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Energy-dependent scattering and the Gross-Pitaevskii equation in two-dimensional Bose-Einstein condensates

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We consider many-body effects on particle scattering in one-, two-, and three-dimensional (3D) Bose gases. We show that at $T=0$ these effects can be modeled by the simpler two-body T matrix evaluated off the energy shell. This is important in 1D and 2D because the two-body T matrix vanishes at zero energy and so mean-field effects on particle energies must be taken into account to obtain a self-consistent treatment of low-energy collisions. Using the off-shell two-body T matrix we obtain the energy and density dependence of the effective interaction in 1D and 2D and the appropriate Gross-Pitaevskii equations for these dimensions. Our results provide an alternative derivation of those of Kolomeisky and co-workers. We present numerical solutions of the Gross-Pitaevskii equation for a 2D condensate of hard-sphere bosons in a trap. We find that the interaction strength is much greater in 2D than for a 3D gas with the same hard-sphere radius. The Thomas-Fermi regime is, therefore, approached at lower condensate populations and the energy required to create vortices is lowered compared to the 3D case.

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I. INTRODUCTION

Recent experiments on the quasicondensation of a two-dimensional gas of atomic hydrogen [3] and the possibilities of confining dilute atomic gases in "low-dimensional" traps [4,5] have stimulated interest in the possibilities of Bose-Einstein condensation in two-dimensional systems. It has long been known that, in the thermodynamic limit, Bose condensation is not possible in two-dimensional homogeneous systems at any finite temperature because long wavelength fluctuations destroy long-range coherence [6]. Instead such a system undergoes a Kosterlitz-Thouless transition [7] and acquires local coherence properties over a length scale dependent on the temperature—a "quasicondensate" [8]. In the limit $T\rightarrow 0$ global coherence is achieved in homogeneous 2D systems and a true condensate then exists. In a trapped 2D system the modifications of the density of states caused by the confining potential enable a true condensate to exist even at finite temperatures [9].

In most treatments of a Bose condensed gas in 3D, particle interactions are described by a δ-function contact potential whose strength is determined by the zero energy and momentum limit of the two-body T matrix (T_{2b}) that describes scattering in a vacuum. This leads to the standard form of the interaction potential $(4\pi\hbar^2 a_{3D}/m)\delta(\mathbf{r})$, where a_{3D} is the s-wave scattering length. At higher order it can be shown that the interactions are actually described by a many-body T matrix (T_{MB}) [10–12] which accounts for the fact that collisions occur in the presence of the condensate rather than in free space. In 2D this correction is critical because the 2D two-body T matrix vanishes in the zero energy limit [2,13], and thus we must include this correction (at least partially) even at leading order [14]. In this paper we develop an expression for the many-body T matrix in terms of the two-body T matrix evaluated at a shifted effective interaction energy. In one and two dimensions we obtain an effective interaction that depends on the energy of the collision, in contrast with three-dimensional gases.

The energy dependence of the effective interaction can be written as a density dependence, in which form the results can be applied to trapped gases. This leads to a Gross-Pitaevskii equation (GPE) describing the condensate wave function that no longer has a cubic non-linearity in ψ, but instead goes as $|\psi|^4\psi$ in 1D and as $(|\psi|^2/\ln|\psi|^2)\psi$ in 2D. Such a modified GPE has already been introduced by Kolomeisky [1,2] and Tanatar [15], using arguments based either on the renormalization group or a Kohn-Sham density-functional approach [16]. Our discussion in this paper is to show how essentially the same results can be obtained by a consideration of many-body effects on particle scattering and to relate this to well-understood treatments of the 3D Bose gas. Indeed, substantially the same treatment as used in 3D applied to the 1D and 2D gases leads to the energy dependent effective interactions. The principle difference is that these effects must be taken into account in leading order, whereas in 3D they can be neglected in the simplest treatments and only become important at finite temperature or high density.

In the following section we discuss the Gross-Pitaevskii equation, and the limits in which a system may be considered two dimensional. In Sec. III we then derive the many-body effective interaction for low-dimensional gases, before considering its implications for 1D gases in Sec. IV. Finally, using this effective interaction we obtain a form of the two-dimensional Gross-Pitaevskii equation, and we present the results of numerical solutions for both ground and vortex states in Sec. VI.

II. THE GROSS-PITAEVSKII EQUATION IN 2D AND QUASI-2D

The macroscopic wave function for a Bose-Einstein condensate (BEC) is found in mean-field theory using a nonlinear Schrödinger equation known as the Gross-Pitaevskii equation—where the nonlinear term arises from interactions between the atoms of the condensate. Obtaining the form of the effective interaction in 2D, and describing its effect on the solutions of this equation are the main concerns of this paper.

Currently, most BEC experiments have created three-dimensional condensates, which are described by a GPE of the form

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r})+V_{\mathrm{trap}}(\mathbf{r})\psi(\mathbf{r})+N_0g_{3\mathrm{D}}|\psi(\mathbf{r})|^2\psi(\mathbf{r})=\mu\psi(\mathbf{r}), \tag{1}$$

where $V_{\mathrm{trap}}(\mathbf{r})$ is the external trapping potential, N_0 is the condensate population, μ the chemical potential, and $g_{3\mathrm{D}}$ is the coupling parameter describing the effective interactions. The coupling parameter is generally taken to be the zero energy and momentum limit of the two-body T matrix that in 3D is a nonzero constant $g_{3\mathrm{D}}=4\pi\hbar^2a_{3\mathrm{D}}/m$, where a is the s-wave scattering length. The T matrix has the contact potential form $T_{2\mathrm{b}}(\mathbf{r},\mathbf{r}')=g_{3\mathrm{D}}\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{r})$ in the limit that all the momenta involved in typical collisions are much less than $1/R_e$, where R_e is the range of the actual interatomic potential (which is not in general equal to the scattering length a).

The obvious extension of these experiments in order to achieve the goal of two-dimensional condensates is to confine a gas in an anisotropic trap such that the gas is tightly confined in the z direction. For a harmonic potential such a trap has the form $V_{\mathrm{trap}}(\mathbf{r})=m\omega^2/2(\rho^2+z^2/\gamma)$, with $l_z\equiv\sqrt{\hbar/2m\omega_z}$ as the characteristic trap length in the tightly confined direction, where $\omega_z\equiv\omega/\gamma^{1/2}$. On decreasing l_z (decreasing γ) the system will pass from being three dimensional to being two dimensional in a variety of senses.

The system can first be called two dimensional once l_z has merely been decreased sufficiently that the mean-field energy of the condensate is small compared to $\hbar\omega_z$. In this case the dynamics of the system in the z dimension are restricted to zero-point oscillations. Nonetheless, if l_z is still much greater than $a_{3\mathrm{D}}$, then two body collisions are hardly affected, and hence interactions can still be described by the three-dimensional contact potential $g_{3\mathrm{D}}$. Therefore, although in this case the third dimension can be factored out of the dynamics of the system, at short length scales the interactions are still three dimensional. This regime can be described using the 3D GPE of Eq. (1) with the assumption that the wave function can be factorized as

$$\Psi(\rho,z)=\psi(\rho)\left(\frac{m\omega_z}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega_z}{2\hbar}z^2\right). \tag{2}$$

Substituting into the 3D GPE, and integrating over z leads to a two-dimensional equation

$$-\frac{\hbar^2}{2m}\nabla_\rho^2\psi(\rho)+\frac{1}{2}m\omega^2\rho^2\psi(\rho)+g'N_0|\psi(\rho)|^2\psi(\rho)=\mu'\psi(\rho), \tag{3}$$

where $\rho=\{x,y\}$, $\mu'=\mu-\hbar\omega_z/2$, and the coupling parameter g' is given by $g'_{3\mathrm{D}}=(m\omega_z/2\pi\hbar)^{1/2}g_{3\mathrm{D}}$. The subscript here refers to the three-dimensional nature of the interactions whilst the prime indicates that $g'_{3\mathrm{D}}$ is a two-dimensional quantity.

The above factorization of the wave function remains valid as l_z is decreased further, but the assumption that the scattering is unaffected begins to break down when l_z is not much greater than $a_{3\mathrm{D}}$. The effect of the confinement on particle interactions has been discussed in detail by Petrov and Shlyapnikov [17,18], who found that a 2D contact potential can still be used but that the strength of the interaction becomes dependent upon the confinement. The coupling parameter that they obtained in this "quasi-2D" regime is

$$g'_{\mathrm{q2D}}=\left(\frac{8\pi\omega_z\hbar^3}{m}\right)^{1/2}\left[\frac{1}{a_{3\mathrm{D}}}+\left(\frac{m\omega_z}{2\pi\hbar}\right)^{1/2}\ln\left(\frac{B\hbar\omega_z}{2\mu\pi}\right)\right]^{-1}, \tag{4}$$

where $B\approx0.915$. This expression is valid when the conditions $mg'_{\mathrm{q2D}}/2\pi\hbar^2, R_e/l_z, 2\mu/\hbar\omega_z \ll 1$ are satisfied. In the large l_z limit the $1/a_{3\mathrm{D}}$ term dominates and the scattering is three-dimensional as considered above. However in the fully 2D limit the logarithmic term in Eq. (4) dominates and g becomes dependent upon μ. Equation (4) was derived from solving the two-body scattering problem within the potential causing the tight z confinement. We will now show how essentially the same result can be obtained in the fully 2D limit by a consideration of the many-body effects on particle scattering.

III. THE *T* MATRIX IN THE GPE

In order to describe the interactions within a truly 2D BEC we must consider 2D scattering in the presence of a condensate. This is described by a many-body T matrix T_{MB}, and the coupling parameter that appears in the GPE is in fact given by the matrix element $\langle\mathbf{k}'|T_{\mathrm{MB}}(E)|\mathbf{k}\rangle$ evaluated in the limit of zero momentum and energy $(\mathbf{k},\mathbf{k}',\mathbf{K},E=0)$. Note that the many-body T matrix is, in principle, also a function of the center-of-mass momentum $\mathbf{K}$, but this will not be explicitly indicated in this paper for notational simplicity. This will not be important for the results presented since we will always take the limit $\mathbf{K}=\mathbf{0}$ in this paper.

Before discussing the many-body T matrix, however, we will first consider the simpler two-body T matrix that describes collisions between two particles in a vacuum and for which analytical expressions exist [19]. We will then show how the many-body T matrix can be obtained from the two-body version in the limit appropriate for the study of BEC.

A. The two-body *T* matrix

The two-body T matrix describing scattering from an interparticle potential $V(\mathbf{r})$ is the solution to the Lippmann-Schwinger equation [20]

$$\langle\mathbf{k}'|T_{2\mathrm{b}}(\overline{E})|\mathbf{k}\rangle=\langle\mathbf{k}'|V(\mathbf{r}_1-\mathbf{r}_2)|\mathbf{k}\rangle+\sum_{\mathbf{q}}\langle\mathbf{k}'|V(\mathbf{r}_1-\mathbf{r}_2)|\mathbf{q}\rangle\times\frac{1}{\overline{E}-(\varepsilon^{sp}_{\mathbf{K}/2+\mathbf{q}}+\varepsilon^{sp}_{\mathbf{K}/2-\mathbf{q}})}\langle\mathbf{q}|T_{2\mathrm{b}}(\overline{E})|\mathbf{k}\rangle, \tag{5}$$

where $\mathbf{k}$ and $\mathbf{k}'$ are the relative momenta of the two particles before and after the collision respectively, and $\mathbf{K}$ is the center-of-mass momentum. The energy of a single-particle state is ε_k^{sp}, where in the homogeneous limit $\varepsilon_k^{sp}=\hbar^2k^2/2m$. The total energy of the collision is $\bar{E}$ and includes a contribution from the center-of-mass momentum $\mathbf{K}$ that cancels the corresponding contribution from the single-particle energies. The two-body T matrix is, therefore, independent of $\mathbf{K}$, as it must be in free space.

The scattering event described here could be a single interaction $\langle\mathbf{k}'|V|\mathbf{k}\rangle$, or alternatively the particles may first make a transition to an intermediate state $|\mathbf{q}\rangle$ (weighted by an energy dependent denominator) before interacting again to emerge in state $|\mathbf{k}'\rangle$. The recursive nature of Eq. (5) sums all possible processes for which $|\mathbf{k}\rangle\rightarrow|\mathbf{k}'\rangle$. For many applications we only need the "on-shell" T matrix where both the energy and momentum conservation laws are fulfilled. However, it is also useful to consider the more general off-shell form shown above, where the momenta and energy may take arbitrary values.

It can be shown that, for interaction potentials of a finite range R_e, the T matrix is independent of the incoming and outgoing momenta (in the limit $kR_e, k'R_e \ll 1$) [19]. In the position representation this corresponds to an effective interaction that is proportional to $\delta(\mathbf{r}_1-\mathbf{r}_2)$. This contact potential approximation is of great utility in solving the GPE where the zero-momentum limit of the T matrix is used to describe particle interactions. In the three-dimensional case the T matrix elements at low energy and momenta are also independent of energy, leading to a constant coupling parameter in the GPE with form $g_{3\mathrm{D}}=4\pi\hbar^2 a_{3\mathrm{D}}/m$ in Eq. (1).

The contact potential approximation is still valid in one and two dimensions, but the T matrix at leading order now depends upon the energy of the collision, as will be shown in the following sections. Thus the scattering terms in the 2D GPE will be quite different from the three-dimensional case.

B. The many-body *T* matrix

The two-body T matrix describes collisions *in vacuo* in which the intermediate states are single particle in nature. However, in a Bose condensed gas collisions occur in the presence of a condensate and a many-body T matrix is needed to describe scattering processes. This is defined by the equation

$$\langle\mathbf{k}'|T_{\mathrm{MB}}(E)|\mathbf{k}\rangle=\langle\mathbf{k}'|V(\mathbf{r}_1-\mathbf{r}_2)|\mathbf{k}\rangle+\sum_{\mathbf{q}}\langle\mathbf{k}'|V(\mathbf{r}_1-\mathbf{r}_2)|\mathbf{q}\rangle \times\frac{(1+n_{\mathbf{K}/2+\mathbf{q}}+n_{\mathbf{K}/2-\mathbf{q}})}{E-(\varepsilon_{\mathbf{K}/2+\mathbf{q}}+\varepsilon_{\mathbf{K}/2-\mathbf{q}})}\langle\mathbf{q}|T_{\mathrm{MB}}(E)|\mathbf{k}\rangle, \tag{6}$$

where E is the interaction energy, and $\varepsilon_{\mathbf{q}}$ is the energy of a quasiparticle state of momentum $\mathbf{q}$, which is given by

$$\varepsilon_p=[(\varepsilon_p^{sp})^2+2\varepsilon_p^{sp}\mu]^{1/2}, \tag{7}$$

in the Bogoliubov approximation [21] for the case of the hard-sphere gas. The corrections included in this many-body T matrix over the two-body version are the occurrence of quasiparticle rather than particle energies for the intermediate states, and the Bose enhancement of scattering into these states. This latter effect results in the presence of population factors $n_{\mathbf{q}}$ in Eq. (6).

Formally, this many-body T matrix is included in the theory of a Bose condensed gas by considering the effect of the so-called anomalous average $\langle\hat{a}_i\hat{a}_j\rangle$ on the condensate evolution, where $\hat{a}_i$ is the noncondensate annihilation operator for state i. This term occurs when terms in the Hamiltonian of higher than quadratic order in $\hat{a}_i, \hat{a}_i^\dagger$ are taken into account [10,29]. We note that a generalization of the many-body T matrix that includes quasiparticle propagator factors for the intermediate states has been proposed [11], but the corrections this includes over and above Eq. (6) are of still higher order.

We note that the energies $\varepsilon_{\mathbf{q}}$ and E in T_{MB} are measured relative to the condensate, whereas the single-particle energies in $T_{2\mathrm{b}}$ are measured relative to the energy of a stationary particle. This means that for collisions between particles in the condensate we take the limit $E=0$ in T_{MB}, which corresponds to $\bar{E}=2\mu$ when measured relative to the same zero of energy as the two-body case [10]. For collisions between condensate atoms, we also take the zero-momentum limit $\mathbf{k},\mathbf{k}',\mathbf{K}=\mathbf{0}$. Interactions between two condensate atoms are, therefore, described by the matrix element $\langle\mathbf{0}|T_{\mathrm{MB}}(0)|\mathbf{0}\rangle$.

C. T_{MB} in terms of $T_{2\mathrm{b}}$, a simple argument

The Lippmann-Schwinger equation for the many-body T matrix is substantially more difficult to solve than the two-body equivalent due to the presence of quasiparticle energies and populations. In the limit of zero temperature we will show that the many-body T matrix can be approximated by an off-shell two-body T matrix evaluated at a negative energy. To see this we consider Eq. (6) for the matrix element $\langle\mathbf{0}|T_{\mathrm{MB}}(0)|\mathbf{0}\rangle$ at $T=0$ where the population terms vanish. Upon comparison with Eq. (5) it can be seen that the only difference between the equations for the two types of T matrix occurs in the energy denominators. Specifically, the quasiparticle energy spectrum appears in the many-body case, whereas the single-particle spectrum appears in the two-body case. Heuristically, if the dominant contribution to the intermediate states in a collision comes from states with energies of order μ or higher, we can proceed by replacing ε_k by $\varepsilon_k^{sp}+\mu$. This is the high-energy limit of the Bogoliubov spectrum of Eq. (7) and it contains a constant shift from the single-particle spectrum due to the mean-field effects of the condensate that do not vanish in the relevant momentum range $k\sim k_0$ for a contact potential interaction (where $\hbar^2k_0^2/2m\equiv\mu$). We are interested in the many-body T matrix at $E=0$, and thus the energy denominator in Eq. (6) becomes

$$\frac{1}{0-(\varepsilon_{\mathbf{K}/2+\mathbf{q}}+\varepsilon_{\mathbf{K}/2-\mathbf{q}})}\approx\frac{1}{0-(\varepsilon^{sp}_{\mathbf{K}/2+\mathbf{q}}+\mu+\varepsilon^{sp}_{\mathbf{K}/2-\mathbf{q}}+\mu)} =\frac{1}{-2\mu-(\varepsilon^{sp}_{\mathbf{K}/2+\mathbf{q}}+\varepsilon^{sp}_{\mathbf{K}/2-\mathbf{q}})}. \tag{8}$$

Comparison with Eq. (5) for the two-body T matrix shows that in this approximation

$$\langle \mathbf{0}|T_{\rm MB}(0)|\mathbf{0}\rangle = \langle \mathbf{0}|T_{\rm 2b}(-2\mu)|\mathbf{0}\rangle. \tag{9}$$

Interestingly, this shows that the effective two-body interaction energy is negative, meaning that the interaction strength is always real. We will see that this is important in the 1D case in the following section. In 3D the two-body T matrix is independent of energy to first order, but in both one and two dimensions it has a nontrivial energy dependence and, therefore, the effective interaction energy becomes important in these lower dimensions.

At first glance the result of Eq. (9) may appear counterintuitive since the energy of a collision between two condensate particles might be thought to be $+2\mu$, and certainly not negative. However, as we have shown, the many-body effects in the system lead to a shift in the quasiparticle energy spectrum and it is this that leads to a shifted effective energy entering the two-body T matrix. Stoof and co-workers [22,23] have also proposed that interactions in low-dimensional condensates can be described by the two-body T matrix evaluated at a negative energy (-2μ), the same result given by our heuristic argument above. In the following section we will use a more rigorous argument and find that this leads to somewhat better values for the effective interaction energy.

D. $T_{\rm MB}$ in terms of $T_{\rm 2b}$, a better argument

Having shown heuristically in the preceding section that the many-body T matrix can be approximated by a two-body T matrix evaluated at a negative energy, we will now present a more formal justification. This will lead to a slight modification to the magnitude of the energy used in the two-body T matrix, but the essential physics of the argument is unchanged.

From Eqs. (5) and (6), it is possible to derive an expression for the many-body T matrix solely in terms of the two-body T matrix [10]

$$\langle \mathbf{k}'|T_{\rm MB}(E)|\mathbf{k}\rangle = \langle \mathbf{k}'|T_{\rm 2b}(\overline{E})|\mathbf{k}\rangle + \langle \mathbf{k}'|T_{\rm corr}(E,\overline{E})|\mathbf{k}\rangle, \tag{10}$$

where

$$\langle \mathbf{k}'|T_{\rm corr}(E,\overline{E})|\mathbf{k}\rangle = \sum_{\mathbf{q}\neq 0} \frac{\langle \mathbf{k}'|T_{\rm 2b}(\overline{E})|\mathbf{q}\rangle (1+n_{\mathbf{K}/2+\mathbf{q}}+n_{\mathbf{K}/2-\mathbf{q}})\langle \mathbf{q}|T_{\rm MB}(E)|\mathbf{k}\rangle}{E-(\varepsilon_{\mathbf{K}/2+\mathbf{q}}+\varepsilon_{\mathbf{K}/2-\mathbf{q}})} - \sum_{\mathbf{q}} \frac{\langle \mathbf{k}'|T_{\rm 2b}(\overline{E})|\mathbf{q}\rangle\langle \mathbf{q}|T_{\rm MB}(E)|\mathbf{k}\rangle}{\overline{E}-(\varepsilon^{sp}_{\mathbf{K}/2+\mathbf{q}}+\varepsilon^{sp}_{\mathbf{K}/2-\mathbf{q}})}. \tag{11}$$

If we now assume that there is a value of $\overline{E}=\overline{E}^*$ for which $\langle \mathbf{k}'|T_{\rm MB}(E)|\mathbf{k}\rangle = \langle \mathbf{k}'|T_{\rm 2b}(\overline{E})|\mathbf{k}\rangle$, we can replace $T_{\rm MB}(E)$ on the right-hand side of Eq. (11) by $T_{\rm 2b}(\overline{E}^*)$. The value of $\overline{E}^*$ may then be found by solving for $\langle \mathbf{k}'|T_{\rm corr}(E,\overline{E}^*)|\mathbf{k}\rangle = 0$. We again take the limit of zero temperature, such that $n_{\mathbf{K}/2+\mathbf{q}}, n_{\mathbf{K}/2-\mathbf{q}}$ are zero, and for collisions between two atoms in the condensate we take the limit $\mathbf{k},\mathbf{k}',\mathbf{K},E=0$. The value of $\overline{E}^*$ is then given in D dimensions by the solution to

$$0=\int_0^\infty \frac{k^{(D-1)}}{-2\varepsilon_k}dk - \int_0^\infty \frac{k^{(D-1)}}{\overline{E}^*-\hbar^2k^2/m}dk. \tag{12}$$

Substituting the Bogoliubov dispersion relationship for the quasiparticle energies using Eq. (7) and carrying out the integrals in Eq. (12) we can obtain expressions for $\overline{E}^*$. We are then able to express the coupling parameter that occurs in the GPE in terms of the two-body T matrix evaluated at the energies $\overline{E}^*$. In two and three dimensions this leads to

$$g=\langle \mathbf{0}|T_{\rm MB}(0)|\mathbf{0}\rangle = \begin{cases} \langle \mathbf{0}|T_{\rm 2b}(-\mu)|\mathbf{0}\rangle & \text{in 2D,} \\ \langle \mathbf{0}|T_{\rm 2b}\left(-\dfrac{16}{\pi^2}\mu\right)|\mathbf{0}\rangle & \text{in 3D.} \end{cases} \tag{13}$$

However, in 1D the situation is more complicated because the first integral is logarithmically divergent. This case will be dealt with in Sec. IV where we show that the results obtained are consistent with known exact results. Prior to that however, we derive in the following section the form of the many-body T matrix in two dimensions and show that the effective interaction energy becomes important in this case.

E. The many-body T matrix in two dimensions

We consider the case of a 2D Bose gas with an interatomic potential $V(\rho)$ that is short range, parameterized by a length $a_{\rm 2D}$, and which admits no bound states. Specifically, we consider the case of a "hard-disk" potential such that $V(\rho)=\infty$ for $|\rho|\leqslant a_{\rm 2D}$ and $V(\rho)=0$ otherwise. In recent work [19] we have derived a full expression for the two-body T matrix for this potential in the general off-shell case. In the limit $ka_{\rm 2D}, k'a_{\rm 2D}\ll 1$ the result is

$$\langle \mathbf{k}'|T_{\rm 2b}(E)|\mathbf{k}\rangle = \frac{4\pi\hbar^2/m}{\pi i - 2\gamma_{\rm EM} - \ln(Ema_{\rm 2D}^2/8\hbar^2)}, \tag{14}$$

where $\gamma_{\rm EM}$ is the Euler-Mascheroni constant. The corrections are of order $(ka_{\rm 2D})^2$ and $(k_Ea_{\rm 2D})^2/\ln(k_Ea_{\rm 2D})$ or greater, where $k_E^2=Em/\hbar^2$. This result agrees with the work of Stoof [24], and also in the half-on-shell limit with the earlier work of Schick [14] and Bloom [25]. It is also of the same form as the results obtained by Fisher and Hohenberg [13] who considered the case of a Gaussian interatomic potential, implying that the result is general for most short-range repulsive potentials that may be parameterized by a length a_{2D}. In this low-momentum limit the T matrix is independent of both $\mathbf{k}$ and $\mathbf{k}'$ and thus it is still represented in position space by a δ-function effective interaction potential. The new feature compared to the 3D case is that the T matrix now depends on energy and, in particular, it vanishes as $E\to 0$. It is, therefore, crucial to take into account the many-body shift in the effective collision energy of two condensate atoms. This is now a self-consistent problem as many-body effects give rise to a nonzero coupling constant. In 3D the two-body T matrix is non-zero as $E\to 0$ and many-body effects can, therefore, be neglected at leading order for dilute gases.

From Eqs. (13) and (14) the many-body T matrix, and, therefore, the coupling parameter, in 2D is found to be

$$g_{2D}=\langle \mathbf{0}|T_{2b}(-\mu)|\mathbf{0}\rangle=-\frac{4\pi\hbar^2}{m}\frac{1}{\ln(\mu m a_{2D}^2/4\hbar^2)}, \tag{15}$$

where terms of order $1/[\ln(\mu m a_{2D}^2/4\hbar^2)]^2$ or greater have been neglected. Note that the evaluation of the two-body T matrix at a negative energy means that the imaginary component in Eq. (14) vanishes, and thus the many-body T matrix is real.

The parameter that appears in this description of the interparticle interactions is the two-dimensional scattering length a_{2D}, analogous to the 3D s-wave scattering length a_{3D} that parametrizes three-dimensional collisions in cold dilute gases. Reliable values of a_{3D} have been obtained in 3D by experimental measurements, and potentially a_{2D} could be measured in this manner. However, in their work on quasi-2D scattering processes Petrov and Shlyapnikov [18] also derived an expression for this parameter in terms of the three dimensional a_{3D}, and the confinement of the trap in the tight direction l_z,

$$a_{2D}=4\sqrt{\frac{\pi}{B}}l_z\exp\left(-\sqrt{\pi}\,\frac{l_z}{a_{3D}}\right), \tag{16}$$

where $B\approx 0.915$. Using this expression for a_{2D} in Eq. (15) we obtain the quasi-2D coupling parameter of Petrov and Shlyapnikov given in Eq. (4), and our approach, therefore, agrees with their results in the genuine 2D limit that is appropriate for $l_z \lesssim a_{3D}$.

Using this expression we are able to compare the strength of the 2D and quasi-2D coupling parameters with the parameter for quasi-2D gases with 3D scattering g'_{3D} described in Sec. II. These quantities are displayed as a function of trap width in the z dimension in Fig. 1. It can easily be seen that the size of coupling parameter appearing in the GPE for the genuine 2D case is over an order of magnitude greater than in the case where the scattering is essentially 3D in nature $(l_z/a_{3D}\gg 1)$. The magnitude of g_{2D} decreases slowly as l_z is decreased beyond $\sim a_{3D}/2$ (not shown on the graph) due to the size of a_{2D} determined from Eq. (16), and it matches the 3D scattering limit for $l_z/a_{3D}\gtrsim 10$.

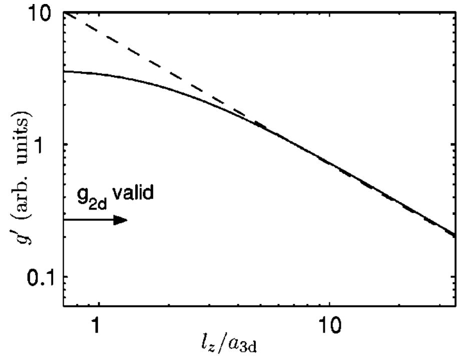

FIG. 1. Log-log graph of the effective 2D interparticle interaction strength as a function of confinement in the third dimension. The solid line shows g'_{q2D} that describes scattering in quasi-2D gases, taken from Ref. [18]. Our results for g_{2D} derived in this paper are consistent with this result and were derived for the region of validity shown. The dashed line shows g'_{3D} that is the expected limit at large l_z/a_{3D}.

IV. THE MANY-BODY *T* MATRIX IN ONE DIMENSION

Before we use the result in the preceding section to solve the two-dimensional GPE, we briefly consider the one-dimensional case. Our discussion in this section is not intended to be rigorous, but is meant instead to demonstrate the importance of including many-body effects, via the many-body T matrix, when considering the properties of a Bose gas in low dimensions.

A one-dimensional condensate is described by the Gross-Pitaevskii equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(x)+V_{\rm trap}(x)\psi(x)+N_0 g_{1D}|\psi(x)|^2\psi(x)=\mu\psi(x), \tag{17}$$

where g_{1D} is the one-dimensional coupling parameter. The use of the GPE necessarily assumes the existence of a condensate, which in one dimension implies that the system must be confined in a trap and, therefore, of a finite size. In a homogeneous 1D system a true condensate may not exist in the thermodynamic limit due to the density of states [6,26]. With this caveat in mind we will use the 1D case to illustrate the importance of the energy dependence of the many-body T matrix. Specifically we will consider the one-dimensional analogue of a hard-sphere gas for which exact results exist. This gas has an interatomic potential of the form

$$V(x)=\begin{cases}0 & \text{for } |x|>a_{1D},\\ \infty & \text{for } |x|\leqslant a_{1D}.\end{cases} \tag{18}$$

In a recent paper [19] we have used an inhomogeneous Schrödinger equation to obtain results for the general off-shell two-body T matrix for hard-sphere gases in one, two, and three dimensions. In one dimension in the limit of zero momenta the result is

$$\langle \mathbf{0}|T_{2b}(E)|\mathbf{0}\rangle = \begin{cases} -\dfrac{2}{a_{1D}}\left(\dfrac{\hbar}{\sqrt{m}} i\sqrt{E}a_{1D}+Ea_{1D}^2\right) & \text{for } E>0, \\ \dfrac{2}{a_{1D}}\left(\dfrac{\hbar}{\sqrt{m}}\sqrt{|E|}a_{1D}-Ea_{1D}^2\right) & \text{for } E<0. \end{cases} \tag{19}$$

As in the two-dimensional case, the T matrix is dependent on the collision energy even at lowest order, and so the shift to an effective interaction energy predicted in Sec. III C due to many-body effects is again important. Furthermore, in the case that $Ea_{1D}^2 \ll 1$, the leading-order term in the T matrix in 1D is imaginary if E is positive. The shift to a *negative* effective interaction energy is, therefore, critical in this one-dimensional case.

In order to obtain the many-body T matrix in terms of this two-body T matrix we must solve Eq. (12). As noted earlier the first integral in this equation is logarithmically divergent in 1D. Physically this arises from the fact that a true condensate does not exist in a homogeneous 1D system. Instead of a single quantum level with a macroscopic occupation (as occurs in a true condensate), in 1D there is a band of low-energy levels that all have large occupations. The same methods as discussed above may still be used in the 1D case, however, provided that we now define the "condensate" as a band of levels in momentum space up to a cutoff at $k_{\max}$, such that the 1D "condensate density" $n_0 \equiv \Sigma_{k_i<k_{\max}} n_i$ satisfies $n_0 \sim n$ (as for a true condensate). Using this definition, the lower limit of the first integral in Eq. (12) should then be $k_{\max}$ and the divergence is removed. This approach is justified for a confined 1D system since we may assume the existence of a condensate due to the modification to the density of states that also removes the divergence.

A reasonable value for $k_{\max}$ may be obtained from the momentum distribution for a system of impenetrable bosons. Such a distribution is discussed in Ref. [27]. We will define $k_{\max}$ by the criterion that $N(k>k_{\max})<1$, which gives $k_{\max} \approx 0.25\pi n_0$ [27]. Using this as the cutoff in Eq. (12), a solution may be found for $\bar{E}^*$ by making the ansatz that $\bar{E}^* = -C\mu$, where C is a constant. For the hard-sphere case considered here the ansatz is satisfied when C is the solution to

$$\tanh^{-1}\left[\frac{2}{\sqrt{(0.25\pi)^2/4C+4}}\right]=\frac{\pi^2}{C}. \tag{20}$$

This can be solved numerically to give $C\approx 3.4$. The expression for the many-body T matrix in 1D to leading order is then

$$g_{1D}=\langle \mathbf{0}|T_{2b}(-C\mu)|\mathbf{0}\rangle=\sqrt{4C\hbar^2\mu/m}. \tag{21}$$

We now consider a homogeneous 1D Bose gas, using the above definition of the condensate. When this system is in the ground state the contributions in the GPE from the curvature of the wave function and the trapping potential both vanish, and, therefore,

$$\mu_{1D}=n_0 g_{1D}=\frac{4C\hbar^2}{m}n_0^2. \tag{22}$$

This form differs from that found in 3D where $\mu \propto n_0$ because of the dependence of g_{1D} on the chemical potential.

This result can also be explained heuristically, as the extra curvature introduced into the wave function by the presence of the other atoms. If we consider a many-body wave function that scatters off a hard-sphere potential of range a_{1D}, then in the limit of zero energy, we need to solve $d^2\psi/dx^2 = 0$. We impose the boundary conditions that $\psi(x)=0$ at $x = a_{1D}$ and $\psi(x)$ approaches an asymptotic value χ at large x. Since ψ is a many particle wave function, the distance at which it must arrive at its asymptotic value will be of the order of the interparticle spacing l_0. This gives a solution to the scattering problem of

$$\psi(x)=\frac{\chi}{l_0-a_{1D}}(x-a_{1D}) \quad \text{for } a_{1D}<x \lesssim l_0. \tag{23}$$

The extra energy caused by the curvature of the wave function in this region is then

$$-\frac{\hbar^2}{2m}\int_a^{l_0}|\nabla\psi(x)|^2 dx \approx -\frac{\hbar^2|\chi|^2}{2ml_0}. \tag{24}$$

And since $l_0 = 1/n_0$ and $|\chi|^2 = n_0$ we have that the interparticle interactions make a contribution to the energy that scales as n_0^2. The same result may be derived from an even simpler argument that considers each particle to be confined in an infinite square well of length $\sim 1/n$ by its nearest neighbors.

The exact result for μ in such a 1D gas has long been known. In solving the system of 1D interacting bosons by demonstrating equivalence with a gas of 1D noninteracting fermions, Girardeau [28] showed that in the strong coupling limit (appropriate to the hard-sphere potential considered above)

$$\mu=\frac{\pi^2}{2}\frac{\hbar^2}{m}n^2. \tag{25}$$

Our result, therefore, shows the correct dependence on n^2, but disagrees on the numerical factor. The disagreement is due to the fact that, as previously mentioned, in a homogeneous 1D system there can never be a true Bose condensate, so significant corrections to the GPE can be expected. The additional uncertainty in the choice of $k_{\max}$ also introduces a source for discrepancy in the numerical factor. However, the agreement with the dependence on n^2 indicates that the energy dependent many-body T matrix appears to deal with the interactions correctly. This is interesting because it means that an intrinsically many-body effect, namely, particle confinement by neighbors, can be modeled by an off-shell two-body T matrix evaluated at a shifted effective interaction energy, which is the essential argument of this paper. This suggests that the method will have at least qualitatively the correct density dependence in the strong coupling limit. A more detailed investigation of this approach in the 1D case will be the subject of a further paper. Although our discussion in this section has been qualitative due to the lack of a true condensate in a 1D homogeneous system even at zero temperature, in a trapped 1D system it is possible for a true condensate to form. We expect, therefore, that semiquantitative results outside the normal BEC regime of validity can be achieved using this method. In two dimensions a true condensate can be formed, even in a homogeneous system, at $T=0$ and so we expect our 2D results in this paper to be quantitatively correct.

V. SCATTERING IN INHOMOGENEOUS GASES

In the previous two sections we presented expressions for the many-body T matrix in one and two dimensions in terms of the two-body T matrix evaluated at shifted effective interaction energies. However, the results obtained are strictly only valid for homogeneous systems since we have not accounted for any modifications of the scattering wave functions due to the presence of a confining potential. We consider here the case of a gas confined tightly in one or two dimensions (in order to reduce the dimensionality, as discussed in Sec. II) and weakly in the remaining dimensions on a length scale $l_{\rm trap}$.

Provided that the range of the interatomic potential R_e is much smaller than $l_{\rm trap}$ then the scattering will be locally homogeneous and we can replace μ where it occurs in Eqs. (15) and (21) by the homogeneous expression $\mu=n_0 g$. This is a form of local-density approximation and, as the density of an inhomogeneous gas is spatially dependent, this leads to spatially dependent coupling parameters. Recognizing that $n_0(\mathbf{r})=N_0|\psi(\mathbf{r})|^2$ the coupling parameters in one and two dimensions are

$$g_{\rm 1D}=\frac{4C\hbar^2 N_0}{m}|\psi(x)|^2, \tag{26}$$

$$g_{\rm 2D}=-\frac{4\pi\hbar^2}{m}[\ln(N_0\pi|\psi(\rho)|^2 a_{\rm 2D}^2)]^{-1} + o\left(\frac{\ln[\ln(n_0 a_{\rm 2D}^2)]}{\ln(n_0 a_{\rm 2D}^2)}\right). \tag{27}$$

These results agree with the work of Kolomeisky and coworkers [1,2] who obtained similar expressions based on a renormalization-group analysis. Such density dependent coupling parameters are also expected from the results of density-functional theory [16] that predict that the energy of the system is a functional of the density only. The same results may be obtained from mean-field theory by incorporating the spatially dependent anomalous average $\langle \hat{a}_i\hat{a}_j\rangle$ into the system of equations governing a condensate and solving self-consistently [29].

VI. 2D SOLUTIONS OF THE NONLINEAR SCHRÖDINGER EQUATION

In this section we present solutions of the GPE for a trapped two-dimensional gas. The solutions are found for a given μ by propagating the time-dependent GPE forward in imaginary time from an initial approximate solution to obtain both the ground-state wave function and the nonlinearity $g_{\rm 2D}N_0$. As mentioned in the preceding section the coupling parameter in two dimensions in a trap is spatially dependent, having a logarithmic dependency on the density. However, since in two dimensions the spatial dependence is merely logarithmic it will have little effect on the solutions of the GPE, except at the very edges of the trap where the wave function vanishes. We, therefore, use the homogeneous system coupling parameter of Eq. (15), which will illustrate the features of most interest.

Using the expression for the 2D coupling parameter found in Eq. (15) we solve the two-dimensional time-independent Gross-Pitaevskii equation for a 2D Bose condensate in a trap with $V_{\rm trap}(\rho)=\frac{1}{2}m\omega^2\rho^2$. We can make the GPE dimensionless, scaling all energies by $\hbar\omega$ and all lengths by $l_\rho=\sqrt{\hbar/(2m\omega)}$, giving

$$-\tilde{\nabla}^2\psi(\tilde{\rho})+\tilde{V}_{\rm trap}(\tilde{\rho})\psi(\tilde{\rho})+N_0\tilde{g}_{\rm 2D}(\tilde{\mu})|\psi(\tilde{\rho})|^2\psi(\tilde{\rho})=\tilde{\mu}\psi(\tilde{\rho}), \tag{28}$$

where $\tilde{g}_{\rm 2D}(\tilde{\mu})=-8\pi/\ln(\tilde{\mu}\tilde{a}_{\rm 2D}^2/8)$ and $\tilde{V}_{\rm trap}(\tilde{\rho})=\frac{1}{4}\tilde{\rho}^2$. Note that the quantity $\tilde{\mu}\tilde{a}_{\rm 2D}^2$ is small compared to unity (or the earlier expansion of the T matrix elements fails) and, therefore, the interaction is repulsive. As shown earlier, for the range of μ and N_0 that we consider here, we find that Eq. (15) leads to a value for $\tilde{g}_{\rm 2D}(\tilde{\mu})$ which is more than an order of magnitude greater than the equivalent value for a quasi-2D gas in which the particle interactions are effectively 3D in nature. Thus the nonlinear term in the GPE is more significant in two dimensions than in the 3D case.

A. Ground-state solutions

Figure 2 presents sample solutions for the ground state of a 2D BEC in a trap for differing values of $\tilde{\mu}$. To illustrate the physical quantities involved we give numbers for a gas in a trap of $\omega=2\pi\times100$ Hz and with a scattering parameter given by $a_{\rm 2D}=6$ nm. This is close to the 3D s-wave scattering length $a_{\rm 3D}$ found for ^{87}Rb, and, therefore, from Eq. (16) this corresponds to a situation where $l_z\approx a_{\rm 3D}$. We see that at low N_0 the solution is approximately the Gaussian wave function that is expected for the noninteracting case. At higher N_0 the Thomas-Fermi approximation found by neglecting the contribution to the GPE from the kinetic energy term as compared to the interaction and trapping terms is expected to be a good description. In two dimensions the Thomas-Fermi approximation gives a density profile in the form of an inverted parabola

$$|\psi(\tilde{\rho})_{TF}|^2=-\frac{\ln(\tilde{\mu}\tilde{a}_{\rm 2D}^2/8)}{N_0 8\pi}[\tilde{\mu}-\tilde{V}_{\rm trap}(\tilde{\rho})]\theta(\tilde{\mu}-\tilde{V}_{\rm trap}(\tilde{\rho})), \tag{29}$$

where $\theta(x)$ is the step function. At higher N_0 the solutions shown are generally very well approximated by the Thomas-Fermi form, except at the boundary region of the condensate. Indeed we find that the Thomas-Fermi approximation works

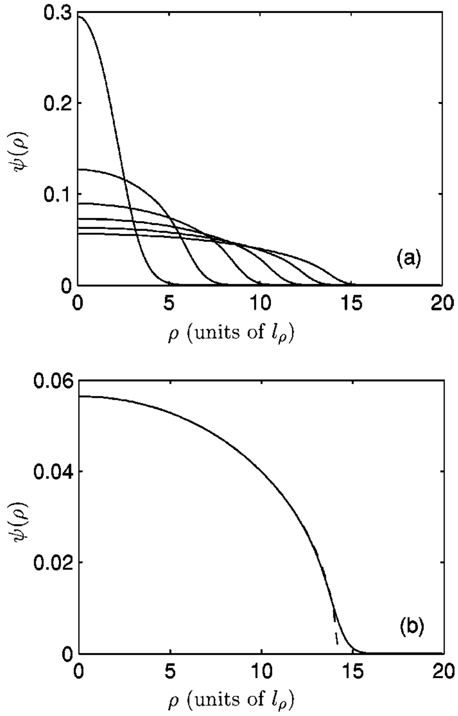

FIG. 2. (a) Ground-state 2D GPE solutions in an axisymmetric trap for $\mu=2$, 10, 20, 30, 40, and $50\hbar\omega$. $\psi(\tilde{\rho})$ is normalized to unity, and populations given assume parameters $\omega=2\pi \times 100$ Hz, $a_{2D}=6$ nm. (b) Comparison of GPE solution for $\tilde{\mu}=50$ (solid line) with Thomas-Fermi approximation (dashed line).

well for the 2D case, due to the high strength of the scattering, as expected from the dimensionless GPE (28). For the nonlinear term to dominate the kinetic-energy term requires that $N_0^{2D} \gg -\ln(\tilde{\mu}\tilde{a}_{2D}^2/8)$ (where $\tilde{\mu}\sim 10$–100), while in the three-dimensional case we require $N_0^{3D} \gg 1/\tilde{a}_{3D}$. Putting typical numbers into this using our parameters we get $N_0^{2D} \gg 10$, while $N_0^{3D} \gg 100$, and thus the Thomas-Fermi regime is reached in 2D with about an order of magnitude fewer atoms than is the case for 3D. As confirmation of this, the Thomas-Fermi approximation for the number of condensate atoms is $N_0 = -\mu^2 \ln(\mu m a_{2D}^2/4\hbar^2)/(2\hbar\omega)^2$ and is found to be in agreement with the numerical results to within one percent once N_0 was greater than 300.

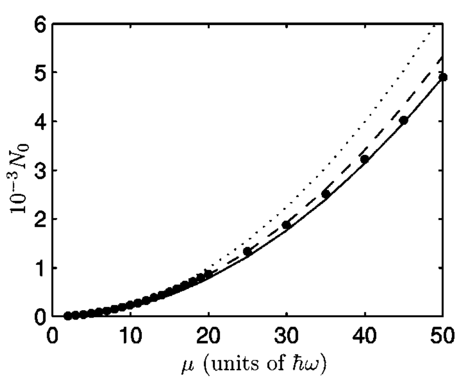

FIG. 3. N_0 vs μ for a 2D Bose gas. The dots represent solutions of the GPE with the full energy dependent interaction given in Eq. (15). The lines are results which assume a constant (independent of μ) coupling parameter g_{2D}. The three constant values of g_{2D} correspond to Eq. (15) evaluated at μ equal to $6\hbar\omega$ (dotted), $25\hbar\omega$ (dashed), and $50\hbar\omega$ (solid).

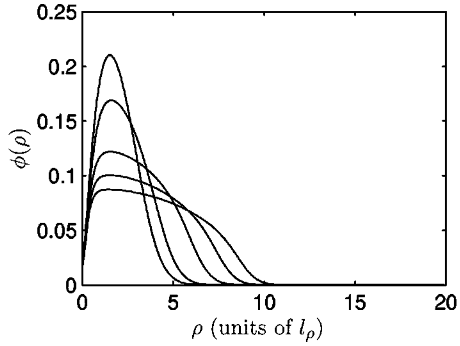

FIG. 4. Sample 2D GPE solutions for a vortex state with $\kappa=1$ and for values of μ of 3, 5, 10, 15, and $20\hbar\omega$. $\phi(\rho)$ is normalized to unity, and populations given assume parameters $\omega=2\pi\times 100$ Hz, $a_{2D}=6$ nm.

In some previous papers [30] the GPE has been solved with g_{2D} approximated by an energy independent constant. This is appropriate to the case where the scattering is three dimensional, but not to the fully 2D case where g_{2D} depends on μ. We find here that the interaction strength given by Eq. (15) increases by about 50% as μ rises from $2\hbar\omega$ to $50\hbar\omega$. Figure 3 shows the possible errors that can arise from making the assumption of a constant coupling parameter. Each line plotted on this graph assumes a constant g_{2D}, the strength of which is chosen to agree with Eq. (15) at a certain value of the chemical potential μ_*. The figure shows that results obtained with a constant $g_{2D}(\mu_*)$ will introduce systematic errors when μ is significantly different from μ_*. In the Thomas-Fermi approximation the relative error incurred in a measurement of N_0 assuming a constant $g_{2D}(\mu_*)$ is given by $\ln(\mu_*/\mu)/\ln(\tilde{\mu}\tilde{a}_{2D}^2/8)$.

B. Vortex state solutions

The 2D GPE can also be solved for the case of a two-dimensional condensate in a symmetric trap containing a vortex at the center by looking for solutions of the form

$$\psi(\rho)=\phi(|\rho|)e^{i\kappa\theta}, \tag{30}$$

where θ is the angle around the vortex core, and the phase wraps around by $2\pi\kappa$, where κ is an integer, as the range of θ is traversed. This adds an "effective potential" to the GPE and we now solve

$$-\frac{\hbar^2}{2m}\nabla^2\phi(\rho)+\frac{\hbar^2\kappa^2}{2mr^2}+V_{\rm trap}(\rho)\phi(\rho) + N_0 g_{2D}(\mu)|\phi(r)|^2\phi(\rho)=\mu\phi(\rho). \tag{31}$$

Solutions of these vortex states are shown in Fig. 4.

Such vortex states, which carry an angular momentum $L_z=N\hbar\kappa$, can be made energetically favorable by rotating

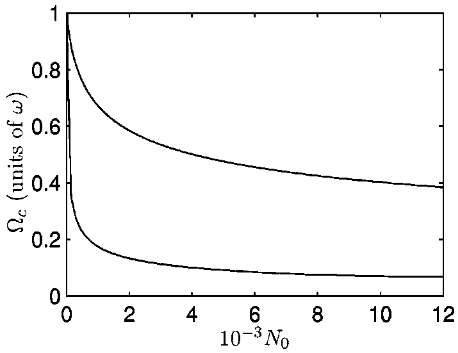

FIG. 5. The critical frequency Ω_c at which vortex formation becomes energetically favorable in 2D (lower) and 3D (upper) gases as a function of condensate population N_0. Results obtained using $a_{3D}=a_{2D}$.

the trap with sufficiently high frequency Ω. The energy functional for a wave function in the nonrotating frame is

$$E[\psi]=\int d\rho\left[\frac{\hbar^2}{2m}|\nabla\psi(\rho)|^2+V_{\text{trap}}(\rho)|\psi(\rho)|^2+\frac{g_{2D}(\mu)}{2}|\psi(\rho)|^4\right]. \tag{32}$$

The point at which $E[\psi_{\kappa=1}]-\Omega L_z$ becomes less than $E[\psi_{\kappa=0}]$ is known as the thermodynamic critical frequency, and this is plotted in Fig. 5 for both 2D and (genuine) 3D condensates. The three-dimensional results were calculated from solutions of the 3D GPE, given by Eq. (1), with a_{3D} taken to be equal to a_{2D} the scattering length used for the 2D results. Creation of a vortex in the center of the trap comes at the cost of increasing the contributions from both the kinetic energy and the trapping potential terms in the GPE, although the nonlinear contribution is reduced by virtue of a lower central density. Stronger nonlinear systems are, therefore, more susceptible to vortex creation, and this becomes energetically favorable at much lower frequencies in 2D than in 3D for the same value of the scattering length a, as seen in Fig. 5.

VII. DISCUSSION AND CONCLUSIONS

In this paper we have found expressions for the many-body T matrix in a dilute Bose gas describing the collisions occurring in a condensate in terms of the simpler two-body T matrix. We have shown that many-body effects of the condensate mean field on such collisions may be incorporated by a shift in the effective interaction energy of a two-body collision, and that such an approach leads to the same results obtained from renormalization-group techniques [1,2].

The fundamental difference to the three-dimensional case is that the first-order term in the T matrix in lower dimensions is dependent not only on the scattering length, but also on the energies of the colliding particles. The coupling parameter in one and two dimensions is, therefore, dependent on the chemical potential of the condensate.

The energy dependent form of the many-body T matrix in 2D found here can be used to obtain a self-consistent form for the 2D Gross-Pitaevskii equation. We have presented sample solutions and have shown that the importance of the nonlinear term is magnified in 2D (as compared to the 3D case) due to the size of the coupling constant in two dimensions. The Thomas-Fermi approximation is, therefore, valid at a much lower number of atoms than in the 3D case, approximately an order of magnitude lower in the case considered here. The critical frequency of vortex formation is also found to decrease with condensate occupation much faster in 2D than in 3D, and so vortices should be comparatively easier to form in 2D.

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