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Phase collapse and excitations in Bose-Einstein condensates

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A study of fragmented condensates is presented to elucidate the interplay between excitations and the collapse of relative phases within single condensates. Implications for experimental observation of interference between weakly coupled condensates are discussed, and means for computation are suggested and applied to a one-dimensional model system. [S1050-2947(98)06207-6]

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I. INTRODUCTION

Bose-Einstein condensation has been observed in trapped dilute gases of rubidium [1], sodium [2], and lithium [3] atoms. The experimental developments have been impressive, and a number of fundamental properties of these many-body systems can be investigated due to the ideal possibilities for manipulation and monitoring of the condensates. Theoretically they are well treated by the simplest approximate theories of many-body physics, and they are therefore ideal for investigating fundamental and generic properties of simple many-body systems. Be it debatable or not whether these studies contribute to the well-established domain of many-body physics, they will certainly serve to spread the techniques and experience of this field into other domains of physics such as atomic physics and quantum optics.

In Sec. II of this paper, we briefly review the derivations of the Gross-Pitaevskii equation. In Sec. III, we address the issue of phase collapse, and we show the explicit agreement between ''particle'' and ''quantum field'' approaches published independently in the literature [4–7]. In Sec. IV we analyze the excitation spectrum of a Bose-Einstein condensate. Excitations and condensate phase collapse are related, and in Sec. V, we consider the collapse of the relative phase between components of a fragmented condensate. Spatial interference has been observed when such fragments are brought together [8], and our work suggests an element to the quantitative analysis of this interference, in particular an analysis of the phase synchronization induced by exchange of particles between the fragments. The analysis is supplemented by a numerical example in Sec. VI.

II. CONDENSATE GROUND STATE

We consider Bose-Einstein condensation of a trapped gas of atoms. The atoms interact by elastic collisions and we assume that the low kinetic energies of the atoms and the short range of their interaction permit the replacement of the potential by a δ function, $V_{int}(\vec{r})\rightarrow g\,\delta(\vec{r})=4\pi\hbar^2 a_{sc}/M\,\delta(\vec{r})$, where a_{sc} is the s-wave scattering length for the binary atomic collision process, and M is the atomic mass.

In the formalism of second quantization, one introduces field operators $\hat{\Psi}(\vec{r})$, $\hat{\Psi}(\vec{r}\,')^\dagger$, which annihilate and create atoms at $\vec{r}$ and $\vec{r}\,'$, respectively. They fulfill the bosonic commutation relations $[\hat{\Psi}(\vec{r}),\hat{\Psi}(\vec{r}\,')^\dagger]=\delta(\vec{r}-\vec{r}\,')$, and, using these operators, the (grand-canonical) Hamiltonian for the system can be written

$$H=\int d^3\vec{r}\,\hat{\Psi}(\vec{r})^\dagger\left[-\frac{\hbar^2}{2M}\nabla^2+V_{ext}(\vec{r})+\frac{1}{2}g\hat{\Psi}(\vec{r})^\dagger\hat{\Psi}(\vec{r})\right]\hat{\Psi}(\vec{r}). \tag{1}$$

The Hartree ansatz for the ground-state wave function of N atoms can be written in terms of the field creation operator applied N times on the vacuum state,

$$|\Psi\rangle=\frac{1}{\sqrt{N!}}\left[\int d^3\vec{r}\,\psi(\vec{r})\hat{\Psi}(\vec{r})^\dagger\right]^N|0\rangle. \tag{2}$$

This expression is analogous to the one for number states in quantum optics, and one finds that the mode function $\psi(\vec{r})$, i.e., the single-particle wave function, minimizing the expectation value of the Hamiltonian (1) is the solution of the Hartree equation:

$$\left[-\frac{\hbar^2}{2M}\nabla^2+V_{ext}(\vec{r})+(N-1)g|\psi(\vec{r})|^2\right]\psi(\vec{r})=\mu\psi(\vec{r}), \tag{3}$$

where μ is the single-particle energy.

The Hamiltonian (1) commutes with the total number operator, the particle number is conserved, and the exact eigenstates for the problem are number eigenstates. Still, it may be beneficial to carry out calculations where one relaxes this condition and instead considers eigenstates of the field operators. This also applies in quantum optics where such states correspond to classical fields. Classical fields replace operators by c numbers, and this can be formulated more rigorously by assuming a state of the system that is an eigenstate of the field annihilation operators, known as the Glauber coherent state in quantum optics.

Let $|\Psi_N\rangle$ denote the eigenstate of field annihilation operators

$$\hat{\Psi}(\vec{r})|\Psi_N\rangle=\Psi_N(\vec{r})|\Psi_N\rangle, \tag{4}$$

with an average number of particles $\int d^3\vec{r}\langle\hat{\Psi}(\vec{r})^\dagger\hat{\Psi}(\vec{r})\rangle=\int d^3\vec{r}\,\Psi_N(\vec{r})^*\Psi_N(\vec{r})=N$. Minimizing the expectation value of the Hamiltonian with respect to variations of the function $\Psi_N(\vec{r})$, one finds that $\Psi_N(\vec{r}) = \sqrt{N}\psi(\vec{r})$, where $\psi(\vec{r})$ solves the equation

$$\left[-\frac{\hbar^2}{2M}\nabla^2 + V_{ext}(\vec{r}) + Ng|\psi(\vec{r})|^2 \right]\psi(\vec{r}) = \mu\psi(\vec{r}). \tag{5}$$

This equation, called the Gross-Pitaevskii equation, is identical to the Hartree equation (3), except for the insignificant difference between N and $N-1$ in the nonlinear term. The state vector $|\Psi_N\rangle$ obeying Eq. (4), however, is very different from the number state (2), since it has a fluctuating number of atoms and it has a nonvanishing expectation value of the field operator $\langle \Psi_N|\hat{\Psi}(\vec{r})|\Psi_N\rangle = \Psi_N(\vec{r})$. Although these properties have a negligible influence on the determination of μ and, e.g., the particle density $N|\psi(\vec{r})|^2$, they are important for the way we describe interference phenomena of condensates.

We can solve Eqs. (3) and (5) by a propagation in imaginary time τ, replacing $\mu\psi(\vec{r})$ by $-(\partial/\partial\tau)\psi(\vec{r},\tau)$: The wave function norm in the long-time limit decays with the rate μ, and the renormalized wave function is the desired solution $\psi(\vec{r})$. In the Thomas-Fermi approximation one neglects the kinetic-energy operator in Eqs. (3) and (5) and divides by the wave function to obtain

$$|\psi^{TF}(\vec{r})|^2 = [\mu - V_{ext}(\vec{r})]/(Ng) \tag{6}$$

for the single-particle density. This expression is applied only when the right-hand side is positive, and μ is determined by the normalization of $\psi^{TF}(\vec{r})$ to unity.

For later convenience we present the results for harmonic-oscillator trapping potentials in one, two, and three dimensions,

$$\mu^{TF}(1\mathrm{D}) = \left[\left(\frac{M\omega^2}{2} \right)^{1/2} \frac{3}{4} Ng \right]^{2/3},$$

$$\mu^{TF}(2\mathrm{D}) = \left[\left(\frac{M\overline{\omega}^2}{2} \right) \frac{2}{\pi} Ng \right]^{1/2},$$

$$\mu^{TF}(3\mathrm{D}) = \left[\left(\frac{M\overline{\omega}^2}{2} \right)^{3/2} \frac{15}{8\pi} Ng \right]^{2/5}, \tag{7}$$

where ω is the oscillator frequency $[\overline{\omega} = (\omega_x\omega_y)^{1/2}$ in 2D and $\overline{\omega} = (\omega_x\omega_y\omega_z)^{1/3}$ in 3D].

III. PHASE FLUCTUATIONS OF THE BOSE-EINSTEIN CONDENSATE

A. Interference, mean fields, and number states

Two condensates, A and B, that overlap at a position-sensitive detector give rise to an interference pattern. Such interferences have been observed experimentally [8], and they follow easily from theory if one assumes that both condensates are in annihilation operator eigenstates: The position-dependent counts at the detector positions $\vec{r}_D$ are proportional to the local number operators, $\langle [\Psi_A^\dagger(\vec{r}_D) + \Psi_B^\dagger(\vec{r}_D)][\Psi_A(\vec{r}_D) + \Psi_B(\vec{r}_D)]\rangle$ containing both direct terms, proportional to the respective condensate densities, and cross terms like $\langle \Psi_A^\dagger(\vec{r}_D)\Psi_B(\vec{r}_D)\rangle$, which are nonvanishing in the coherent-state case; and if the atoms in the condensates have different momenta $k\vec{e}_x$ and $-k\vec{e}_x$, an interference pattern at $\cos(2kx+\gamma)$ appears, where γ accounts for the phase difference between the two condensates.

If both condensates are in number states, the cross terms vanish, but an interference pattern builds up anyway [9]: After the detection of the first atom at a random position, we cannot tell from which condensate the atom was absorbed by the detector. The state vector after the detection is therefore a superposition of the ones where the atom was taken from one and from the other condensate, and in this state the cross terms do not vanish anymore. When more and more atoms are detected, a stable interference pattern builds up that is indistinguishable from the one obtained from condensates in coherent states. For further discussions of these interferences see [10,11].

The interference pattern appears with a random positioning of the fringes, which is determined either by the random relative phase of the coherent-state fields $\Psi(\vec{r}) = e^{i\gamma}|\Psi(\vec{r})|$ or by the first few random detection events (particle picture). If the intereference pattern is determined at $t=0$, and the condensates are left for their own free evolution for a certain time, what is the probability that a shift in the interference pattern has occurred if detection is recommenced? Both the ''particle'' and the ''quantum field'' analysis of this problem have been presented in the literature, and we shall briefly review both and show that they produce identical results.

In addition to the discussion of phase collapse, one must perform a calculation with the correct matter wave propagation, since the momentum dispersion of the condensates may wash out interferences as well. This effect adds to the experimental difficulty of investigating the phase diffusion of condensates. Here we merely recall that interference fringes *have been observed*, and in fact, a more detailed theoretical analysis including the momentum dispersion of the condensates has shown good agreement with the experimental findings [12].

B. Particle picture of phase diffusion

A number state has no phase, but due to back action a phase-sensitive measurement will introduce a dispersion in the number of atoms remaining in the condensate and make the equivalent of a phase appear. If the measurement is done by interference with the N_{st} atoms of another larger condensate, the entangled state of both condensates after n atomic detections can be written $\Sigma_{k=0}^{n} c_k|N-k\rangle \otimes |N_{st}-(n-k)\rangle$, in a suggestive quantum optics notation [10]. Assuming that the big condensate has a chemical potential that does not vary with the number of atoms, the amplitudes c_k of the entangled state acquire different phase factors $\exp(-i\mu_{N-k}t/\hbar)$, and the interference of the terms in the sum is modified when $\Delta\mu t/\hbar \sim 1$, where $\Delta\mu$ denotes the variation in μ over the particle number distribution. In Refs. [6,7], the number of atoms in the condensate is assumed to fluctuate following a Poisson distribution. Estimating thus the variation in chemical potential by $\sqrt{N}\partial\mu/\partial N$, one obtains the ''collapse'' time τ_c,

$$\tau_c = \hbar / (\sqrt{N} \partial \mu / \partial N). \tag{8}$$

For the harmonic-oscillator trap in 1D, 2D, and 3D, we get within the Thomas-Fermi approximation (7)

$$h/\tau^{TF}(1\text{D}) = \left[\left(\frac{M\omega^2}{2} \right)^{1/2} \frac{3}{4} g \right]^{2/3} \frac{2}{3} N^{1/6},$$

$$h/\tau^{TF}(2\text{D}) = \left[\left(\frac{M\overline{\omega}^2}{2} \right) \frac{2}{\pi} g \right]^{1/2} \frac{1}{2} N^{0},$$

$$h/\tau^{TF}(3\text{D}) = \left[\left(\frac{M\overline{\omega}^2}{2} \right)^{3/2} \frac{15}{8\pi} g \right]^{2/5} \frac{2}{5} N^{-1/10}, \tag{9}$$

where typical experimental values inserted in the 3D expression yield a time scale of 100 ms.

C. Quantum field picture of phase collapse

Although the state vector is assumed to be an eigenstate of the field annihilation operators, there are quantum fluctuations around their eigenvalues, following, for example, from the field commutator relations. A standard procedure, applied also in quantum optics, is to expand the field operators as a mean-field (c-number) and a ‘‘noise’’ operator part

$$\hat{\Psi}(\vec{r}) = \sqrt{N}\psi(\vec{r}) + \delta\hat{\Psi}(\vec{r}). \tag{10}$$

After elimination of a simple rotation, the c-number part represents a static component with no phase or number fluctuations associated with it. Fluctuations are described by the noise part, and, for any location $\vec{r}$ in space, the atomic field can be pictorially described as a point $\psi(\vec{r})$ in the complex plane with an uncertainty cloud around it. In the annihilation operator eigenstate at $t=0$, this cloud is circular, and its subsequent dynamics yields the phase collapse of the atomic field.

The requirement that the Hamiltonian (1) have no terms linear in the noise operators is fulfilled if $\psi(\vec{r})$ solves the Gross-Pitaevskii equation (5). Assuming that the noise terms are smaller than the mean-field terms, we omit contributions to the Hamiltonian (1) of order higher than 2 in noise operators, leaving us with the quantum noise contribution to the energy of the system:

$$\begin{aligned} \delta H = \int d^3\vec{r} [& \delta\hat{\Psi}(\vec{r})^\dagger (L + 2Ng|\psi(\vec{r})|^2) \delta\hat{\Psi}(\vec{r}) \\ & + \tfrac{1}{2} Ng\psi(\vec{r})^2 \delta\hat{\Psi}(\vec{r})^\dagger \delta\hat{\Psi}(\vec{r})^\dagger \\ & + \tfrac{1}{2} Ng\psi^*(\vec{r})^2 \delta\hat{\Psi}(\vec{r}) \delta\hat{\Psi}(\vec{r})], \end{aligned} \tag{11}$$

where $L = -(\hbar^2/2M)\nabla^2 + V_{ext}(\vec{r}) - \mu$.

If we introduce the the Bogoliubov transformation,

$$\delta\hat{\Psi}(\vec{r}) = \sum_k [U_k(\vec{r})\hat{g}_k - V_k^*(\vec{r})\hat{g}_k^\dagger], \tag{12}$$

and the canonically conjugated ‘‘position’’ and ‘‘momentum’’ operators

$$\hat{Q} = i \int d^3\vec{r} \phi(\vec{r}) (\delta\hat{\Psi}(\vec{r}) - \delta\hat{\Psi}(\vec{r})^\dagger),$$

$$\hat{P} = \int d^3\vec{r} \psi(\vec{r}) [\delta\hat{\Psi}(\vec{r}) + \delta\hat{\Psi}(\vec{r})^\dagger], \tag{13}$$

the Hamiltonian (11) takes the canonical form [4,5],

$$\delta H = \alpha \hat{P}^2/2 + \sum_{k\neq 0} \hbar\omega_k g_k^\dagger g_k, \tag{14}$$

where $[g_k, g_{k'}^\dagger] = \delta_{kk'}$, provided the functions $U_k(r), V_k(r)$ fulfill the coupled Bogoliubov–de Gennes equations, discussed in Sec. IV A below.

The function $\phi(\vec{r})$ satisfies [4,5] the equation

$$[L + 3Ng|\psi(\vec{r})|^2]\phi(\vec{r}) = \alpha\psi(\vec{r}) \tag{15}$$

and the constraint

$$2\int d^3\vec{r} \phi(\vec{r})\psi(\vec{r}) = 1, \tag{16}$$

which determine the value of α in Eq. (14).

We can solve Eq. (15) by propagation of the inhomogeneous equation, $d\phi(\vec{r},\tau)/d\tau = -\{[L + 3Ng|\psi(\vec{r})|^2]\phi(\vec{r},\tau) - \alpha\psi(\vec{r})\}$. We first take $\alpha = 1$, and we subsequently determine the correct value as the reciprocal of the normalization integral in Eq. (16). If we neglect the kinetic-energy operator in Eq. (15) we obtain a Thomas-Fermi approximation for ϕ:

$$\begin{aligned} \phi^{TF}(\vec{r}) &= [V_{ext}(\vec{r}) - \mu + 3Ng|\psi^{TF}(\vec{r})|^2]^{-1} \alpha\psi^{TF}(\vec{r}) \\ &= (2Ng\psi^{TF}(\vec{r}))^{-1}\alpha. \end{aligned} \tag{17}$$

Within this approximation the integrand in Eq. (16) is a constant, and independently of the external potential $V_{ext}(\vec{r})$ we can express α in terms of N, g, and the volume $\mathcal{V}$ of space in which the atomic density is nonvanishing:

$$\alpha = Ng/\mathcal{V}. \tag{18}$$

The excitation of the condensate described by $\alpha\hat{P}^2/2$ is the gapless Goldstone mode resulting from the U(1) symmetry breaking [13]. In [4] it is argued how $\hat{P}$ and $\hat{Q}$ are amplitude and phase noise operators of the atomic field, and that the variance in $\hat{P}$ should be taken on the order of unity. The variance of $\hat{Q}$ grows with time, and, following [4], we replace $\sqrt{N}\psi(\vec{r}) - i\psi(\vec{r})\hat{Q}$ by $\sqrt{N}\psi(\vec{r})\exp(-i\hat{Q}/\sqrt{N})$; i.e., the uncertainty cloud in the pictorial representation introduced above first attains the shape of an ellipse, but then it is gradually being bent along a circle with radius $\sqrt{N}\psi(\vec{r})$ in the complex plane. The expectation value of the field operator is the center of gravity of the cloud, and we understand how this gradually converges towards the origin. The commutator of $\hat{Q}$ and the Hamiltonian (11) is given as $i\alpha\hat{P}$, and the phase spreading $\sim\hat{Q}/\sqrt{N}$ with time thus causes the expectation value of the field to vanish on a time scale τ_c where

$$\tau_c = \sqrt{N}/\alpha. \tag{19}$$

We shall see that this collapse time coincides *exactly* with the one determined in the particlelike description (8).

D. Identity of particle and quantum field predictions for phase collapse

The two approaches to phase collapse lead to identical results. The proof of this leads to an identification of various quantities in the two approaches, in particular of the function $\phi(\vec{r})$. We introduce the ''macroscopic'' wave function $\Psi_N(\vec{r})=\sqrt{N}\psi(\vec{r})$, obeying the equation

$$[L+g|\Psi_N(\vec{r})|^2]\Psi_N(\vec{r})=0. \tag{20}$$

The energy μ and the wave function $\Psi_N(\vec{r})$ depend on N, and if we take the derivative of Eq. (20) with respect to N we obtain the equation

$$[L+3g|\Psi_N(\vec{r})|^2]\,\frac{\partial\Psi_N(\vec{r})}{\partial N}-\frac{\partial\mu}{\partial N}\Psi_N(\vec{r})=0. \tag{21}$$

The similarity with Eq. (15) is striking: we treat $\partial\mu/\partial N$ as an unknown, like α in Eq. (15), and note that $2\int d^3\vec{r}[\partial\psi_N(\vec{r})/\partial N]\psi_N(\vec{r})=(\partial/\partial N)\int d^3\vec{r}\,\psi_N(\vec{r})^2=1$ enforces the value of $\partial\mu/\partial N$ to the value of α/N; Eqs. (8) and (19) are thus identical definitions.

Equation (21) reveals a connection between the $\phi(\vec{r})$ function and the condensate wave function:

$$\phi(\vec{r})=\sqrt{N}\partial[\sqrt{N}\psi(\vec{r})]/\partial N. \tag{22}$$

The field approach to lowest order assumes the same one-particle (mode) function for all occupation numbers within a Poisson distribution. The function $\phi(\vec{r})$ describes the first-order change of $\psi(\vec{r})$ when N is varied. If atoms are added to the condensate it grows in size, and the wave function $\psi(\vec{r})$ particularly changes value near the edge of the condensate, so this is where the function $\phi(\vec{r})$ is maximal, cf. also the Thomas-Fermi approximation (17). A more drastic incorporation of such a change assuming different ''mode functions'' depending on the occupation number, has recently been applied in the description of Schrödinger-cat states of bicondensates [14].

We note that also within the Thomas-Fermi approximation the two expressions for τ_c, Eqs. (8) and (19), are identical. This follows from a replicate of the general proof of agreement between the two approaches in which the kinetic-energy part in the operator L is omitted. The function $\phi(\vec{r})$, and the functions describing discrete excitations, have important contributions on the edge of the condensate, where the Thomas-Fermi ansatz for the wave function is particularly ill-suited, but it follows from the reliable prediction of $\mu(N)$ that this has little effect on the quality of the quantitative prediction for the collapse time. Our use of the Thomas-Fermi approximation in the following, supplemented with numerical results, is based on this quantitative observation rather than on a physical expectation of its validity.

IV. EXCITATIONS OF THE BOSE-EINSTEIN CONDENSATE

Work on phase collapse and on excitations has so far dealt exclusively with one or the other effect. Our aim in the following sections, and a major purpose of the paper, is to show how closely related these two phenomena are, and in particular how we may use this relationship to formulate a quantitative analysis of local phase collapse within a single condensate.

A. Excitations in the field and particle picture

To obtain the excitation spectrum of the condensate we solve the coupled Bogoliubov–de Gennes equations [4]

$$[L+2gN|\psi(\vec{r})|^2]U_k(\vec{r})-gN|\psi(\vec{r})|^2V_k(\vec{r})=\hbar\omega_kU_k(\vec{r}),$$

$$[L+2gN|\psi(\vec{r})|^2]V_k(\vec{r})-gN|\psi(\vec{r})|^2U_k(\vec{r})=-\hbar\omega_kV_k(\vec{r}), \tag{23}$$

subject to the normalization and (bi)orthogonality relations:

$$\int d^3\vec{r}[U_k(\vec{r})U^*_{k'}(\vec{r})-V_k(\vec{r})V^*_{k'}(\vec{r})]=\delta_{kk'}. \tag{24}$$

The Bogoliubov transformation mixes annihilation and creation operators, so that within a given number-state subspace, we qualitatively identify components where the atomic density is depleted in one region [function $V_k(\vec{r}_1)$], and increased in another [function $U_k(\vec{r}_2)$], and vice versa. The many-particle state where the particle numbers in different regions are oscillating in this highly entangled way are very economically described within the quantum field picture. Some spurious expectation values are introduced, and particle number conservation is violated, but as long as discussions are restricted to measurable operators, e.g., the energy of the system, these introduce negligible errors, as discussed in the seminal BCS paper on superconductivity [15] and in later more philosophical digressions [16,17].

If a solution for $V_k(\vec{r})$ is small in magnitude compared to $U_k(\vec{r})$ the excitation is particlelike, cf. Eq. (12), and the first of the Bogoliubov–de Gennes equations becomes an ordinary Schrödinger equation for the excited state $U_k(\vec{r})$. Particlelike excitations out of the condensate experience twice the interaction term. This effect is well-known and incorporated in the so-called Popov approximation applied at finite temperatures [18]; see also [19].

Let us rewrite the Bogoliubov–de Gennes equations,

$$[L+Ng|\psi(\vec{r})|^2]\psi_k(\vec{r})=\frac{\hbar\omega_k}{\eta}\phi_k(\vec{r}),$$

$$[L+3Ng|\psi(\vec{r})|^2]\phi_k(\vec{r})=\hbar\omega_k\eta\psi_k(\vec{r}), \tag{25}$$

where we have introduced

$$\psi_k(\vec{r})=\frac{1}{\sqrt{2\eta}}[U_k(\vec{r})+V_k(\vec{r})],$$

$$\phi_k(\vec{r})=\sqrt{\frac{\eta}{2}}\,[U_k(\vec{r})-V_k(\vec{r})], \tag{26}$$

and where η is a constant ensuring unit normalization of $\psi_k(\vec{r})$.

These equations are interesting. If we focus on a situation with $U_k(\vec{r})$ and $V_k(\vec{r})$ comparable in magnitude and $\hbar\omega_k$ negligible, we recognize the upper equation as the Gross-Pitaevskii equation (5), and, if the proper limit is taken, the lower equation becomes equivalent to Eq. (15), yielding the free phase collapse of the condensate in the mean-field ground state. Due to the normalization condition (24), we have $2\int d^3\vec{r}\phi_k(\vec{r})\psi_k(\vec{r})=1$, just like Eq. (16).

B. Numerical treatment of excitations

One method to solve the Bogoliubov–de Gennes equations numerically is to rewrite the equations as an eigenvalue problem for the eigenvalues $\hbar\omega_k$ and the expansion coefficients of $U_k(\vec{r})$ and $V_k(\vec{r})$ on, e.g., a harmonic-oscillator basis [20,21]. One may also apply the operator $[L+3Ng|\psi(\vec{r})|^2]$ on both sides of the first equation in Eq. (25), resulting in a fourth-order equation for ψ_k, which is readily solved numerically as an eigenvalue problem with the eigenvalues $(\hbar\omega_k)^2$. This method was applied to obtain the 1D results presented below.

For problems where only the lowest excited state is required, it is useful to have a method that is effective in 3D, and we propose a quantum Monte Carlo variational method, in which the the values of the functions are specified on a grid in position space. One chooses a random position $\vec{r}_i$ on the grid and a small random number δ. One of the two functions $W=U$ or V is modified: $W(\vec{r}_i)\rightarrow W(\vec{r}_i)+\delta$, and based on whether the functional

$$\left(\int d^3\vec{r}\{U(\vec{r})LU(\vec{r})+Ng|\psi(\vec{r})|^2[2U(\vec{r})-V(\vec{r})]U(\vec{r})\}+[U\leftrightarrow V]\right)\Big/\int d^3\vec{r}[U(\vec{r})^2-V(\vec{r})^2]\equiv E_{var} \tag{27}$$

is reduced or not, the change is accepted. To obtain excited states with this method, we assume a symmetry $\hat{S}W(\vec{r})=sW(\vec{r})$, for the initial trial wave functions, and reinforce it at each step of the computation by applying the change to the wave function in all grid points connected by the symmetry [if $\hat{S}$ is the parity operator, an odd parity solution experiences both the change $W(\vec{r}_i)\rightarrow W(\vec{r}_i)+\delta$ and $W(-\vec{r}_i)\rightarrow W(-\vec{r}_i)-\delta$].

C. Thomas-Fermi approximation to excitations

One can use the information available from the Thomas-Fermi approximation for $\psi(\vec{r})$ to obtain a good approximation for the lowest excitations of a condensate in a harmonic-oscillator potential [22]. In three dimensions the excitation spectrum obtained in this way is identical to the one obtained by a hydrodynamic analysis [23]. We present a brief derivation following a slightly different route than Refs. [22,23].

The idea is to neglect the kinetic energy in places where it is relatively less significant. In the operator $[L+3Ng|\psi(\vec{r})|^2]$ the kinetic energy may be neglected in comparison with the remaining term equal to $2[\mu-V_{ext}(\vec{r})]$ in the Thomas-Fermi approximation. Thus, the second equation in Eq. (25) can be formally solved for $\phi_k(\vec{r})$ and upon insertion in the first equation we obtain a single eigenvalue equation,

$$2[\mu-V_{ext}(\vec{r})][L+Ng|\psi(\vec{r})|^2]\psi_k(\vec{r})=(\hbar\omega_k)^2\psi_k(\vec{r}). \tag{28}$$

Subsequently we make the ansatz $\psi_k(\vec{r})=W_k(\vec{r})\psi(\vec{r})$, and use the fact that $\psi(\vec{r})$ solves the Gross-Pitaevskii equation, to get the equation

$$-\frac{\hbar^2}{M}[\mu-V_{ext}(\vec{r})][\psi(\vec{r})\nabla^2W_k(\vec{r})+2\vec{\nabla}\psi(\vec{r})\cdot\vec{\nabla}W_k(\vec{r})]$$
$$=(\hbar\omega_k)^2W_k(\vec{r})\psi(\vec{r}). \tag{29}$$

As the last step, we replace $\psi(\vec{r})$ by $\psi^{TF}(\vec{r})$ and we note that $\vec{\nabla}\psi^{TF}(\vec{r})/\psi^{TF}(\vec{r})=-\vec{\nabla}V_{ext}(\vec{r})/\{2[\mu-V_{ext}(\vec{r})]\}$, so that we get the equation

$$-\frac{\hbar^2}{M}[\mu-V_{ext}(\vec{r})]\nabla^2W_k(\vec{r})+\frac{\hbar^2}{M}\vec{\nabla}V_{ext}(\vec{r})\cdot\vec{\nabla}W_k(\vec{r})$$
$$=(\hbar\omega_k)^2W_k(\vec{r}). \tag{30}$$

Equation (30) generalizes the result of Ref. [22] to arbitrary potentials.

In case of a 1D harmonic oscillator the equation for $W_k(\vec{r})$ is solved by polynomials of varying maximum power, and assuming x^k to be the highest power in such a polynomium we obtain for the x^k component of Eq. (30),

$$\frac{\hbar^2}{M}[\tfrac{1}{2}M\omega^2k(k-1)+M\omega^2k]x^k=(\hbar\omega_k)^2x^k, \tag{31}$$

and therefore the excitation energies

$$\hbar\omega_k=\hbar\omega\sqrt{k(k+1)/2}. \tag{32}$$

The lowest excitation corresponds to the center-of-mass oscillation of the condensate in the trap, and the eigenvalue $\omega_1=\omega$ is exact for the harmonic oscillator, whereas for the higher excited modes a small discrepancy appears between the analytical spectrum (32) and the exact results. We observe that the spectrum is compressed (by a factor of $\sqrt{2}$) compared to the spectrum of noninteracting particles; a similar compression has also been observed in numerical 3D calculations [21].

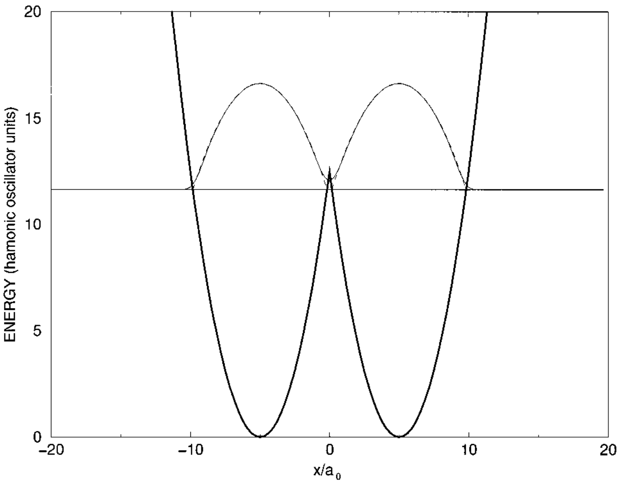

FIG. 1. Model potential (38) is shown for $x_0 = 5a_0$. The single-particle density $|\psi(x)|^2$ is shown: solid curve, exact numerical result; dashed curve, the Thomas-Fermi approximation; and the single-particle energy μ is indicated by a solid (exact) and a dashed line (Thomas-Fermi approximation). The parameters of the calculation are $N = 1000$ atoms, $g = 0.15\hbar\omega a_0$.

V. EXCITATION AND PHASE COLLAPSE OF A FRAGMENTED CONDENSATE

A. Interference between well separated fragments

Consider a single condensate, broken into two noninteracting parts due to a change of the external potential $V_{ext}(\vec{r})$. If the final potential has two local minima, and if the atomic density is entirely localized in two nonoverlapping regions around these minima, we may treat the future evolution of the system as that of two independent condensates. One may, for example, wait for a certain time T, after which the two trapped condensates are released from their traps, and one may observe a spatial interference pattern emerge when they overlap. We may imagine that in the interference region, the atomic density is so low that no collective effects appear due to atom-atom interactions in this part of the experiment. This situation is not so different from the one realized in experiments [8]. If the delay time T is short, one would expect that the phases of the condensates are still given by the phase of the nonfragmented condensate and the interference pattern should have a definite location of the fringes, so that averages over repeated experiments yield a signal with high visibility. If, on the other hand, T is large, the two components have lost their phase relationship. In individual experiments interference will be observed but the fringe location varies at random from experiment to experiment.

The particle picture yields a simple description of the relative phase diffusion of the two components. If a condensate with exactly N atoms is split in two, the resulting quantum-mechanical state will be a superposition state involving a binomial distribution over components with a given population of one or the other condensate. In a binomial distribution the variance is proportional to the mean, as in the Poisson distribution, and the dephasing is readily obtained, and it is quantitatively similar to the one obtained by the quantum field theory [24].

In the quantum field description the coherent-state atomic field in the single well-potential is deformed, as the trap potential is modified, and eventually it attains a form where two localized components can unambiguously be defined. The two mean fields at this stage are in phase, but in both wells we have a phase collapse, as described quantitatively in Sec. III C.

B. Phase collapse of weakly coupled condensates

What interests us here is the magnitude of the relative phase collapse when the separation of the condensate into two fragments is not complete. During separation the first excited state, where the wave function $\psi_1(\vec{r})$ has opposite signs in the regions around the potential minima, becomes degenerate with the ground state of the double-well condensate. A small population of such a state is already equivalent to a degradation of the phase between the two condensates, and we shall cast this in a formulation equivalent to the Goldstone mode discussion above.

From the analysis we shall recover the limit of well-separated condensates, but we shall also get a quantitative theory applicable to the situation of weakly interacting condensates. In this way we can supplement the existing quantum optics ‘‘toy-models’’ of Josephson-like coupling of condensates [5] by a quantitative analysis for the full matter wave problem.

We shall focus on the solutions (ψ_1, ϕ_1) corresponding to the lowest excited state of the condensate. The ground state of the single condensate adiabatically transforms into the state where the wave function has the same sign in both fragments, and in this limit the wave functions ψ_1 and ϕ_1 are the antisymmetric partners of ψ and ψ.

1. Superposition and product states

There is no obvious role played by superpositions of the solutions to a nonlinear Schrödinger equation, but in the limit of well-separated condensates it is indeed meaningful to construct localized wave functions by $[\psi(\vec{r}) \pm \psi_1(\vec{r})]/\sqrt{2}$. Mathematically the algebraic structure of the state vector Hilbert space includes both addition (superposition principle) and multiplication (product states).

States with a definite number of atoms can be represented as an Nth power of a single particle state, e.g., the ground state $\psi(\vec{r})$ of a condensate in a double-well potential. If this state is expanded on components localized in either well, the Nth power leads to a binomial splitting of the atoms in the two wells.

The eigenstates of the annihilation operator, are *exponentials* of one-particle states [25]. Thus, when the single-particle state is written as a superposition, the coherent state is the exponential of this superposition, i.e., a product of two coherent-state solutions, as follows from the fundamental property of the exponential function,

$$\exp(x+y) = \exp(x)\exp(y). \tag{33}$$

2. Relative phase, ‘‘Goldstone boson with variable mass’’

Restricting ourselves to the gapless excitation and the excitation with the lowest discrete excitation energy, we can rewrite δH [Eq. (14)],

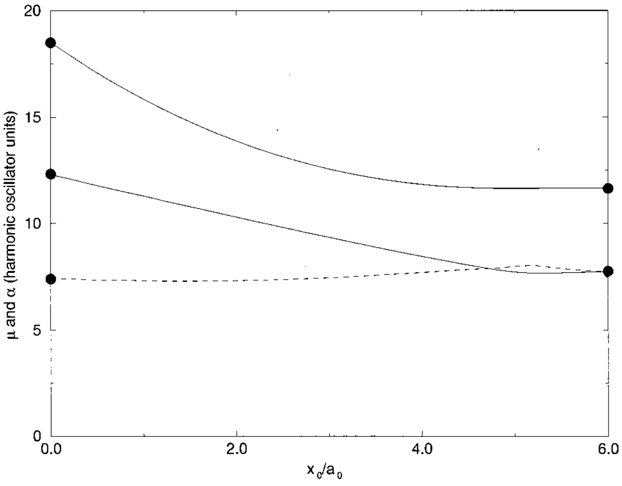

FIG. 2. The dependence of μ (upper curve) and α on the potential displacement x_0. The dashed curve indicates the value of α_1 determined in Sec. V. The physical parameters are as in Fig. 1. The filled circles present the Thomas-Fermi predictions for simple oscillator potentials, and as observed they are excellent approximations when $x_0=0$ and $x_0>6a_0$.

$$\delta H=\alpha\hat{P}^2/2+\alpha_1\hat{P}_1^2/2+\frac{1}{2\alpha_1}\omega_1^2\hat{Q}_1^2. \tag{34}$$

$\hat{Q}_1/\sqrt{N}$ is the relative phase operator of the two condensate fractions, and when $\omega_1\neq 0$, this quantum phase is seen to be a harmonically bound variable, in contrast to the overall phase, which is free.

Quantitatively, we must determine the properties of this oscillator: We first determine ω_1 by solving the Bogoliubov–de Gennes equations. Subsequently we compute the number η normalizing $\psi_1(\vec{r})$. And, finally, we obtain $\alpha_1=\eta\hbar\omega_1$, according to Eq. (25).

The ground-state width of the $\hat{Q}_1$ oscillator divided by $\sqrt{N}$ is a measure of the steady-state phase fluctuations $\delta\gamma$ between the fragments, and with our suggested procedure for obtaining the excitation energy and wave functions we are able to compute their characteristic variation

$$\delta\gamma\sim\sqrt{\alpha_1/(\hbar\omega_1 N)}. \tag{35}$$

In the case of a weak coupling, the relative phase variable moves freely over a wide range, and if this range exceeds 2π we conclude that the relative phase collapses as for the free condensate case with a collapse time $\tau_c=\sqrt{N}/\alpha_1$. In this limit $\alpha_1=\alpha$, and the Hamiltonian (34) may be rewritten as a sum of two free kinetic energies, corresponding to the phases of the two separated condensates rather than the symmetric (overall phase) and antisymmetric (relative phase) collapse terms.

When the excitation frequency is gradually increased (corresponding to a lowering of the barrier between the two potential minima and an increased passage of particles between the two fragments), $\mathrm{Var}(\hat{Q}_1)$ becomes an oscillating rather than quadratically growing function, and in the limit the relative phase is limited to fluctuations of magnitude $\delta\gamma$ smaller than 2π: there is no collapse of the relative phase, only a finite smearing.

C. Relative phase within a single condensate, long-range order, and condensate fraction

When the barrier is lowered our association of operators with the left- and the right-hand sides is no longer precise, and we can hence not take this theory too far quantitatively. But it is appealing to keep the qualitative picture that within a single condensate the relative phase in different regions may fluctuate within a finite interval identified by the equations given above.

For example, the left- and right-hand sides of a condensate in a simple 1D harmonic oscillator may experience a relative quantum phase fluctuation within the interval, $\delta\gamma\sim\sqrt{\alpha_1/(\hbar\omega_1 N)}$, where $\omega_1=\omega$. Within the Thomas-Fermi approximation, the lowest excitation in a 1D harmonic-oscillator trapping potential is described by $W_1(x)\propto x$, and a straightforward calculation gives

$$\eta=\frac{2}{5}\mu/\hbar\omega,\quad \alpha_1=\frac{2}{5}\mu, \tag{36}$$

confirmed by our numerical calculation of α_1 described in the next section (value at $x_0=0$). The Thomas-Fermi approximation for the value of μ is given in Eq. (7). For an interaction dominated condensate with μ significantly larger than ω, the phase uncertainty is in excess (but not necessarily by much) of the value enforced by complementarity between phase and particle number and what can conceivably be determined experimentally.

What we are discussing here is in fact the off-diagonal long-range order [26], suitably defined for an inhomogeneous system. In homogeneous systems, like superfluid ^{4}He, the order parameter, defined through the expectation value $\langle\hat{\Psi}^\dagger(\vec{r}_1)\hat{\Psi}(\vec{r}_2)\rangle$, is used to identify the condensate fraction f_c, i.e., the probability, or the fraction of time, that an atom spends in the condensate. It is natural for an inhomogeneous problem to define this fraction heuristically by the following equation:

$$\langle\hat{\Psi}(\vec{r})^\dagger\hat{\Psi}(\vec{r}\,')\rangle=Nf_c\psi(\vec{r})^*\psi(\vec{r}\,'), \tag{37}$$

where $\vec{r},\vec{r}\,'$ are chosen on opposite sides of the condensate. With this identification, we obtain $f_c\sim\langle\exp(i\hat{Q}_1/\sqrt{N})\rangle\sim\exp(-\delta\gamma^2/2)=\exp[-\alpha_1/(2\hbar\omega_1 N)]$.

If we insert the N dependence of $\alpha_1\sim\mu$ we get a scaling of the argument in the exponential as $N^{-1/3}$ (1D), $N^{-1/2}$ (2D), and $N^{-3/5}$ (3D), which is thus the large-N dependence of the noncondensed fraction suggested by this phase collapse argument. We recall the heuristic character of our definition of ''long'' range order and our inclusion of only the lowest excitation (in the 1D problem higher-order excitations yield values of $\alpha_k/\omega_k\sim k^{-2}$), so these estimates should be taken at most as a suggestion for the noncondensed fraction at zero temperature.

In the particle picture, the existence of a noncondensed fraction at zero temperature reflects the only approximate character of the Hartree ansatz. A proper treatment involves excitations out of this state due to atom-atom interactions, and the amount of such excitations may be estimated from the expectation value of the interaction term relative to the excitation energies. This, in fact, suggests the same combi-

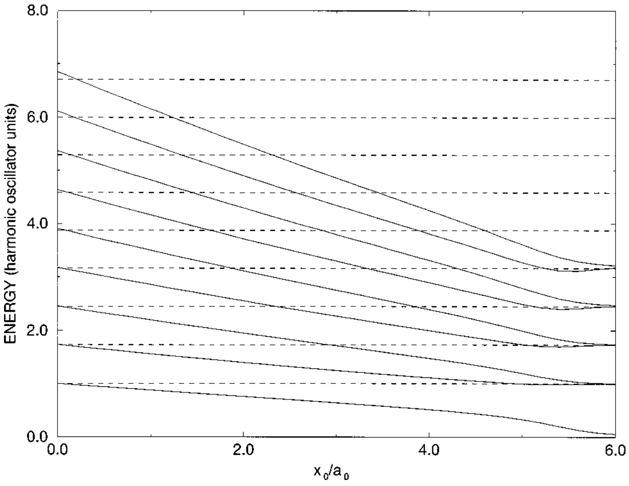

FIG. 3. Nine lowest excitation energies $\hbar\omega_k$ as a function of x_0. The parameters are as in the other figures. The dashed lines indicate the analytical expression (32) obtained by use of the Thomas-Fermi approximation.

nation of parameters α (or $\partial\mu/\partial N$) and ω_1 and hence the same N dependence as above.

One may speculate that the off-diagonal order could be made the subject of experimental investigations by cutting the condensate into pieces and subsequently performing an interference experiment. For small regions, the information available from higher excitation modes enters, although their higher and higher energies may suppress their individual contributions. If there are too few atoms in each piece, the precision on the phase measurement is limited, but one may make a compromise so that the level of discrimination is sufficient to probe the expected phase fluctuations.

VI. 1D MODEL SYSTEM

We consider atoms confined by a potential that we can modify through a single control parameter so that it changes continuously from a single harmonic oscillator into two separate oscillator potentials with the same oscillator frequency ω as the single potential. For simplicity we assume the following model potential,

$$V_{ext}(x)=\frac{1}{2}M\omega^2(x\pm x_0)^2, \tag{38}$$

where the $+$ $(-)$ sign applies for x negative (positive), and where the positive quantity x_0 provides the location of the potential minima at $\pm x_0$. When the potential barrier $E_0=(1/2)M\omega^2x_0^2$ at $x=0$ exceeds the energy of the particles μ, the two fragments are separated. The potential is illustrated in Fig. 1, the figure also indicates the square of the ground-state wave function and the chemical potential μ obtained both within the Thomas-Fermi approximation and exactly. Results in this section are presented for a specific choice of parameters (in harmonic-oscillator units); we assume $N=1000$ atoms and $g=0.15\hbar\omega a_0$, where the width of the oscillator ground state is $a_0=\sqrt{\hbar/M\omega}$. Positions are presented in units of a_0. The results in Fig. 1 assume $x_0=5a_0$.

Within the Thomas-Fermi approximation it is not difficult to obtain the ground-state wave function and the energy μ for the potential (38). Normalizing the particle density to the desired number of atoms, we obtain a third-order equation relating μ and x_0. For large x_0, μ becomes smaller than the barrier height E_0, and μ is then given by the result (7) for a single harmonic oscillator with $N/2$ atoms (the number of atoms in each harmonic well). The value of μ (and of α) is accordingly reduced by a factor of $(1/2)^{2/3}\sim 0.63$ when the condensate is split. Within the Thomas-Fermi approximation the splitting is completed when $x_0>(3Ng/4M\omega^2)^{1/3}\sim 4.83a_0$ for the applied parameters, but this approximation of course underestimates the wave function in the classically forbidden region between the two fragments.

In Fig. 2 is shown the dependence of μ and α on x_0, obtained for a fixed number of particles $N=1000$. The relative phase collapse parameter α_1 is determined from the functions associated with the lowest excitation energy, and its dependence on x_0 is shown as a dashed line in the figure. As predicted α_1 and α converge to the same value for large separations. The filled circles indicate the Thomas-Fermi predictions applicable in the case of simple harmonic-oscillator potentials.

We present in Fig. 3 the variation of the nine lowest excitation frequencies with the parameter x_0. We clearly identify the convergence of pairs of levels corresponding to degenerate even and odd solutions. The dashed lines in Fig. 3 show the excitation energies predicted analytically by application of the Thomas-Fermi approximation, and applicable both for $x_0=0$ and for large x_0. We have applied the quantum Monte Carlo variational procedure and verified that it very efficiently yields the same results as the diagonalization procedure for the first excitation of the condensate.

This excitation frequency decreases, and, as discussed above, in the limit of two separated fragments, the relative phase between the two is unbounded. The relative phase uncertainty $\delta\gamma$ is shown in Fig. 4 as a function of x_0.

We have assured ourselves of the rapid convergence of the lowest excitation to zero as both the height and the width of the barrier increase with x_0. There is a close relationship between the energy difference between odd and even states of double-well systems and the probability T of tunneling through the barrier. This establishes a connection between the relative phase fluctuations determined above and a particlelike picture where the passage of atoms among different regions ensures the entanglement responsible for the relative phase. In case of a tunnel barrier with a transmission coefficient of T, setting $\omega_1\sim T\omega$, we can interpret the phase synchronization as a result of N atoms ‘‘knocking’’ on the barrier with a frequency ω and a fraction T of them actually getting through to communicate the phase of the condensate from one to the other side of the barrier. The tunneling of atoms between condensates has recently been studied in some detail [27]. In competition with the relative phase collapse, we may understand how this process limits the phase fluctuations as predicted by Eq. (35).

VII. DISCUSSION

We have considered the phase of a Bose condensate and the means for calculating the time scale for its collapse under

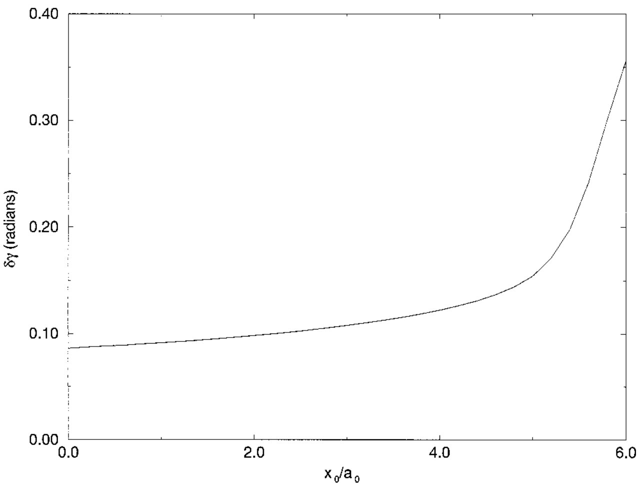

FIG. 4. The characteristic magnitude of fluctuations of the relative phase between the two fragments of the condensate. For x_0 small, the identification of two components is ambiguous, and the values of $\delta\gamma$ should only be understood in a qualitative sense.

different circumstances. We have demonstrated the strong connection between phase collapse and excitations of the condensate, which is of course evident as both are described by the Bogoliubov–de Gennes equations in the quantum field picture. We have in particular identified how separately collapsing phases emerge from the gapless excitation and the first discrete excitation when a condensate is broken up. Nonsymmetry-breaking analyses of the dynamics of very-low-temperature condensates have recently been proposed [28,29]. Explicitly time-dependent analyses may contribute even further to our understanding of the relations between excitation and phase collapse; see also [30].

We have considered only the case of zero temperature. As shown in [4], temperature-dependent phase collapse rates can be evaluated within the Popov approximation. In our problem of weakly coupled condensates, a closer scrutiny is necessary to determine the influence of the transfer of thermally excited atoms among the condensates.

It has been proposed that a mechanism similar to the phase collapse can account for the observed damping of oscillations in condensates in time-dependent traps. The proposed mechanism refers to the spreading in number of quanta in the excited mode and the mode anharmonicity, which causes a dephasing of the superposition of ground- and excited-state wave functions [31,32]. The calculations that we have particularly carried out for the lowest excited state can be straightforwardly applied to higher excited states, and we imagine that this may be a promising avenue for further studies.

In a recent study [33] it was shown how a model with a transmission barrier inserted in a simple box of nucleons may account for the congruence energy, a contribution to nuclear binding associated with the granularity of nucleonic density and not obtainable from the Thomas-Fermi model of the nucleus. The relevance of phase in connection with nuclear excitation and fission may be an interesting line of research, with parallels to the study of Bose condensates.

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