin}}}{\hbar\omega N^{3/2}} &= \frac{\sqrt{2}}{3} - \frac{128}{105\pi} 2^{1/4} \epsilon N^{1/4}, \\ \frac{E_{\text{trap}}}{\hbar\omega N^{3/2}} &= \frac{\sqrt{2}}{3} + \frac{128}{105\pi} 2^{1/4} \epsilon N^{1/4}, \\ \frac{E_{\text{dd}}^{(1)}}{\hbar\omega N^{3/2}} &= \frac{512}{315\pi} 2^{1/4} \epsilon N^{1/4} \approx 0.615 \epsilon N^{1/4}. \end{aligned} \quad (50)$$

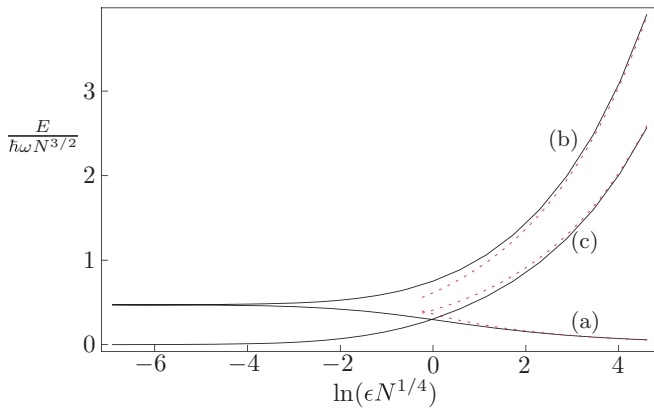


FIG. 2. (Color online) The energy contributions (a) E_{kin} , (b) E_{trap} , and (c) $E_{\text{dd}}^{(1)}$ (in units of $\hbar\omega N^{3/2}$) as functions of $\epsilon N^{1/4}$ (in logarithmic scale). The solid lines show the full solutions of Eqs. (48) and (49), and exhibit the correct weak interaction of Eqs. (50) on the far left-hand side. The short-dashed lines indicate the asymptotic forms of Eqs. (51) for large values of $\epsilon N^{1/4}$.

Note that the sum of E_{kin} and E_{trap} has no first-order correction.

The asymptotic values in the limit of large $\epsilon N^{1/4}$ —shown as dashed lines in Fig. 2—are given by

$$\begin{aligned} \frac{E_{\text{kin}}}{\hbar\omega N^{3/2}} &\sim (\epsilon N^{1/4})^{-2/5}, \\ \frac{E_{\text{trap}}}{\hbar\omega N^{3/2}}, \frac{E_{\text{dd}}^{(1)}}{\hbar\omega N^{3/2}} &\sim (\epsilon N^{1/4})^{2/5}, \\ \frac{E_{\text{dd}}^{(2)}}{\hbar\omega N^{3/2}} &\sim (\epsilon N^{1/4})^{-1.58}, \end{aligned} \quad (51)$$

where the final power law is obtained by a numerical fit. Note that E_{trap} and $E_{\text{dd}}^{(1)}$ have the same large- $\epsilon N^{1/4}$ behavior.

VII. SPIN-DENSITY MATRIX

While the above treatment yields the TFD-approximated ground-state density profile and energy for a 2D cloud of spin-1/2 fermions that are polarized along the axial direction and are hence repelling each other, the lack of spherical symmetry of the magnetic-dipole interaction, which is the source of some interesting predictions [26], is not well reflected due to the peculiarity of both the configuration and the low dimension.

In order to take the spin-dependent nature of the magnetic-dipole interaction into consideration, we extend the treatment by (i) introducing an external magnetic field strong enough to define a local quantization axis, and (ii) constructing spin-dependent Wigner functions and hence the corresponding one-body and two-body spin-density matrices.

For an arbitrary time-independent external magnetic field,

$$\mathbf{B}(\mathbf{r}) = B(\mathbf{r}) \mathbf{e}(\mathbf{r}), \quad (52)$$

the magnetic energy of a single dipole is given by

$$-\mathbf{B}(\mathbf{r}) \cdot \boldsymbol{\mu} = -B(\mathbf{r}) \boldsymbol{\mu} \mathbf{e}(\mathbf{r}) \cdot \boldsymbol{\sigma} \equiv -v(\mathbf{r}) \mathbf{e}(\mathbf{r}) \cdot \boldsymbol{\sigma}. \quad (53)$$

The TF-approximated Wigner function is then

$$\begin{aligned} \underline{v}(\mathbf{r}, \mathbf{p}) &= \eta \left(-\zeta - \frac{p^2}{2M} - V(\mathbf{r}) + v(\mathbf{r}) \mathbf{e}(\mathbf{r}) \cdot \boldsymbol{\sigma} \right) \\ &= \frac{1 + \mathbf{e}(\mathbf{r}) \cdot \boldsymbol{\sigma}}{2} \eta(P_+(\mathbf{r}) - p) \\ &\quad + \frac{1 - \mathbf{e}(\mathbf{r}) \cdot \boldsymbol{\sigma}}{2} \eta(P_-(\mathbf{r}) - p), \end{aligned} \quad (54)$$

with

$$P_{\pm}(\mathbf{r}) = \{2M[-\zeta - V(\mathbf{r}) \pm v(\mathbf{r})]\}^{1/2}, \quad (55)$$

and $-\zeta$ is the chemical potential. The underscore is a reminder that this Wigner function is 2×2 -matrix valued. As a result, the single-particle density also has a corresponding spin dependence,

$$\begin{aligned} \underline{n}(\mathbf{r}) &= \frac{1 + \mathbf{e}(\mathbf{r}) \cdot \boldsymbol{\sigma}}{2} \pi \left[\frac{P_+(\mathbf{r})}{2\pi\hbar} \right]^2 \\ &\quad + \frac{1 - \mathbf{e}(\mathbf{r}) \cdot \boldsymbol{\sigma}}{2} \pi \left[\frac{P_-(\mathbf{r})}{2\pi\hbar} \right]^2 \\ &\equiv \frac{1}{2} [n(\mathbf{r}) + s(\mathbf{r}) \mathbf{e}(\mathbf{r}) \cdot \boldsymbol{\sigma}]. \end{aligned} \quad (56)$$

We observe that now there are two functions present here, the total density, $n(\mathbf{r})$, and the spin-imbalance density, $s(\mathbf{r})$, which are constrained by

$$|s(\mathbf{r})| \leq n(\mathbf{r}), \quad (57)$$

but are otherwise independent of each other. Therefore, the minimization to achieve the ground-state energy has to be done over both functions under the constraints of normalization and positivity, Eqs. (19) and (57), respectively.

We can then evaluate the trap, kinetic, and magnetic energy accordingly,

$$\begin{aligned} E_{\text{trap}} &= \text{tr}_{2 \times 2} \int (d\mathbf{r}) \frac{1}{2} M \omega^2 r^2 \underline{n}(\mathbf{r}) \\ &= \int (d\mathbf{r}) \frac{1}{2} M \omega^2 r^2 n(\mathbf{r}), \\ E_{\text{kin}} &= \text{tr}_{2 \times 2} \int (d\mathbf{r}) \frac{(d\mathbf{p})}{(2\pi\hbar)^2} \frac{p^2}{2M} \nu(\mathbf{r}, \mathbf{p}) \\ &= \int (d\mathbf{r}) \frac{\pi\hbar^2}{2M} [n(\mathbf{r})^2 + s(\mathbf{r})^2], \end{aligned} \quad (58)$$

$$\begin{aligned} E_{\text{mag}} &= -\text{tr}_{2 \times 2} \int (d\mathbf{r}) \boldsymbol{\mu} \cdot \mathbf{B}(\mathbf{r}) \underline{n}(\mathbf{r}) \\ &= - \int (d\mathbf{r}) v(\mathbf{r}) s(\mathbf{r}). \end{aligned}$$

To compute the dipole interaction energy, we construct an approximation to the two-body spin-density matrix $\underline{\underline{n}}^{(2)}(\mathbf{r}', \mathbf{r}''; \mathbf{r}', \mathbf{r}'')$ in the spirit of Eq. (8), starting with the single-particle orbital,

$$\phi_m(x) = \begin{pmatrix} \alpha_m(\mathbf{x}) \\ \beta_m(\mathbf{x}) \end{pmatrix}, \quad (59)$$

where α_m and β_m are the spin-up and spin-down components, \mathbf{x} is the position variable, while x denotes the combination of the position and spin variables, so that the ground-state wave function of a N fermion system can be constructed as a Slater determinant,

$$\psi(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \det[\phi_m(x_l)]. \quad (60)$$

When expressing the one-body and two-body spin-density matrices in terms of single-particle orbitals, we get

$$\begin{aligned} \underline{n}(\mathbf{x}; \mathbf{y}) &= N \int dx_2 \cdots dx_N \psi(x, x_2, \dots, x_N) \psi(y, x_2, \dots, x_N)^* \\ &= \sum_m \begin{pmatrix} \alpha_m(\mathbf{x}) \alpha_m(\mathbf{y})^* & \alpha_m(\mathbf{x}) \beta_m(\mathbf{y})^* \\ \beta_m(\mathbf{x}) \alpha_m(\mathbf{y})^* & \beta_m(\mathbf{x}) \beta_m(\mathbf{y})^* \end{pmatrix} \equiv \begin{pmatrix} n_{\uparrow\uparrow}(\mathbf{x}; \mathbf{y}) & n_{\uparrow\downarrow}(\mathbf{x}; \mathbf{y}) \\ n_{\downarrow\uparrow}(\mathbf{x}; \mathbf{y}) & n_{\downarrow\downarrow}(\mathbf{x}; \mathbf{y}) \end{pmatrix}, \\ \underline{\underline{n}}^{(2)}(\mathbf{x}, \mathbf{y}; \mathbf{x}', \mathbf{y}') &= \frac{N(N-1)}{2} \int dx_3 \cdots dx_N \psi(x, y, x_3, \dots, x_N) \psi(x', y', x_3, \dots, x_N)^* \\ &= \frac{1}{2} \sum_{l, m} \begin{pmatrix} \alpha_l(\mathbf{x}) \\ \beta_l(\mathbf{x}) \end{pmatrix} \otimes \begin{pmatrix} \alpha_m(\mathbf{y}) \\ \beta_m(\mathbf{y}) \end{pmatrix} \left[\begin{pmatrix} \alpha_l(\mathbf{x}') \\ \beta_l(\mathbf{x}') \end{pmatrix} \otimes \begin{pmatrix} \alpha_m(\mathbf{y}') \\ \beta_m(\mathbf{y}') \end{pmatrix} - \begin{pmatrix} \alpha_m(\mathbf{x}') \\ \beta_m(\mathbf{x}') \end{pmatrix} \otimes \begin{pmatrix} \alpha_l(\mathbf{y}') \\ \beta_l(\mathbf{y}') \end{pmatrix} \right]^\dagger \\ &= \frac{1}{2} \left(\underline{n}(\mathbf{x}; \mathbf{x}') \otimes \underline{n}(\mathbf{y}; \mathbf{y}') - [\underline{n}(\mathbf{x}; \mathbf{y}') \otimes \underline{n}(\mathbf{y}; \mathbf{x}')]_{T_{23}} \right), \end{aligned} \quad (61)$$

where T_{23} means interchanging the second and the third columns. The double summation in $\underline{\underline{n}}^{(2)}$ includes the $l = m$ summands of the self-energy, which has equal contributions to the direct and exchange terms and hence does not contribute to the sum.

The contact term in the dipole interaction potential is nonvanishing only in the singlet state,

$$\begin{aligned} E_{\text{dd},s} &= \text{tr}_{4 \times 4} \int (d\mathbf{r}') (d\mathbf{r}'') \frac{1}{l_z \sqrt{2\pi}} \underline{\underline{n}}^{(2)}(\mathbf{r}', \mathbf{r}''; \mathbf{r}', \mathbf{r}'') \\ &\quad \times \frac{\mu_0}{4\pi} \boldsymbol{\mu} \cdot \left[-\frac{8\pi}{3} \delta(\mathbf{r}' - \mathbf{r}'') \right] \boldsymbol{\mu} \\ &= \frac{\sqrt{2\pi}}{l_z} \frac{\mu_0 \mu^2}{4\pi} \int (d\mathbf{r}) [n(\mathbf{r})^2 - s(\mathbf{r})^2], \end{aligned} \quad (62)$$

where the prefactor $\sqrt{2\pi}/l_z$ originates in the reduction of dimensionality. We observe that, owing to the $1/l_z$ scaling, the relative strength of this term can be tuned by adjusting the stiffness of the z -confining trap.

On the other hand, the triplet state interacts according to the remaining terms in the dipole potential. Since the state is symmetric under particle exchange, we use, instead of the $\underline{\underline{n}}^{(2)}$ in Eq. (61), an alternative two-body density,

$$\tilde{\underline{\underline{n}}}^{(2)}(\mathbf{r}', \mathbf{r}''; \mathbf{r}', \mathbf{r}'') = \frac{1}{2} [\underline{n}(\mathbf{r}') \otimes \underline{n}(\mathbf{r}'') - \underline{n}(\mathbf{r}'; \mathbf{r}'') \otimes \underline{n}(\mathbf{r}''; \mathbf{r}')], \quad (63)$$

which yields the same energy but greatly simplifies the computation due to its tensor product structure.

The triplet interaction energy is then given by

$$\begin{aligned} E_{\text{dd},t} &= \text{tr}_{4 \times 4} \frac{\mu_0 \mu^2}{4\pi} \int (d\mathbf{r}') (d\mathbf{r}'') \tilde{\underline{\underline{n}}}^{(2)}(\mathbf{r}', \mathbf{r}''; \mathbf{r}', \mathbf{r}'') \\ &\quad \times \frac{\boldsymbol{\rho}^2 \boldsymbol{\sigma} \cdot \boldsymbol{\tau} - 3 \boldsymbol{\sigma} \cdot \boldsymbol{\rho} \boldsymbol{\rho} \cdot \boldsymbol{\tau}}{\rho^5}, \end{aligned} \quad (64)$$

with $\boldsymbol{\rho} = \mathbf{r}' - \mathbf{r}''$, and $\boldsymbol{\tau}$ denotes the Pauli vector for the second atom. To evaluate this expression, we apply the same procedure

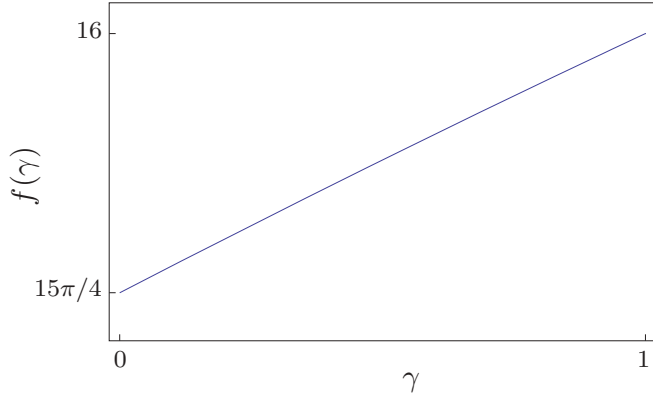


FIG. 3. (Color online) $f(\gamma)$ at relevant values of γ . It can be shown that $15\pi/4 < f(\gamma) < 16$ for $0 < \gamma < 1$.

as that used to obtain Eq. (29) and find

$$E_{\text{dd,t}}^{(1)} = \frac{32}{45} \sqrt{2\pi} \frac{\mu_0 \mu^2}{4\pi} \int (d\mathbf{r}) \frac{3e_z(\mathbf{r})^2 - 1}{2} \times \left\{ [n(\mathbf{r}) + s(\mathbf{r})]^{5/2} + [n(\mathbf{r}) - s(\mathbf{r})]^{5/2} - \frac{f(\gamma)}{8} [n(\mathbf{r}) + s(\mathbf{r})]^{3/2} [n(\mathbf{r}) - s(\mathbf{r})] \right\}, \quad (65)$$

$$E_{\text{dd,t}}^{(2)} = -\frac{1}{2} \frac{\mu_0 \mu^2}{4\pi} \int (d\mathbf{r})(d\mathbf{r}') \times \frac{\nabla s_z(\mathbf{r}) \cdot \nabla' s_z(\mathbf{r}') - \nabla \cdot \mathbf{s}(\mathbf{r}) \nabla' \cdot \mathbf{s}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|},$$

where $\gamma = [P_-(\mathbf{r})/P_+(\mathbf{r})]^2$ is essentially the ratio between the Fermi energies of the minority and majority spin components, and

$$f(\gamma) = (\gamma^{-1} + 14 + \gamma)E(\gamma) + (-\gamma^{-1} - 6 + 7\gamma)K(\gamma) \quad (66)$$

is a combination of elliptic integrals that is smooth and finite for $0 < \gamma < 1$. It is clear from Fig. 3 that $f(\gamma)$ can be replaced by a linear function $\tilde{f}(\gamma) = \frac{15}{4}\pi + (16 - \frac{15}{4}\pi)\gamma$ to simplify computations.

In passing, we note that a magnetic field with a large component in the xy plane, such that $3e_z(\mathbf{r})^2 - 1 < 0$ in Eq. (65) for some region, may lead to an energy that is not bounded from below. The system is then unstable and will collapse and explode within milliseconds (this catastrophe was observed in dipolar Bose gases [27,28]). When this happens, so much energy is made available that the 2D confinement will be lost.

For the simple case of a constant external magnetic field, we have

$$\mathbf{B}(\mathbf{r}) = B_0 \mathbf{e}_z, \quad v(\mathbf{r}) = B_0 \mu \equiv v_0. \quad (67)$$

In the dimensionless quantities, we reparametrize the spin-imbalance density in accordance with

$$h(\mathbf{x}) = \frac{a^2}{N} s(\mathbf{r}) \equiv \cos[\vartheta(\mathbf{x})]g(\mathbf{x}), \quad (68)$$

so that Eq. (57) is automatically fulfilled. In the limit of weak interaction, we obtain the total energy as a functional of both $g(\mathbf{x})$ and $\vartheta(\mathbf{x})$,

$$\begin{aligned} \frac{E_{\text{TFD}}^{(2D)}[g, \vartheta]}{\hbar \omega N^{3/2}} &= \frac{\pi}{2} \int (d\mathbf{x}) g(\mathbf{x})^2 \{1 + \cos^2[\vartheta(\mathbf{x})]\} \\ &+ \frac{1}{2} \int (d\mathbf{x}) x^2 g(\mathbf{x}) \\ &- \frac{1}{\sqrt{N}} \frac{v_0}{\hbar \omega} \int (d\mathbf{x}) g(\mathbf{x}) \cos[\vartheta(\mathbf{x})], \end{aligned} \quad (69)$$

and the variation of $g(\mathbf{x})$ and $\vartheta(\mathbf{x})$, with $\frac{1}{2}X^2$ as the Lagrange multiplier, yields

$$\begin{aligned} \pi g(\mathbf{x}) + \cos[\vartheta(\mathbf{x})] \left\{ \pi g(\mathbf{x}) \cos[\vartheta(\mathbf{x})] - \frac{1}{\sqrt{N}} \frac{v_0}{\hbar \omega} \right\} &= \frac{1}{2}(X^2 - x^2), \\ g(\mathbf{x}) \sin[\vartheta(\mathbf{x})] \left\{ \pi g(\mathbf{x}) \cos[\vartheta(\mathbf{x})] - \frac{1}{\sqrt{N}} \frac{v_0}{\hbar \omega} \right\} &= 0. \end{aligned} \quad (70)$$

There are two nontrivial solutions, one for a spin-polarized (SP) system and the other allowing a spin mixture (SM). The SP solution yields the TF profile equivalent to Eq. (46). The SM solution gives

$$g(\mathbf{x}) = \begin{cases} \frac{1}{2\pi} (2\sqrt{1-A^2} - x^2) & \text{for } 0 \leq x \leq x_-, \\ \frac{1}{2\pi} (A + \sqrt{1-A^2} - \frac{x^2}{2}) & \text{for } x_- \leq x \leq x_+, \end{cases} \quad (71)$$

with

$$A = \frac{v_0}{\hbar \omega} \frac{1}{\sqrt{N}} = \frac{B_0 \mu}{\pi \sqrt{N}}, \quad (72)$$

together with a constant spin-imbalance density in the center,

$$g(\mathbf{x}) \cos[\vartheta(\mathbf{x})] = \frac{A}{\pi}, \quad (73)$$

where x_{\pm} are the radii of the SM (lower sign) and the entire cloud (upper sign), respectively, given by

$$x_{\pm}^2 = 2(\sqrt{1-A^2} \pm A). \quad (74)$$

These matters are illustrated in Fig. 4.

However, the existence of a SM requires an extremely weak external magnetic field, such that

$$\frac{v_0}{\hbar \omega} \frac{1}{\sqrt{N}} \leq \frac{1}{\sqrt{2}}. \quad (75)$$

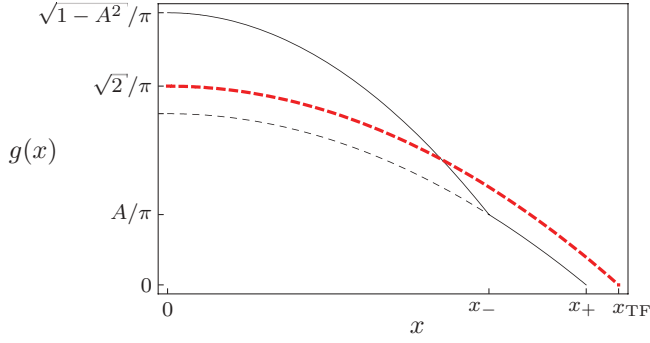


FIG. 4. (Color online) The dimensionless density profile of a SM (thin solid line) with $A = 0.25$, in comparison with the TF profile (i.e., SP solution, thick dashed line). The thin dashed line indicates the density of the majority component in the spin mixture. For greater values of A while keeping $A \leq 1/\sqrt{2}$, the density profile approaches that of the SP solution with a lowering central density and an increasing x_{\pm} . In the opposite limit, we recover a mixture of equal spin components when there is no external magnetic field, i.e., $A = 0$.

This condition arises from the positivity of the radii x_{\pm} . In usual experimental setups, this translates into $B \sim 10$ mG for a system of $N = 10^6$ atoms with a radial harmonic confinement of $\omega = 2\pi \times 20$ Hz. In other words, a SP cloud is readily attainable. This justifies the treatment of a SP system before Sec. VII.

VIII. SUMMARY AND OUTLOOK

Table I summarizes the kinetic and the dipole-dipole interaction energies as functionals of the single-particle density for a fully SP gas in 1D, 2D, and 3D. It is clear that the structure of the density functionals depends crucially on the spatial dimension. The procedure used here to reduce dimensionality is by no means unique, but fairly well justified by the strong confinement of a stiff harmonic trap in a possible experimental setup.

In 2D, the total energy with TFD approximation depends on both the dimensionless interaction strength ϵ , and the number of particles N , as it does in 3D, but the N dependence is slightly more complicated. Namely, as one piece of the interaction

energy is proportional to $\epsilon N^{1/4}$, while the other piece is proportional to $\epsilon N^{-1/4}$, the latter is always a factor of \sqrt{N} smaller, inviting a perturbative treatment.

For large $\epsilon N^{1/4}$, the potential energy and the first piece of the interaction energy dominate, and are of the order of $\hbar\omega N^{3/2} \times (\epsilon N^{1/4})^{2/5}$, while the kinetic energy is of the order of $\hbar\omega N^{3/2} \times (\epsilon N^{1/4})^{-2/5}$. Numerical results suggest that the second piece of the interaction energy is of the order $\hbar\omega N^{3/2} \times (\epsilon N^{1/4})^{-1.58}$, which makes it the most slowly growing term in the total energy.

In the limiting case of $\epsilon \rightarrow 0^+$, the kinetic and potential energies are both $\hbar\omega N^{3/2} \frac{\sqrt{2}}{3}$, where the equality is well predicted by the virial theorem applied to a simple harmonic oscillator. The two pieces of the interaction energy are of the order $N^{7/4}$ and $N^{5/4}$ respectively, even though both are vanishing due to small ϵ .

In addition to the fully spin-polarized situation, we also dealt with partially polarized gases, allowing for inhomogeneous polarization. By considering the spin-density matrix, we found the energy as a functional of the total density and the spin-imbalance density, and then determined the implied ground-state density profile. For typical experimental parameters and a modest number of trapped atoms, a spin mixture can only exist for an extremely weak external magnetic field. In other words, a fully spin-polarized gas is readily attainable.

Having thus established the TFD functionals, we intend to investigate the excitation energies of the system for small deviation from the equilibrium. On the other hand, it is well known that the TF approximation is problematic at the boundary of the system. We will follow up on the gradient corrections of von Weizsäcker type. It is perceivable that once the corrections are included, $E_{\text{dd}}^{(2)}$ may no longer be negligible. Lastly, we would like to explore other external trapping potentials, such as anisotropic harmonic traps, possibly with an optical lattice superimposed.

ACKNOWLEDGMENTS

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TABLE I. Summary of the density functionals for the kinetic energy and the dipole-dipole interaction energy in 1D, 2D, and 3D. In 1D, the spins are polarized normal to the z axis, along which the atoms align. $\text{erfc}()$ denotes the complementary error function, and $t = |z - z'|/(\sqrt{2}l_{\perp})$. Note that further simplification of the 1D expression of E_{dd} involves taking the limit of $l_{\perp} \rightarrow 0^+$ which should be done with extreme care. In 2D and 3D, the spins are polarized along the z direction, and θ in 3D refers to the azimuthal angle of the vector $\mathbf{r} - \mathbf{r}'$.

	E_{kin}	E_{dd}
1D	$\int dz \frac{\pi^2 \hbar^2}{6M} n(z)^3$	$\frac{\mu_0 \mu^2}{4\pi} \int dz dz' [n(z)n(z') - n(z; z')n(z'; z)] \frac{1}{\sqrt{2}l_{\perp}^3} \left[\left(\frac{1}{2} + t^2 \right) \sqrt{\pi} e^{t^2} \text{erfc}(t) - t \right]$
2D	$\int (d\mathbf{r}_{\perp}) \frac{\pi \hbar^2}{2M} n(\mathbf{r}_{\perp})^2$	$\frac{\mu_0 \mu^2}{4\pi} \int (d\mathbf{r}_{\perp}) \left[\frac{256}{45} \sqrt{\pi} n(\mathbf{r}_{\perp})^{5/2} - \pi n(\mathbf{r}) \sqrt{-\nabla^2} n(\mathbf{r}_{\perp}) \right]$
3D	$\int (d\mathbf{r}) \frac{\hbar^2}{20\pi^2 M} [6\pi^2 n(\mathbf{r})]^{5/3}$	$\frac{\mu_0 \mu^2}{4\pi} \int (d\mathbf{r})(d\mathbf{r}') \frac{1}{2} n(\mathbf{r}) \frac{1 - 3 \cos^2 \theta}{ \mathbf{r} - \mathbf{r}' ^3} n(\mathbf{r}')$

APPENDIX A: CALCULATING THE INTERACTION ENERGY

The splitting of the dipole-dipole interaction energy into direct and exchange energy at the level of the one-particle

density and the one-particle density matrix turns out to be inconvenient as it stands, since this yields two integrals, which both diverge individually but together sum up to a finite value. This prompts us to express everything in terms of the one-particle Wigner function,

$$\begin{aligned}
 E_{\text{dd}} &= \frac{1}{2} \frac{\mu_0 \mu^2}{4\pi} \int \frac{(d\mathbf{r}')(d\mathbf{r}'')(d\mathbf{p}_1)(d\mathbf{p}_2)}{(2\pi\hbar)^4} \frac{1}{|\mathbf{r}' - \mathbf{r}''|^3} \left[v(\mathbf{r}', \mathbf{p}_1) v(\mathbf{r}'', \mathbf{p}_2) - v\left(\frac{\mathbf{r}'+\mathbf{r}''}{2}, \mathbf{p}_1\right) v\left(\frac{\mathbf{r}'+\mathbf{r}''}{2}, \mathbf{p}_2\right) e^{i(\mathbf{p}_1 - \mathbf{p}_2) \cdot (\mathbf{r}' - \mathbf{r}'')/\hbar} \right] \\
 &= \frac{1}{2} \frac{\mu_0 \mu^2}{4\pi} \int \frac{(d\mathbf{r})(d\boldsymbol{\rho})(d\mathbf{p}_1)(d\mathbf{p}_2)}{(2\pi\hbar)^4} (d\mathbf{k}_1)(d\mathbf{k}_2) \frac{1}{\rho^3} e^{i(\mathbf{k}_1 + \mathbf{k}_2) \cdot \mathbf{r}} \bar{v}(\mathbf{k}_1, \mathbf{p}_1) \bar{v}(\mathbf{k}_2, \mathbf{p}_2) (e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \boldsymbol{\rho}/2} - e^{i(\mathbf{p}_1 - \mathbf{p}_2) \cdot \boldsymbol{\rho}/\hbar}), \quad (\text{A1})
 \end{aligned}$$

where we have used the substitution $\mathbf{r} = \frac{1}{2}(\mathbf{r}' + \mathbf{r}'')$, $\boldsymbol{\rho} = \mathbf{r}' - \mathbf{r}''$, and the Fourier transform in 2D,

$$\begin{aligned}
 v(\mathbf{r}, \mathbf{p}) &= \int (d\mathbf{k}) \bar{v}(\mathbf{k}, \mathbf{p}) e^{i\mathbf{k} \cdot \mathbf{r}}, \\
 \bar{v}(\mathbf{k}, \mathbf{p}) &= \int \frac{(d\mathbf{r})}{(2\pi)^2} v(\mathbf{r}, \mathbf{p}) e^{-i\mathbf{k} \cdot \mathbf{r}}. \quad (\text{A2})
 \end{aligned}$$

The integration over $\boldsymbol{\rho}$ can be evaluated with the outcome

$$\int (d\boldsymbol{\rho}) \frac{1}{\rho^3} [e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \boldsymbol{\rho}/2} - e^{i(\mathbf{p}_1 - \mathbf{p}_2) \cdot \boldsymbol{\rho}/\hbar}] = 2\pi (|\mathbf{p}_1 - \mathbf{p}_2|/\hbar - |\mathbf{k}_1 - \mathbf{k}_2|/2). \quad (\text{A3})$$

We recognize that the interaction energy is split into two pieces,

$$\begin{aligned}
 E_{\text{dd}} &= E_{\text{dd}}^{(1)} + E_{\text{dd}}^{(2)}, \\
 E_{\text{dd}}^{(1)} &\equiv \frac{1}{2} \frac{\mu_0 \mu^2}{4\pi} 2\pi \int (d\mathbf{r}) \frac{(d\mathbf{p}_1)}{(2\pi\hbar)^2} \frac{(d\mathbf{p}_2)}{(2\pi\hbar)^2} (d\mathbf{k}_1)(d\mathbf{k}_2) e^{i(\mathbf{k}_1 + \mathbf{k}_2) \cdot \mathbf{r}} \bar{v}(\mathbf{k}_1, \mathbf{p}_1) \bar{v}(\mathbf{k}_2, \mathbf{p}_2) \frac{|\mathbf{p}_1 - \mathbf{p}_2|}{\hbar}, \quad (\text{A4}) \\
 E_{\text{dd}}^{(2)} &\equiv -\frac{1}{2} \frac{\mu_0 \mu^2}{4\pi} 2\pi \int (d\mathbf{r}) \frac{(d\mathbf{p}_1)}{(2\pi\hbar)^2} \frac{(d\mathbf{p}_2)}{(2\pi\hbar)^2} (d\mathbf{k}_1)(d\mathbf{k}_2) e^{i(\mathbf{k}_1 + \mathbf{k}_2) \cdot \mathbf{r}} \bar{v}(\mathbf{k}_1, \mathbf{p}_1) \bar{v}(\mathbf{k}_2, \mathbf{p}_2) \frac{|\mathbf{k}_1 - \mathbf{k}_2|}{2},
 \end{aligned}$$

but this is *not* the splitting into the direct and exchange terms, as the integration of a single exponential term in Eq. (A3) will not converge.

A closer look at $E_{\text{dd}}^{(1)}$ tells us that the $\int (d\mathbf{k}_1)$ and $\int (d\mathbf{k}_2)$ integrations recover the Wigner functions, which impose an upper limit of $P = \hbar\sqrt{4\pi n(\mathbf{r})}$ on the length of p_1 and p_2 , so that

$$E_{\text{dd}}^{(1)} \equiv \frac{1}{2} \frac{\mu_0 \mu^2}{4\pi} 2\pi \int (d\mathbf{r}) \frac{(d\mathbf{p}_1)}{(2\pi\hbar)^2} \frac{(d\mathbf{p}_2)}{(2\pi\hbar)^2} |\mathbf{p}_1 - \mathbf{p}_2|/\hbar = \frac{\mu_0 \mu^2}{4\pi} \int (d\mathbf{r}) \frac{256}{45} \sqrt{\pi n(\mathbf{r})}^{5/2}. \quad (\text{A5})$$

On the other hand, $E_{\text{dd}}^{(2)}$ needs to be treated differently. The $\int (d\mathbf{p}_1)$ and $\int (d\mathbf{p}_2)$ integrations yield the form factor

$$\bar{n}(\mathbf{k}) = \int \frac{(d\mathbf{p})}{(2\pi\hbar)^2} \bar{v}(\mathbf{k}, \mathbf{p}) = \int \frac{(d\mathbf{r})}{(2\pi)^2} e^{-i\mathbf{k} \cdot \mathbf{r}} n(\mathbf{r}), \quad (\text{A6})$$

while the $\int (d\mathbf{r})$ integration gives rise to a 2D Dirac delta function,

$$\int (d\mathbf{r}) e^{i(\mathbf{k}_1 + \mathbf{k}_2) \cdot \mathbf{r}} = (2\pi)^2 \delta(\mathbf{k}_1 + \mathbf{k}_2).$$

This then takes care of one of the integrations over \mathbf{k}_1 or \mathbf{k}_2 , and we arrive at

$$E_{\text{dd}}^{(2)} = -\frac{1}{2} \frac{\mu_0 \mu^2}{4\pi} (2\pi)^3 \int (d\mathbf{k}) \bar{n}(\mathbf{k}) k \bar{n}(-\mathbf{k}) = -\frac{\mu_0 \mu^2}{4\pi} \pi \int (d\mathbf{r}) n(\mathbf{r}) \sqrt{-\nabla^2} n(\mathbf{r}), \quad (\text{A7})$$

where the short-hand notation of $\sqrt{-\nabla^2}$ for the integral operator (30) is used in recognition that it is equivalent to the integral operator $-\nabla^2$ when applied twice. This completes the derivation of Eqs. (29).

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