Ground state and excitations of a Bose gas: From a harmonic trap to a double well

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(Received 19 June 2011; published 23 September 2011)

We determine the low-energy properties of a trapped Bose gas split in two by a potential barrier over the whole range of barrier heights and asymmetry between the wells. For either weak or strong coupling between the wells, our two-mode theory yields a two-site Bose-Hubbard Hamiltonian with the tunneling, interaction, and bias parameters calculated simply using an explicit form of two mode functions. When the potential barrier is relatively low, most of the particles occupy the condensate mode and our theory reduces to a two-mode version of the Bogoliubov theory, which gives a satisfactory estimate of the spatial shape and energy of the lowest collective excitation. When the barrier is high, our theory generalizes the standard two-site Bose-Hubbard model into the case of asymmetric modes, and correctly predicts a full separation of the modes in the limit of strong separation of the wells. We provide explicit analytic forms for the number squeezing and coherence as a function of particle number and temperature. We compare our theory to other two-mode theories for bosons in a double well and discuss their validity in different parameter regimes.

DOI: 10.1103/PhysRevA.84.033630 PACS number(s): 03.75.Gg, 03.75.Lm, 05.30.Jp, 95.30.Dr

I. INTRODUCTION

A Bose-Einstein condensate (BEC) of ultracold atoms in a double-well potential is a model system for the study of matter-wave coherence for atom interferometry [1–4], and tunneling and entanglement in few-body and many-body systems [5–7]. Its equivalence with a Josephson junction of two superconductors separated by a tunneling barrier was demonstrated experimentally [8,9]. As long as the two parts of the Bose gas are well connected (i.e., the tunneling rate is high) and the temperature is very low, most of the atoms occupy a single spatial mode with a well-defined phase, satisfying the Gross-Pitaevskii equation (GPE) [10], while excitations and higher-temperature effects are described by Bogoliubov theory [11–13]. However, when the tunneling rate between the two wells is low, the single condensate breaks down into separate modes occupying each of the two wells, and the GPE and Bogoliubov theories cease to be valid. In this case, the system is best described in terms of a two-mode theory, e.g., the Bose-Hubbard model or the Josephson model [14–22], giving rise to many-body effects such as squeezing, entanglement [6], and phase diffusion [23–25].

The standard two-mode model for a Bose gas in a double well [14,16] replaces the single condensate wave function by a superposition of two mode functions,

$$\psi(\mathbf{r},t) = c_1(t)\phi_1(\mathbf{r}) + c_2(t)\phi_2(\mathbf{r}), \tag{1}$$

where ϕ_1 and ϕ_2 are taken to be time-independent spatial modes, and c_1, c_2 are time-dependent amplitudes which carry the mutual phase and occupation probability of the two modes. This theory has proven to successfully describe effects such as Josephson oscillations and self-trapping. A second-quantized version of this theory, where the wave function ψ is replaced by the field operator, and c_1, c_2 are replaced by bosonic annihilation operators, is capable of describing many-body effects beyond the GPE, which involve phase uncertainty between the two wells, and number squeezing in the steady-state properties or in the time evolution of a Bose gas.

If interactions between the particles at each well are weak compared to the splitting between the single-particle energy levels in each well, then the two mode functions ϕ_1 and ϕ_2 may be taken to be the two lowest-energy single-particle eigenmodes in the double-well potential. For two symmetric wells, their even and odd superpositions will mainly occupy each of the two wells. However, in usual traps of ultracold atoms in a BEC, the repulsive interaction drastically changes the spatial shape of the condensate, so that single-particle modes are not really relevant. It was first suggested to take the two modes as solutions of the GPE in the two isolated traps [14], but then it is not clear how the tunneling rate should be calculated based on the overlap between these modes. Later it was proposed to use the symmetric and antisymmetric solutions of the GPE in the total potential [16,20,26]. This choice is applicable only to the case of weak coupling between the two wells and a nearly symmetric potential, because in a potential with an arbitrary symmetry, different solutions of the GPE are nonorthogonal.

In general, the standard two-mode theories are valid only for weak tunneling between the two wells, while the GPE together with Bogoliubov excitations allow a good description of the Bose gas in the case of a low barrier. A self-consistent two-mode method based on Hartree-Fock (HF) mean-field theory was developed in the last few years [27–33] and applied to various steady-state and time-dependent physical situations. This theory purports to provide a calculation method that is applicable to the case of double wells with either low or high barriers and to describe, for example, the process of splitting a single harmonic trap into a double well. However, results using this method have not been validated by a quantitative comparison with either experimental results or with results using other existing theories in the regimes where they are known to be valid. Furthermore, reports on these results often concentrate on specific numerical examples and do not provide a more general picture which extends over a large range of parameters.

Here we address the steady-state properties of a zero-temperature and low-temperature quantum gas, where only the ground state and lowest excitations of the gas of interacting

bosons in a double-well potential are populated, and develop a two-mode theory, which is applicable over the whole range of barrier heights. Our theory shows satisfactory agreement with the Gross-Pitaevskii and Bogoliubov theories for low barrier heights or large particle numbers, and agrees with the standard Bose-Hubbard or Josephson theories in the case of symmetric double wells with weak coupling. However, it also provides a continuous picture of the properties of the Bose gas over the whole range of parameters, including an asymmetric double-well potential with an arbitrary level of asymmetry. Numerical examples in one and three dimensions are presented that cover the whole range of barrier heights.

The structure of this paper is as follows. In Sec. II, we set up the general framework and define the essential criteria for validating a theory of a Bose gas in a single and double well. In Sec. III, we describe the Bogoliubov theory of a Bose gas and justify its reduction to a two-mode theory to describe the condensate and the lowest-energy excitation. In Sec. IV, we show how the two-mode Bogoliubov theory transforms into the two-mode Bose-Hubbard model that satisfies the validity criteria over the whole range of parameters. We give explicit expressions for the parameters of the Bose-Hubbard model. In Sec. V, we derive the Josephson form of the Hamiltonian and describe the excitation spectrum, number squeezing, and coherence properties of a Bose gas at low temperatures, with emphasis on a complementary description in the condensate-excitation basis and in the left-right mode basis. In Sec. VI, we compare our theory with the standard approach to a weakly coupled double-well system and the two-mode HF theory, and discuss their ranges of validity. A summary and discussion are presented in Sec. VII.

II. GENERAL FRAMEWORK

Here we introduce the full theory of a Bose gas in a trapping potential using a multimode representation, and specify the validity criteria for a theory with a reduced number of modes. We examine its results in the two extreme limits of a single harmonic trap and a double-well potential with large separation.

A. The second-quantized Hamiltonian

We consider N bosons of mass m in a trapping potential $V(\mathbf{r})$. At low temperature, collisions between the particles are described by s-wave scattering and the Hamiltonian can be written as

$$H = \sum_i \left[\frac{p_i^2}{2m} + V(\mathbf{r}_i)\right] + \frac{1}{2}\sum_{i\neq j} U(\mathbf{r}_i - \mathbf{r}_j), \tag{2}$$

where we take the usual contact interaction potential $U(\mathbf{r}_i - \mathbf{r}_j) = g\delta(\mathbf{r}_i - \mathbf{r}_j)$ with $g = 4\pi\hbar^2 a/m$, and with a being the s-wave scattering length. A field-theoretical form of the Hamiltonian uses the field operator $\hat{\Psi}(\mathbf{r})$,

$$\hat{H} = \int d^3\mathbf{r}\hat{\Psi}^\dagger(\mathbf{r})\left[H_0 + \frac{g}{2}\hat{\Psi}^\dagger\hat{\Psi}\right]\hat{\Psi}(\mathbf{r}), \tag{3}$$

where $H_0 = p^2/2m + V$ is the single-particle Hamiltonian. $\hat{\Psi}(\mathbf{r})$ can be expanded in single-particle spatial modes $\phi_j(\mathbf{r})$ and annihilation operators $\hat{a}_j$,

$$\hat{\Psi}(\mathbf{r}) = \sum_i \hat{a}_i\phi_i(\mathbf{r}), \tag{4}$$

to yield the multimode form of the Hamiltonian,

$$\hat{H} = \sum_{ij}\epsilon_{ij}\hat{a}_i^\dagger\hat{a}_j + \frac{1}{2}\sum_{ijkl}U_{ijkl}\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_k\hat{a}_l, \tag{5}$$

where $\epsilon_{ij} = \int d^3\mathbf{r}\phi_i^* H_0\phi_j$ and $U_{ijkl} = g\int d^3\mathbf{r}\phi_i^*\phi_j^*\phi_k\phi_l$. As long as the mode functions ϕ_i form a complete orthogonal set spanning the relevant space, Hamiltonian (5) is exact. However, a realizable numerical solution of such a system is possible only for a few particles (up to ~10 particles) [34–37], so that for applications using a large number of particles, one must assume that only a single mode or a restricted number of modes is macroscopically occupied. It is then important to know how to choose these mode functions and make the appropriate assumptions in a way that at least reproduces the correct behavior of the system at some important limits.

B. Validity criteria

We are interested in the steady-state properties of a Bose gas at very low temperatures over the whole range of potentials from a single (harmonic) trap to a deep double-well trap. Under these circumstances, it is known (as we demonstrate below in Sec. V) that a single condensate satisfying the GPE provides an accurate approximation for the single-particle density $n(\mathbf{r}) = \langle\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})\rangle$. However, we seek a theory that will also correctly reproduce the excitation energies and the two-particle correlations. These correlations determine the coherence of the Bose gas when the condensate is split into two weakly coupled parts by a tunneling barrier. Hence we set three requirements:

(a) Excitation energy of a harmonic trap. In an external harmonic potential $V(\mathbf{r}) = \frac{m}{2}(\omega_x^2x^2 + \omega_y^2y^2 + \omega_z^2z^2)$, the lowest excitation along each of the major axes involves motion of all the particles as a rigid body. This excitation mode follows from the fact that Hamiltonian (2) with an external harmonic potential V can be separated into the motion of the center of mass and the motion relative to the center of mass, which has exactly the same form as in (2). As shown previously [38], this kind of motion is expected when a fully harmonic trap is shaken while the trapping frequency is unchanged. The lowest excitation energy along axis i should then be $\hbar\omega_i$, regardless of the strength of the interparticle interaction. In the limit where $\{\omega_i\} \to 0$ (a homogeneous Bose gas), this requirement is equivalent to demanding a gapless excitation spectrum at the limit of the long wavelength. This requirement leads to the Popov approximation in the Bogoliubov theory of bosons at finite temperature [11]. It has raised a good deal of dispute, as it implies abandoning full self-consistency. We do not require that our two-mode theory reproduce the exact value of the excitation energy, but that it predict results close to the exact value, even as the interaction strength is increased.

(b) Fragmentation at high barrier separation. In a double-well potential with high barrier separation, theory should

predict the existence of two spatial modes ("left" and "right" modes), such that the overlap between them decreases with increased barrier height and vanishes in the limit of very large barrier separation (vanishing tunneling rate). For a symmetric potential, this implies that the symmetric and antisymmetric modes, which are even and odd superpositions of the left and right modes, become degenerate in the high barrier limit.

(c) Mode orthogonality. The theory should be valid also in the case of an asymmetric potential. The two main modes should stay orthogonal, even in the case where each of them has no definite symmetry. A natural way to achieve such orthogonality is to take the modes to be eigenstates of an effective Hamiltonian, rather than solutions of nonlinear equations.

While the Bogoliubov theory for trapped bosons accurately fulfills the first and third requirements, it breaks down in the high barrier separation limit where more than one mode becomes macroscopically occupied. On the one hand, as we show in Sec. VI, the standard two-mode theory does not yield accurate predictions for a low barrier, or no barrier, and it also does not yield accurate spatial modes in the asymmetric case. On the other hand, the self-consistent Hartree-Fock two-mode theory does not satisfy the first two requirements. Here we will show how a two-mode theory that fulfills the above validity criteria can be constructed.

III. BOGOLIUBOV THEORY

A. Multimode theory

In a gas of many trapped bosons at very low temperatures (far below the critical temperature for condensation, T_c), we may assume that most of the particles occupy only a single mode ϕ_0, which satisfies the time-independent Gross-Pitaevskii equation (GPE)

$$(H_0 + gN|\phi_0|^2 - \mu)\phi_0 = 0, \tag{6}$$

where μ is the chemical potential. A convenient set of orthogonal modes, which constitutes a complete set, are the solutions of the equation

$$(H_0 + gN|\phi_0|^2 - \mu)\phi_j = \epsilon_j\phi_j, \tag{7}$$

where ϕ_0 is the solution with $\epsilon_0 = 0$, and ϕ_j with $j > 0$ are single-particle excitation modes. With this choice, Hamiltonian (5) becomes

$$\begin{aligned}\hat{H} = E_C + \sum_j \bar{\epsilon}_j\hat{n}_j + \frac{1}{2}\sum_{jk} U_{jk}(2\hat{a}_j^\dagger\hat{a}_0^\dagger\hat{a}_0\hat{a}_k + \hat{a}_j^\dagger\hat{a}_k^\dagger\hat{a}_0\hat{a}_0 \\ + \hat{a}_0^\dagger\hat{a}_0^\dagger\hat{a}_j\hat{a}_k) + \sum_{ijk}(U_{ijk0} - U_{i000}\delta_{jk})(\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_k\hat{a}_0 \\ + \hat{a}_0^\dagger\hat{a}_j^\dagger\hat{a}_k\hat{a}_i) + \frac{1}{2}\left(U_{00}\hat{\tilde{n}}^2 + \sum_{ijkl} U_{ijkl}\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_k\hat{a}_l \right. \\ \left. - 2\sum_{jk} U_{jk}\hat{a}_j^\dagger\hat{\tilde{n}}\hat{a}_k\right),\end{aligned} \tag{8}$$

where $\hat{n}_j = \hat{a}_j^\dagger\hat{a}_j$, $\bar{\epsilon}_j = \epsilon_j + U_{0000}/2$, $U_{jk} \equiv U_{0jk0}$, and the operator $\hat{\tilde{n}} \equiv \sum_j \hat{n}_j$ counts the number of noncondensate particles. The constant energy term E_C is the condensate energy

$$E_C = \mu N - \tfrac{1}{2}U_{00}N^2. \tag{9}$$

The Bogoliubov approach, which is suitable for a high number of particles and very low temperature, consists of two approximations. First, terms of the order higher than quadratic in the annihilation and creation operators $\hat{a}_j$ and $\hat{a}_j^\dagger$ for $j > 0$ are omitted. Second, one defines the operators $\hat{b}_j = \hat{a}_0^\dagger\hat{a}_j/\sqrt{N_0}$, where $N_0 = \langle\hat{a}_0^\dagger\hat{a}_0\rangle$. These operators satisfy the commutation relations $[\hat{b}_j,\hat{b}_k^\dagger] \approx \delta_{jk} - \hat{b}_k^\dagger\hat{b}_j/N_0$, which is a canonical bosonic commutation relation in the limit of large N, and one assumes relatively small occupation numbers of the excited modes. The Hamiltonian then takes the Bogoliubov form

$$\hat{H}_{\rm Bog} = E_C + \sum_i \tilde{\epsilon}_i\hat{b}_i^\dagger\hat{b}_i + \frac{1}{2}\sum_{ij} U_{ij}(2\hat{b}_i^\dagger\hat{b}_j + \hat{b}_i\hat{b}_j + \hat{b}_i^\dagger\hat{b}_j^\dagger). \tag{10}$$

Hamiltonian (10) is diagonalized by using the Bogoliubov transformation

$$\hat{b}_i = \sum_k (u_{ik}\hat{\alpha}_k + v_{ik}\hat{\alpha}_k^\dagger), \tag{11}$$

where $\hat{\alpha}_k$ are operators satisfying canonical bosonic commutation relations. Note that both $\hat{b}_i$ and $\hat{\alpha}_i$ are number-conserving operators, which transfer particles from a single-particle excited mode into the condensate mode, or vice versa. Within the number-conserving formalism [39], the field operator $\hat{\Psi}(\mathbf{r})$ can then be written in terms of the new operators $\{\hat{\alpha}_k\}$,

$$\hat{\Psi}(\mathbf{r}) = \left\{\phi_0(\mathbf{r}) + \frac{1}{\sqrt{N_0}}\sum_k [u_k(\mathbf{r})\hat{\alpha}_k + v_k(\mathbf{r})\hat{\alpha}_k^\dagger]\right\}\hat{a}_0, \tag{12}$$

where $u_k(\mathbf{r}) = \sum_i \phi_i(\mathbf{r})u_{ik}$ and $v_k(\mathbf{r}) = \sum_i \phi_i(\mathbf{r})v_{ik}$ are solutions of the Bogoliubov-de Gennes equations,

$$\begin{pmatrix} \mathcal{L} - E_k & gN\phi_0^2 \\ gN(\phi_0^*)^2 & \mathcal{L} + E_k \end{pmatrix}\begin{pmatrix} u_k(\mathbf{r}) \\ v_k(\mathbf{r}) \end{pmatrix} = 0, \tag{13}$$

with $\mathcal{L} \equiv H_0 + 2gN|\phi_0|^2 - \mu$. The frequencies $\omega_k = E_k/\hbar$ are the plasma oscillation frequencies of a BEC when it is slightly driven out of equilibrium. In this case, the solutions of the time-dependent GPE are represented by Eq. (12) with classical amplitudes $\hat{a}_0 \to \sqrt{N_0}$ and $\hat{\alpha}_k \to \alpha_k e^{-i\omega_k t}$, and u_k, v_k satisfying Eq. (13). More generally, E_k are the energies of collective excitations of the many-particle system when N is large. The plasma frequencies ω_k in a double-well potential were measured in a recent experiment [40].

After performing the transformation (11), the Hamiltonian (10) then becomes diagonal in the quasiparticle operators $\hat{\alpha}_j$,

$$H_{\rm Bog} = E_C - \sum_k E_k\sum_i |v_{ik}|^2 + \sum_k E_k\hat{\alpha}_k^\dagger\hat{\alpha}_k. \tag{14}$$

The first two terms define the ground-state energy. The ground state consists of a superposition of states where most of the atoms are in the condensate mode, while pairs of particles occupy the excited single-particle modes with an average

occupation $\langle \hat{n}_j \rangle = \sum_k |v_{jk}|^2 = \int d^3\mathbf{r}\, |v_k(\mathbf{r})|^2$. Within the Bogoliubov theory, the total number of excited particles in the ground state, or in any other state with collective excitations, does not depend on the total number of particles. This implies that for a given number N, the Bogoliubov approximation may break down if the total number of excitations becomes of the same order or larger than the total number of particles. This may happen when the interaction coefficient g is large or, as we shall see below, when a barrier separates two parts of the condensate such that the excitation energy ϵ_1 of the first excited mode is much smaller than the collisional interaction energy per particle.

More elaborate theories using the Bogoliubov approximation have been developed which are suitable for calculating particle density and excitations at finite temperatures where many excitations are thermally occupied. However, here we concentrate on very low temperatures and in the following we show how a two-mode theory, which yields a satisfactory approximation to the first Bogoliubov excitation when the condensate is well connected (high tunneling), may be continued to the regime where more than one mode is macroscopically occupied.

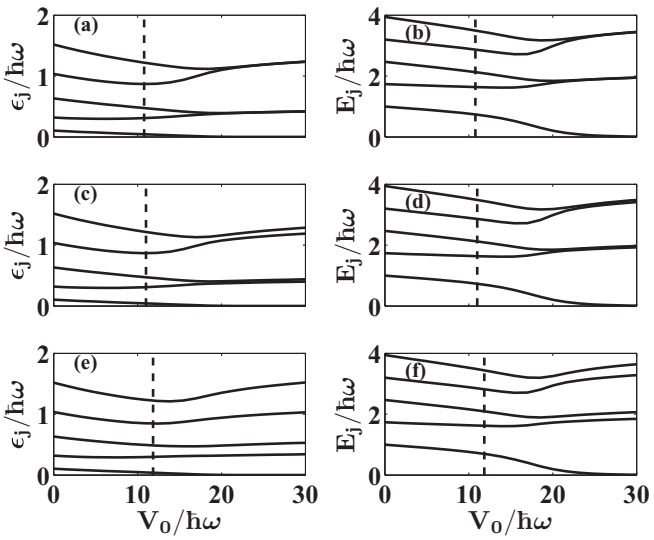

FIG. 1. Energies of single particle (left) and collective (right) excitations in a double-well potential of the form (15): a harmonic trap of frequency $\omega = 2\pi \times 100$ Hz, plus a Gaussian barrier of width $d = 5$ μm and variable height V_0. Here the particle-particle interaction strength reduced to one dimension is $g_{1D}N = 69.7\, l_{\rm ho}\hbar\omega$, where $l_{\rm ho} = \sqrt{\hbar/m\omega}$, and $g_{1D}N = 4.98 \times 10^{-36}$ J m for ^{87}Rb atoms. The dashed vertical line shows the barrier height for which $V_0 = \mu$. (a) and (b) are for a symmetric potential ($x_0 = 0$): when the barrier grows, pairs of symmetric and antisymmetric modes become nearly degenerate. (c) and (d) are for a slightly asymmetric potential ($x_0 = 0.1$ μm), whereas (e) and (f) have a stronger asymmetry ($x_0 = 0.5$ μm): pairs of modes sustain a constant energy splitting when the barrier grows, which indicates the suppression of tunneling between higher modes in the two wells. Yet, due to collisional repulsion, the first excited-state single-particle energy still tends to zero for a high barrier. A two-mode approximation is justified under these circumstances.

Figure 1 shows the single-particle energy levels ϵ_j and the collective Bogoliubov excitations for a one-dimensional (1D) trap of the form

$$V(x) = \tfrac{1}{2}m\omega^2(x - x_0)^2 + V_0 \exp[-(2x/d)^2], \qquad (15)$$

i.e., a harmonic oscillator potential ($\omega = 2\pi \times 100$ Hz) with a Gaussian barrier ($1/e$-width $d = 5$ μm). The trap is symmetric if $x_0 = 0$, and asymmetric otherwise. The barrier height V_0 varies from $V_0 = 0$ (harmonic trap) to about twice the chemical potential (vertical dashed line). The interparticle coupling constant g is replaced by a 1D parameter $g_{1D} = g/A$, where A is the area of the transverse mode. For the demonstration, we take $g_{1D}N = 4.98 \times 10^{-36}$ J m. When $V_0 = 0$, the energy of the first collective excitation is exactly $E_1 = \hbar\omega$. With increased barrier height, the single-particle energy ϵ_1, as well as the energy of the first Bogoliubov excitation, decreases until it becomes very small when the height of the barrier exceeds the chemical potential μ. This implies that even at very low temperature, the first Bogoliubov excitation becomes populated. The fact that the single-particle energy ϵ_1 becomes very small implies that the ground state becomes an entangled state with high occupation of the first excited spatial mode, while the higher spatial modes' population stays small. In what follows, we show how these properties enable us to develop a two-mode model for low energies which involves only the condensate mode and the first excitation.

B. Two-mode approximation

In general, the quasiparticle wave functions $u_{\mathbf{k}}(\mathbf{r})$ and $v_{\mathbf{k}}(\mathbf{r})$ do not have the same spatial form. Let us write these functions as

$$u_k(\mathbf{r}) = \tilde{u}_k \phi_{u,k}(\mathbf{r}), \quad v_k(\mathbf{r}) = \tilde{v}_k \phi_{v,k}(\mathbf{r}), \qquad (16)$$

such that $\tilde{u}_k^2 - \tilde{v}_k^2 = 1$, and $\phi_{u,k}$ and $\phi_{v,k}$ are normalized functions of space which may be found by solving the Bogoliubov-de Gennes equations. The well-known theory of a homogeneous Bose gas [$V(\mathbf{r}) = 0$] with periodic boundary conditions yields the form $\phi_{u,\mathbf{k}} \propto e^{i\mathbf{k}\cdot\mathbf{r}}$ and $\phi_{v,\mathbf{k}} \propto e^{-i\mathbf{k}\cdot\mathbf{r}}$. In that case, or any case where $|\phi_{u,k}| \sim |\phi_{v,k}|$, the Bogoliubov-de Gennes equations yield (see [41] for an experimental demonstration)

$$E_k \approx \sqrt{\epsilon_k(\epsilon_k + 2NU_{kk})}, \qquad (17)$$

$$\tilde{v}_k \approx -\sqrt{\frac{1}{2}\left(\frac{\epsilon_k + NU_{kk}}{E_k} - 1\right)}, \quad \tilde{u}_k \approx \sqrt{1 + \tilde{v}_k^2}. \qquad (18)$$

Here we show that the approximation $\phi_{v,k} \sim \phi_{u,k}$ is relevant for the lowest-energy solution of the Bogoliubov-de-Gennes equations ($k = 1$) and becomes more and more accurate when the barrier height V_0 increases.

The top panels of Fig. 2 show the deviation of ϕ_{u1} and ϕ_{v1} of the first Bogoliubov excitation from ϕ_1, which is the lowest positive energy solution of Eq. (7). Both for a symmetric potential (a) and an asymmetric potential (b), the deviation $1 - |\langle\phi_1|\phi_{u,v}\rangle|^2$ is small, even for a harmonic potential (<0.3% for ϕ_{v1} and <3% for ϕ_{u1}) and reduces significantly with growing barrier height, such that both ϕ_{u1} and ϕ_{v1} become similar to ϕ_1 at large well separation. A more rigorous analytical derivation of this deviation is given in the Appendix.

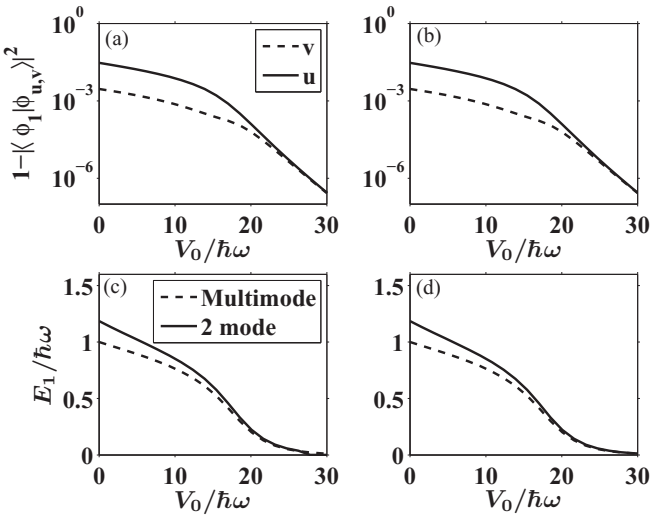

FIG. 2. Comparison of the multimode Bogoliubov theory to the two-mode approximation. Top panels show the deviation $1-|\langle\phi_{u,v}|\phi_1\rangle|^2$ of $\phi_{u,v}$ (normalized u_1 and v_1 quasiparticle functions) in the multimode theory from the single-particle modes ϕ_1 used for the two-mode approximation: (a) for a symmetric trap and (b) for an asymmetric trap ($x_0 = 0.5\ \mu$m). The bottom panels compare the first excitation energy in the two-mode theory to the multimode Bogoliubov theory for the two cases: (c) symmetric and (d) asymmetric. The maximum deviation is ∼19% in the harmonic case ($V_0 = 0$).

In the bottom panel of Fig. 2, we present a comparison of the first excitation energy obtained from the Bogoliubov theory with the excitation energy of Eq. (17), which is obtained when the Hamiltonian (10) is reduced to contain only the lowest single-particle excitation mode ($\hat{b}_1$ and $\hat{b}_1^\dagger$ only). The difference between the two calculations is not larger than 20% for a harmonic potential ($V_0 \to 0$) and reduces to zero for high barrier separations.

Based on the observations of Figs. 1 and 2, we now restrict ourselves to the second-quantized Hamiltonian (5) with only two modes satisfying Eq. (7); the condensate mode ϕ_0 with $\epsilon_0 = 0$ and the first excited mode ϕ_1 with corresponding energy ϵ_1. On the one hand, the resulting Hamiltonian is a reduction of the Bogoliubov Hamiltonian (10) to only one excitation mode, but on the other hand, we include terms involving this excited mode to all orders, so as to take into account situations when this mode becomes macroscopically occupied. We then obtain the two-mode Hamiltonian

$$\hat{H}_{TM} = E_C + \tilde{\epsilon}_1\hat{n}_1 + \frac{U_{11}}{2}(2\hat{n}_1\hat{n}_0 + \hat{a}_0^\dagger\hat{a}_0^\dagger\hat{a}_1\hat{a}_1 + \hat{a}_1^\dagger\hat{a}_1^\dagger\hat{a}_0\hat{a}_0) + K(\hat{a}_0^\dagger\hat{n}_1\hat{a}_1 + \hat{a}_1^\dagger\hat{n}_1\hat{a}_0) + Fn_1^2, \quad (19)$$

where $\tilde{\epsilon}_1 = \epsilon_1 + (U_{0000} - U_{1111})/2$ is the slightly corrected single-particle energy of the lowest excited mode, $K = U_{0111} - U_{0001}$ is an interaction term that vanishes if the potential is symmetric, and $F = \frac{1}{2}(U_{0000} + U_{1111} - 2U_{11})$ gives the self-interaction of the excited mode.

It is clear that retaining terms to all orders in the excitation ϕ_1, while neglecting the effect of all other modes ($j > 1$), is justified only in the high barrier limit, where ϵ_1 is much smaller than the energies of the other modes. On the other hand, we have demonstrated that a single-mode form of Hamiltonian (10), where mixed terms U_{jk} ($j \neq k$) are neglected, provides a reasonable approximation to the energy and shape of the first Bogoliubov excitation, even in the limit of no barrier. We therefore seek an approximation that neglects the self-interaction of the excitation when the barrier is low, but takes into account the full Hamiltonian in the high barrier limit.

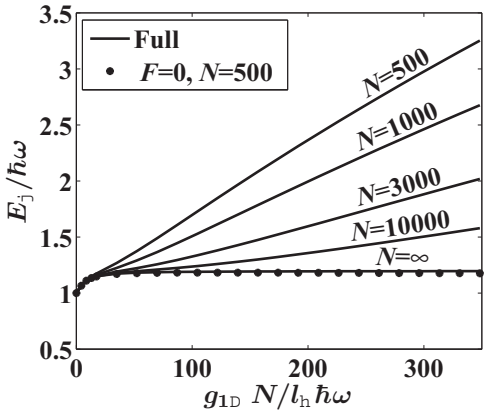

FIG. 3. First excitation energy following from the Hamiltonian (19) as a function of the interaction energy for a harmonic trap. For relatively low particle numbers ($N = 500$), the excitation energy grows linearly with the interaction energy. The excitation energy stays close to the correct value $E_1 = \hbar\omega$ only in the limit $N \to \infty$. Neglecting the last term in Hamiltonian (19) leads to an excitation energy that stays close to the correct value, $\hbar\omega$, with less than 19% deviation (curve with solid circles).

Let us first examine the effect of the self-interaction of the mode ϕ_1 on the eigenstates and eigenvalues of the Hamiltonian (19) for N particles in a harmonic trap as a function of the interaction constant g. In the thermodynamic limit, where $N \to \infty$, with gN kept finite, we expect that the last two terms of the Hamiltonian will be negligible and the lowest eigenvalues of the Hamiltonian will correspond to the two-mode solutions (17) of the Bogoliubov Hamiltonian.

Figure 3 shows the first excitation energy, which is the energy difference between the two lowest eigenvalues of the Hamiltonian (19) for a harmonic trap with varying interaction strengths $g_{1D}N$ for different values of N. It shows that the excitation energy stays close to the correct value of $\hbar\omega$ only in the limit $N \to \infty$. However, if the last term, which is proportional to F, is dropped, then the excitation energy stays close to the correct value for all interaction strengths. Neglecting F makes the Hamiltonian similar to the Bogoliubov Hamiltonian with a single excitation mode. In the next section, we show how this insight can be continued to the whole range of barrier heights in a way that satisfies the validity criteria in Sec. II B.

IV. FROM BOGOLIUBOV TO THE BOSE-HUBBARD HAMILTONIAN

As we have seen in the previous section, the full form of the two-mode Hamiltonian (19) does not provide the right excitation energy for a harmonic trap with a finite number of bosons. In order to facilitate a theory that gives rise to a good

approximation both in the harmonic and the double-well case, we now use the two-mode representation of an ensemble of N bosons as a system with spin $N/2$. First, we define the spin operators

$$\hat{S}_{x'} = \frac{1}{2}(\hat{a}_1^\dagger \hat{a}_0 + \hat{a}_0^\dagger \hat{a}_1), \tag{20}$$

$$\hat{S}_{y'} = \frac{1}{2i}(\hat{a}_1^\dagger \hat{a}_0 - \hat{a}_0^\dagger \hat{a}_1), \tag{21}$$

$$\hat{S}_{z'} = \frac{1}{2}(\hat{n}_1 - \hat{n}_0), \tag{22}$$

which satisfy the canonical commutation relations for spin operators $[\hat{S}_i, \hat{S}_j] = \epsilon_{ijk}\hat{S}_k$, and $\hat{S}_{x'}^2 + \hat{S}_{y'}^2 + \hat{S}_{z'}^2 = N/2(N/2+1)$. In terms of these spin $N/2$ operators, the Hamiltonian (19) becomes

$$\hat{H}_{TM} = (\tilde{\epsilon}_1 + NF)\hat{S}_{z'} + 2U_{11}\hat{S}_{x'}^2 + K(N-1)\hat{S}_{x'} + K(\hat{S}_{x'}\hat{S}_{z'} + \hat{S}_{z'}\hat{S}_{x'}) + F\hat{S}_{z'}^2. \tag{23}$$

This Hamiltonian can be transformed into a simpler form by performing a rotation by an angle θ about the y' axis: $\hat{S}_i \to e^{i\hat{S}_{y'}\theta}\hat{S}_i e^{-i\hat{S}_{y'}\theta}$. This is equivalent to

$$\begin{pmatrix} \hat{S}_{x'} \\ \hat{S}_{z'} \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \hat{S}_x \\ \hat{S}_z \end{pmatrix}, \tag{24}$$

while $\hat{S}_{y'} = \hat{S}_y$. We require that the mixed products of $\hat{S}_x$ and $\hat{S}_z$ in the transformed Hamiltonian vanish. This implies a rotation angle θ that satisfies

$$\tan 2\theta = -\frac{K}{U_{11} - F/2}. \tag{25}$$

The following Hamiltonian is then obtained:

$$\hat{H}_{TM} = \epsilon\hat{S}_z - J\hat{S}_x + U\hat{S}_z^2 + G\hat{S}_x^2, \tag{26}$$

where

$$G = 2U_{11}\cos^2\theta - K\sin 2\theta + F\sin^2\theta, \tag{27}$$

$$U = 2U_{11}\sin^2\theta + K\sin 2\theta + F\cos^2\theta, \tag{28}$$

$$\epsilon = (\tilde{\epsilon}_1 + NF)\cos\theta + K(N-1)\sin\theta, \tag{29}$$

$$J = (\tilde{\epsilon}_1 + NF)\sin\theta - K(N-1)\cos\theta. \tag{30}$$

We find that F and K can be expressed in terms of the new parameters U and G as

$$F = U\cos^2\theta + G\sin^2\theta, \tag{31}$$

$$K = (U - G)\sin\theta\cos\theta, \tag{32}$$

such that the parameters J and ϵ can now be written as

$$\epsilon = [\tilde{\epsilon}_1 + (N - \sin^2\theta)U + \sin^2\theta\, G]\cos\theta, \tag{33}$$

$$J = [\tilde{\epsilon}_1 + (N - \cos^2\theta)G + \cos^2\theta\, U]\sin\theta. \tag{34}$$

Note that in the case of a symmetric potential, such that $K = 0$, the rotation angle is $\theta = \pi/2$ and the parameters of the Hamiltonian become much simpler,

$$U = 2U_{11}, \quad G = F, \qquad J = \tilde{\epsilon}_1, \quad \epsilon = 0. \tag{35}$$

The rotation by an angle θ that led to the Hamiltonian (26), which has a diagonal quadratic form in the spin operators, is equivalent to a rotational transformation into linear superpositions of the annihilation operators $\hat{a}_0, \hat{a}_1$ by a rotation angle of $\theta/2$. This transformation corresponds to a change of wave-function basis, such that the condensate mode ϕ_0 and the first excitation ϕ_1 are transformed into a left-right basis,

$$\begin{pmatrix} \phi_0 \\ \phi_1 \end{pmatrix} = \begin{pmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{pmatrix} \begin{pmatrix} \phi_L \\ \phi_R \end{pmatrix}, \tag{36}$$

where ϕ_L and ϕ_R are called the "left" and "right" modes, respectively. One can verify by direct calculation that the same rotation angle θ that satisfies Eq. (25) is the one that minimizes the overlap integral

$$\int d^3\mathbf{r}\, |\phi_L(\mathbf{r})|^2 |\phi_R(\mathbf{r})|^2 = \frac{G}{2g}, \tag{37}$$

where G is defined in Eq. (27). It follows that the mode functions ϕ_L and ϕ_R are those that exhibit maximum separation, namely, they can be interpreted as the best choice of modes for which each mode occupies the opposite side of the trap. The transformed spin operators can now be defined in terms of the annihilation operators of the left and right modes as

$$\hat{S}_x = \tfrac{1}{2}(\hat{a}_R^\dagger \hat{a}_L + \hat{a}_L^\dagger \hat{a}_R), \tag{38}$$

$$\hat{S}_y = \tfrac{1}{2i}(\hat{a}_R^\dagger \hat{a}_L - \hat{a}_L^\dagger \hat{a}_R), \tag{39}$$

$$\hat{S}_z = \tfrac{1}{2}(\hat{n}_R - \hat{n}_L). \tag{40}$$

In our last step, we examine the role of the left-right overlap parameter G in the two limits of a harmonic trap and a well-separated double-well potential. In the case where there is no barrier and the potential is harmonic, the potential is symmetric, so $\theta = \pi/2$ and $G = F$. As we have shown at the end of the previous section, a correct scaling of the excitation energy is obtained only when F, which is the self-interaction of the excited state, is dropped from the Hamiltonian. In the other limit, Eq. (37) and the demonstration of Fig. 4 show that G as an overlap integral between the left and right modes becomes very small compared with other parameters. Although a two-mode model is mostly justified in this limit, it follows that dropping G from the Hamiltonian has a minor effect. We therefore suggest that the final form of the Hamiltonian and its parameters should be those given above with $G \to 0$. Then, for the whole regime of barrier heights, we obtain the Bose-Hubbard form for the Hamiltonian,

$$\hat{H} = \epsilon\hat{S}_z - J\hat{S}_x + U\hat{S}_z^2. \tag{41}$$

Here the parameters U, J, and ϵ are given in terms of the left and right modes by

$$U = \frac{g}{2}\int d^3\mathbf{r}\,(|\phi_L|^2 - |\phi_R|^2)^2, \tag{42}$$

$$J = \epsilon_1 \sin\theta = \langle\phi_L|h_0|\phi_R\rangle, \tag{43}$$

$$\epsilon = [\epsilon_1 + NU]\cos\theta = \langle\phi_R|h_0|\phi_R\rangle - \langle\phi_L|h_0|\phi_L\rangle + UN\cos\theta, \tag{44}$$

where $h_0 \equiv H_0 + gN|\phi_0|^2 - \mu$ is the effective single-particle Hamiltonian that leads to Eq. (7) for the modes. Here U follows

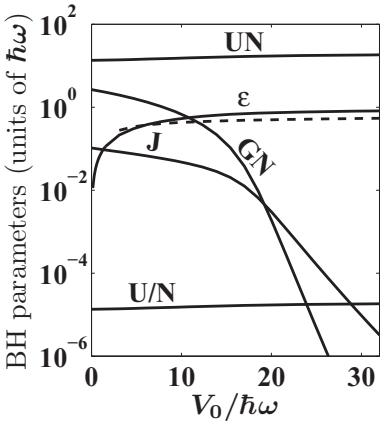

FIG. 4. Parameters of the Bose-Hubbard Hamiltonian (41) as a function of barrier height V_0, asymmetric case ($x_0 = 0.1$ μm), with $N = 1000$, and other parameters as used in Fig. 1. The ratio UN/J determines the degree of number squeezing (see Sec. V). The ratio U/NJ determines ground-state coherence, which drops significantly when $J \sim U/N$. The parameter G, which measures the overlap between the left and right modes, was neglected in the Hamiltonian. At low barrier heights, its neglect is justified by compatibility with the Bogoliubov theory when most of the particles are in the condensate, which satisfies requirement (a) in Sec. II B. At high barrier heights, G drops quickly to negligible values. The dashed line denotes the energy difference between the two minima of the double well, which does not coincide with the bias parameter ϵ.

directly from Eq. (28) and the definition of ϕ_L,ϕ_R, while J and ϵ follow, respectively, from Eqs. (34) and (33) by setting $G = 0$ and neglecting terms of the order unity relative to terms of the order N (implying $\tilde{\epsilon}_1 \to \epsilon_1$).

For later comparison, we also note that the condensate-excitation interaction energy can be written in terms of U (neglecting G) as

$$U_{11} = \tfrac{1}{2} U \sin^2\theta. \tag{45}$$

Figure 4 shows the parameters of the Bose-Hubbard Hamiltonian (41) as a function of the height of the barrier, V_0, for the asymmetric example of Fig. 1. The parameter GN, which was dropped from the Hamiltonian, seems to be important at low barrier heights, but neglecting it in that region was justified by the requirement of compatibility with the scaling of the excitation energy, as correctly predicted by the Bogoliubov theory. In the region where the Bogoliubov model fails, i.e., at high barrier heights, this parameter drops very quickly to zero, which justifies its neglect in that region. The ratio between J and U/N determines the coherence of the Bose gas at the two wells. The coherence drops near the intersection point between J and U/N. The relative number of particles in the two sides of the barrier is determined by the ratio between the parameter ϵ and UN. The parameter ϵ vanishes in the symmetric case, or in the case where $V_0 = 0$ (a single trap).

In order to demonstrate that our method is valid for realistic three-dimensional potentials, we present in Fig. 5 the parameters of the Hamiltonian for a symmetric realistic trap with ^{87}Rb atoms and the single-particle and collective-excitation energies. Again, the collective excitation

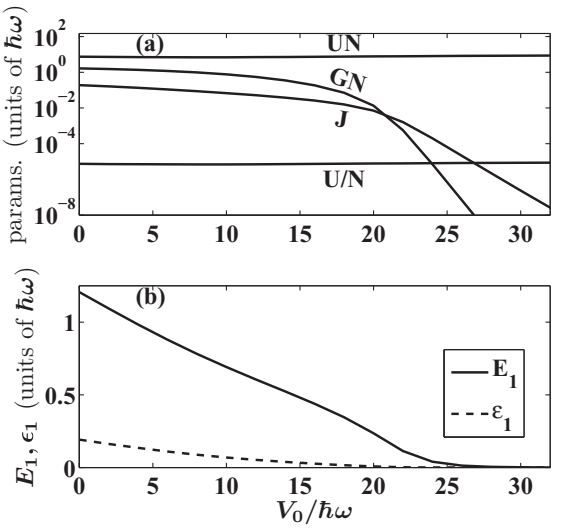

FIG. 5. (a) Parameters of the Bose-Hubbard Hamiltonian as in Fig. 4 for a gas of ^{87}Rb atoms in a three-dimensional harmonic potential with longitudinal frequency $\omega_x = 2\pi \times 500$ Hz and transverse frequencies $\omega_y = \omega_z = 2\pi \times 1.5$ kHz. The barrier parameters are as in Fig. 1. (b) Single-particle (dashed) and collective (solid) excitation energies as a function of barrier height. As in the one-dimensional example, the excitation energy for the harmonic potential ($V_0 = 0$) differs from the expected value $E_1 = \hbar\omega_x$ by ~20%.

for the harmonic trap ($V_0 = 0$) differs from the exact value by ~20%.

To conclude this section, we summarize the algorithm for obtaining the Bose-Hubbard Hamiltonian (41) for an arbitrary potential similar to the form (15): (i) Solve the GPE for the condensate ϕ_0 and find the lowest positive energy solution ϕ_1 of Eq. (7). (ii) For a symmetric potential, ϕ_L and ϕ_R are obtained right away as $\phi_{L,R} = 2^{-1/2}(\phi_0 \pm \phi_1)$ ($\theta = \pi/2$). For an asymmetric potential, the left and right modes are obtained by the transformation (36), with θ obtained either from Eq. (25) or by minimizing the overlap integral (37). (iii) Calculate the parameters U, J, and ϵ of the Hamiltonian by using Eqs. (42)–(44).

In the next section, we give a brief derivation of the solutions of the Hamiltonian and add some more insight concerning coherence and squeezing of the ground state and lowest excitations over the whole range of barrier heights.

V. PHYSICAL PROPERTIES

The steady-state properties and time evolution due to the Hamiltonian (41) were extensively studied in previous works in the weak-coupling regime, where the tunneling between the wells is small. Here we extend the description to the full range of barrier heights and provide a direct connection between the shape of the potential and these properties. However, we restrict ourselves to the ground state and the lowest excitations at very low temperatures. In this context, we also provide two complementary descriptions of the transition from a state where most of the particles occupy a single condensate mode, with a well-defined relative phase when the barrier is low, to the fragmented state when the barrier is high. The fragmented state is a product state of two modes, one in each of the two wells,

with no phase correlation between particles in the two wells. One complementary description relies on the condensate-excitation representation and shows how, with increasing barrier height, the condensate depletion, i.e., the occupation of the first excited mode, grows until the Bogoliubov description breaks down. The other complementary description is based on the left-right representation, and shows how, for low barrier heights, most of the particles are in a coherent superposition of the left and right modes, and how this superposition state becomes a fragmented state through number squeezing when the barrier grows.

A. The Josephson model

Hamiltonian (41) can be solved numerically for a given number of particles. However, to facilitate an intuitive understanding of the solutions, together with analytical approximations for the solutions, we first transform Hamiltonian (41) into the Josephson form. We introduce two conjugate operators: the number operator $\hat{n} \equiv \hat{S}_z$, which measures the difference between the occupations of the two modes, and the phase operator $\hat{\varphi}$, which measures the phase between them. These operators are defined in the Fock basis of eigenestates of the operator $\hat{n}$, namely, $|n\rangle \equiv |n_L,n_R\rangle$, with $n_R = N - n_L$ and $n = (n_R - n_L)/2$, as follows:

$$\hat{n}|n\rangle = n|n\rangle, \quad e^{i\hat{\varphi}}|n\rangle = |n+1\rangle, \tag{46}$$

except for the state $|N/2\rangle$, which is transformed as $e^{i\hat{\varphi}}|N/2\rangle = |-N/2\rangle$. The number and phase operators satisfy (as long as the extreme state $|N/2\rangle$ is excluded) canonical commutation relations $[\hat{\varphi},\hat{n}] = i$, similar to the position and momentum operators.

As we shall see below, the lowest-energy eigenstates of Hamiltonian (41) are superpositions of Fock states $|n\rangle$ around a central value $\bar{n}$, such that the width of the probability distribution in the Fock space is of the order of $\sqrt{N/2}$ or less, and the average phase between the modes in the ground state is $\langle\hat{\varphi}\rangle = 0$. For large N, we may therefore approximate $\hat{S}_x \approx \sqrt{\hat{n}_L\hat{n}_R}\cos\hat{\varphi}$ and estimate $\bar{n}$ of the ground state and lowest-energy excitations by minimizing the energy $\langle\hat{H}\rangle$. This yields the equation

$$\bar{n} = -\frac{\epsilon/2}{U + J/N\eta}, \tag{47}$$

with

$$\eta = \sqrt{1 - 4\bar{n}^2/N^2}. \tag{48}$$

It follows from Eqs. (43) and (44) that

$$\eta = \sin\theta, \quad \bar{n} = -\frac{N}{2}\cos\theta. \tag{49}$$

By expanding the Hamiltonian around the central value $\bar{n}$, we then obtain the Josephson Hamiltonian

$$\hat{H}_J = \tilde{U}(\hat{n} - \bar{n})^2 + \tfrac{1}{2}JN\eta(1 - \cos\hat{\varphi}), \tag{50}$$

where

$$\tilde{U} = U + J/N\eta^3. \tag{51}$$

The eigenstates of the Josephson Hamiltonian are well known. When $J < \tilde{U}/N$, the Hamiltonian is governed by the first term, whose eigenstates are the Fock states $|n\rangle$, for which there is no phase relation between the two sides of the barrier. However, when $J > \tilde{U}/N$, it follows that the lowest eigenstates of the Hamiltonian satisfy $\Delta\varphi \ll 1$, so that the second term may be approximated by $1 - \cos\hat{\varphi} \approx \frac{1}{2}\hat{\varphi}^2$. The quadratic form of the Hamiltonian suggests that its eigenstates are similar to harmonic oscillator states with constant energy splitting $\hbar\omega$, where ω is the Josephson frequency,

$$\hbar\omega_J = \sqrt{JN\eta\tilde{U}}. \tag{52}$$

It may be verified by using Eqs. (43) and (45) that $\hbar\omega_J = E_1$ from Eq. (17), which is the excitation energy of the two-mode Bogoliubov theory in Sec. III.

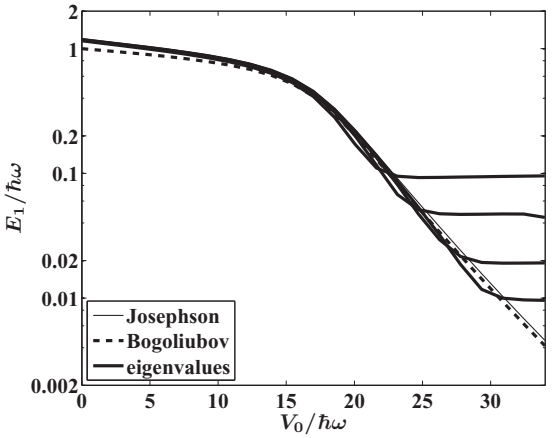

FIG. 6. Energy of the lowest excitation as a function of barrier height for a slightly asymmetric double well, as in Fig. 1, and the Bose-Hubbard parameters of Fig. 4. The Josephson excitation energy $\hbar\omega_J$ of Eq. (52) (thin solid curve) is similar to the two-mode Bogoliubov energy in Fig. 2(d). It is higher, by ∼18% at $V_0 = 0$ and ∼10% at high V_0, than the multimode Bogoliubov energy (dashed curve), which predicts the lowest oscillation frequency of a slightly perturbed initial particle distribution around the equilibrium state, as measured in Ref. [40]. The thick solid curves give the excitation energy obtained numerically by averaging over the eigenvalues of the Hamiltonian (41) over few values of N around $\bar{N} = 100$, 200, 500, and 1000 (top to bottom), such that UN is fixed. In the low tunneling regime $J < U/N$, the ground state becomes a Fock (number) state with average excitation energy $\bar{E}_1 \approx \frac{1}{2}U$. In this case, oscillations around ground-state populations of the two wells are suppressed because all number states are eigenstates of the Hamiltonian.

In Fig. 6, we compare the Josephson energy $\hbar\omega_J$, which is similar to the two-mode Bogoliubov excitation energy in Fig. 2(d), to the excitation energy of the full Bogoliubov model that gives the lowest plasma oscillation frequency when a BEC is slightly driven out of equilibrium. As in Fig. 2, the excitation energy following from the two-mode model is higher by ∼18% than the exact result in the case of a harmonic potential, and by ∼10% in the high barrier regime. Together with the results in Fig. 3, this indicates that the two-mode model provides a satisfactory estimate to the lowest excitation frequency for the full range of barrier heights and interaction strengths, but yet the effect of higher modes on this frequency does not become negligible, even in the limit of weak coupling between the wells. For a relatively small number of particles and strong particle-particle interaction, Fig. 6 shows that the excitation

energy averaged over odd and even numbers N stays fixed on $\bar{E}_{\rm ex} \approx \frac{1}{2}U$ in the weak tunneling regime. In this regime (the Fock regime), the eigenstates of the Hamiltonian are number states and oscillations between the wells can occur if the initial state is a superposition of two different number states, whereas an initial imbalanced number state will not lead to oscillations between the wells. This effect may be interpreted as self-trapping for a population imbalance as small as a single particle.

B. Number squeezing

By analogy of the quadratic form of the Josephson Hamiltonian with a harmonic oscillator Hamiltonian in the conjugate number and phase operators, the number uncertainty in the kth excited state of the Hamiltonian [including the ground state ($k = 0$)] is

$$\langle \Delta n^2 \rangle_k = \sigma^2 \left(k + \frac{1}{2} \right), \tag{53}$$

where

$$\sigma^2 = \sqrt{JN\eta/4\tilde{U}}. \tag{54}$$

In the noninteracting case $U = 0$, we have $\hbar\omega_J = J/\eta$ and $\sigma_0^2 = N\eta^2/2$, which yields the usual Poisson number distribution. However, when the interaction is finite, the number uncertainty is squeezed with squeezing factor

$$\xi \equiv \frac{\sigma}{\sigma_0} = \frac{1}{(1 + NU\eta^3/J)^{1/4}}, \tag{55}$$

so considerable squeezing appears when $UN/J > 1$. This regime covers, in our example of Fig. 4, all the range of barrier heights.

In a noninteracting system ($U = 0$), the ground state is the state where all the particles occupy the condensate mode ϕ_0. In the left-right representation, this ground state is represented by a coherent state with Poissonian number distribution. Left-right number squeezing due to interactions is equivalent, in the condensate-excitation representation, to the appearance of pairs of particles in single-particle excited modes. In the two-mode Bogoliubov model, these pairs are represented by the quasiparticle nonzero coefficient $\tilde{v}_1$, whose square $\bar{v}_1^2$ measures the average occupation of the excited mode. Note that the quasiparticle factors of Eq. (16) may be written explicitly in terms of the squeezing factor as

$$\tilde{v}_1 = \tfrac{1}{2}(1/\xi - \xi), \quad \tilde{u}_1 = \tfrac{1}{2}(1/\xi + \xi). \tag{56}$$

The Bogoliubov approximation breaks down when $\bar{v}_1^2 \approx 1/4\xi^2 \sim N/2$, which corresponds to the limit where $U\eta^3/NJ \sim 1$. As we show below, this limit is characterized by a drop of the coherence and the transition to a fragmented left-right state.

C. Phase uncertainty and coherence

The spatial density of particles is given by

$$n(\mathbf{r}) = n_L|\phi_L|^2 + n_R|\phi_R|^2 + 2\mathrm{Re}(\langle \hat{S}_+ \rangle \phi_L^* \phi_R), \tag{57}$$

where $\hat{S}_+ = \hat{S}_x + i\hat{S}_y \approx \sqrt{\hat{n}_L \hat{n}_R} e^{i\hat{\varphi}}$. The last term in Eq. (57) represents interference between the two modes ϕ_L and ϕ_R, whose contribution is proportional to $\langle e^{i\hat{\varphi}} \rangle$, which we call the *coherence* [18]. If the trapping potential is turned off, then the two modes expand and overlap, so that ϕ_L and ϕ_R become expanding wave packets with spatial phase dependence. Under conditions where particle-particle interaction is not significant during this process, the many-body dynamics will stay frozen and the visibility of the interference pattern that follows from the last term in Eq. (57) is determined by the initial expectation value $\langle e^{i\hat{\varphi}} \rangle$.

In general, the coherence $\langle e^{i\hat{\varphi}} \rangle$ is related to the phase uncertainty as follows [42]:

$$\langle e^{i\hat{\varphi}} \rangle = e^{i\langle \hat{\varphi} \rangle} e^{-\langle (\Delta\varphi)^2 \rangle/2}. \tag{58}$$

The phase uncertainty in the quadratic approximation is equal to

$$\langle (\Delta\varphi)^2 \rangle_k = \sigma^{-2} \left(k + \frac{1}{2} \right). \tag{59}$$

This implies that in a thermal state, where the excitation probability of the kth excited state is $P_k \propto e^{-k\hbar\omega_J/k_BT}$, the phase uncertainty is

$$\langle (\Delta\varphi)^2 \rangle_T = \sigma^{-2} \left[n_T(\hbar\omega_J/k_BT) + \tfrac{1}{2} \right], \tag{60}$$

where

$$n_T(\hbar\omega_J/k_BT) = \frac{1}{e^{\hbar\omega_J/k_BT} - 1} \tag{61}$$

is the total occupation of collective excitations. It follows from Eq. (58) that for $\langle \hat{\varphi} \rangle = 0$, the coherence is

$$\langle e^{i\hat{\varphi}} \rangle_T = \exp\left[-\frac{1}{2\sigma^2} \left(n_T + \frac{1}{2} \right) \right]. \tag{62}$$

Figure 7(a) shows the coherence as a function of barrier height for the ground state ($T = 0$) for different total number of particles N, while $g_{1D}N$ is kept constant, and Fig. 7(b) is for a fixed number of particles ($N = 1000$) at different temperatures. The level of coherence may be attributed to either ground state [in Fig. 7(a)] or thermal relative population of the excited single-particle mode ϕ_1 [in Fig. 7(b)].

The results presented in Fig. 7 and the above equations are valid whenever the phase uncertainty is small compared to unity, in which case the quadratic approximation for the Josephson Hamiltonian is appropriate. However, for states in which $\Delta\varphi \sim 1$ (or equivalently $\Delta n \sim 1$), the system is close to the Fock regime, where eigenstates are number states for which, in general, $\langle \hat{n} \rangle \neq \bar{n}$ and the number and phase uncertainties differ from those given in the above equations. It follows that the coherence plots of Fig. 7 in the regime where they drop below $\sim 1/2$ should be taken as rough estimations that demonstrate the general behavior as a function of number and temperature. It is easy to calculate the more exact values by numerically solving for the eigenstates of the full Bose-Hubbard Hamiltonian (41). Discussion of this regime is beyond the scope of this paper and therefore we do not present these results here.

Note also that in the opposite limit of noninteracting particles, the coherence as defined above does not identically become unity, but rather $\langle e^{i\hat{\varphi}} \rangle = e^{-1/2N\eta^2}$. This follows from the fact that the expression $\langle e^{i\hat{\varphi}} \rangle$ for the coherence is only a

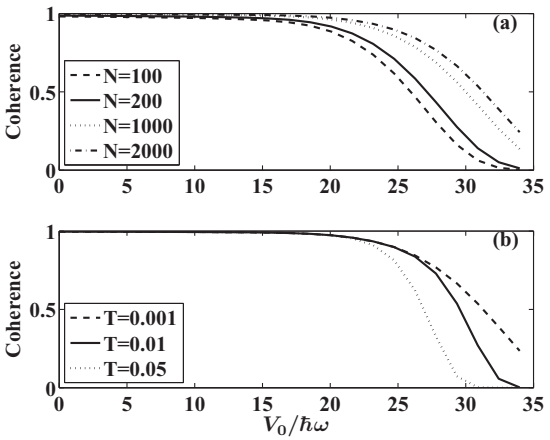

FIG. 7. Coherence $\langle e^{i\hat{\varphi}}\rangle$ between the left and right modes as follows from the parameters of the Bose-Hubbard Hamiltonian in Fig. 4 according to the quadratic approximation for the Josephson model [Eq. (62)]. (a) At zero temperature, for different numbers of particles, such that $g_{1D}N$ is kept constant. (b) For $N = 1000$ for different temperatures (in units of $\hbar\omega/k_B$). At low barrier height, most of the particles are in a superposition of the left and right mode and the coherence is close to 1. The deviation from 1 indicates the existence of single-particle excitations in the ground state (condensate depletion). When the barrier grows, the ground state in (a) becomes incoherent due to the growth of the population of the excited single-particle mode in the ground state or due to thermal excitation of this mode in (b).

large N approximation for the more accurate definition of the coherence as $\langle \hat{S}_+\rangle/\sqrt{n_L n_R}$.

D. Particle density

It is important to examine the deviation of the particle density in steady state from the value $n_0(\mathbf{r}) = N|\phi_0|^2$ that was used here for the mean-field interaction. In terms of the condensate and excitation modes, the density is given by

$$n(\mathbf{r}) = N_0|\phi_0|^2 + N_1|\phi_1|^2 + 2\mathrm{Re}(\langle \hat{a}_0^\dagger \hat{a}_1\rangle \phi_0^* \phi_1). \quad (63)$$

We find that within the Josephson approximation,

$$N_1 \equiv \langle \hat{a}_1^\dagger \hat{a}_1\rangle = \frac{N}{2}\eta^2(1 - \langle e^{i\hat{\varphi}}\rangle), \quad (64)$$

which tends to 0 for a fully coherent gas and to $N\eta^2/2$ in the limit where the coherence vanishes. In the asymmetric case, where $\cos\theta \neq 0$, coherence forms between the condensate and excitation modes,

$$\langle \hat{a}_0^\dagger \hat{a}_1\rangle = \bar{n}\eta(1 - \langle e^{i\hat{\varphi}}\rangle) = -\cot\theta\, N_1. \quad (65)$$

This coherence explicitly goes beyond the Bogoliubov approximation, as it implies that $\langle \hat{b}\rangle \neq 0$, following from a third-order term in the Hamiltonian (19). The resulting spatial density is

$$n(\mathbf{r}) = N|\phi_0|^2 - \frac{2}{\eta}N_1\phi_L\phi_R. \quad (66)$$

If the separation between the two wells is not too large and the temperature is not too high compared to the excitation energy $\hbar\omega_J$, then $N_1 \ll N$, so the deviation from the condensate density is negligible. If the separation is large, the overlap between the modes is quite small and occurs only in the middle of the barrier, where the density is exponentially small. It follows that the particle density deviates from that of the condensate only in the overlap region, such that at full separation, when $N_1 \to N/2$, the density at the center becomes $N|\phi_0|^2/2$, but otherwise the density stays that of the condensate even when the many-body state is fully fragmented.

VI. COMPARISON WITH ALTERNATIVE THEORIES

Let us now compare our theory with the standard approach to a weakly coupled double-well system and with the two-mode HF theory, and discuss the various ranges of validity of these theories.

A. Eigenmodes of the Gross-Pitaevskii equation

Since the beginning of the coupled-mode theory of bosons in a double well, suggestions have been made to use solutions of the GPE in each separated well [14] or to use two stationary solutions of the GPE in the full double-well potential [16,17,26]. In a symmetric double-well potential, it is possible to use the symmetric and antisymmetric solutions of the GPE:

$$\left[\frac{\hat{p}^2}{2m} + V(\mathbf{r}) + gN|\phi_\pm(\mathbf{r})|^2\right]\phi_\pm = E_\pm\phi_\pm. \quad (67)$$

The orthogonality of these modes is ensured by their symmetry. The left and right modes $\phi_{L,R} = 2^{-1/2}(\phi_+ \pm \phi_-)$ are then used even when the potential is not symmetric, under the assumption that the shape of these two modes is not sensitive to their occupation. This assumption is valid as long as the asymmetry is weak enough so that the interaction energy is not significantly different on the two sides of the barrier. A theory based on these modes may be valid when the tunneling rate is low and the coupling between the modes is weak.

In Fig. 8, we compare the tunneling rate J that follows from this theory [20] with our theory. The two approximations coincide in the deep tunneling limit but differ considerably in the low barrier regime, where the value predicted by our theory matches the calculation based on the semiclassical Josephson theory [15]. It follows that the theory based on the stationary eigenmodes of the GPE does not fulfill requirement (a) in Sec. II B. Further demonstration of the compatibility of this approach in the two regimes of weak and strong coupling between the wells is presented in Fig. 9. The shape of the asymmetric solution of the GPE is very different from the shape of the asymmetric Bogoliubov excitation in the low barrier regime, but it becomes very similar to it and to the mode calculated by our theory in the high barrier regime.

Regarding the treatment of asymmetric potentials, our calculations show that the tunneling rate for asymmetric potentials does not significantly differ from that of a symmetric potential with the same parameters except x_0 of Eq. (15) [10% difference for $x_0 = 0.5$ μm, where the population difference is $(n_L - n_R)/N \approx 22\%$]. This implies that for medium asymmetry levels, the parameters of the Bose-Hubbard that result from the symmetric- antisymmetric basis modes may serve as a fair approximation for the asymmetric case. However, as shown in Fig. 4, the bias parameter ϵ is not equal to the potential bias (energy difference between potential minima), so that it

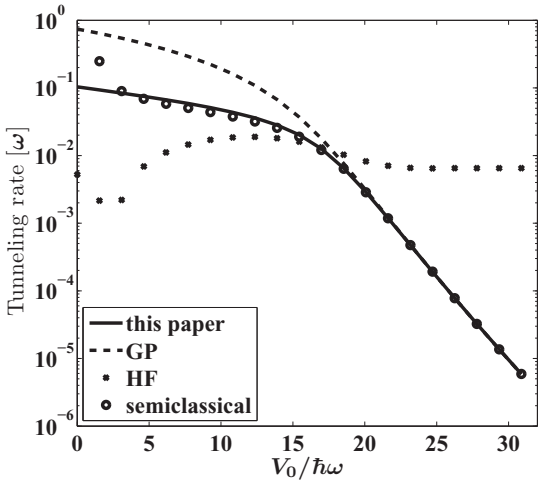

FIG. 8. Tunneling rate J in a symmetric double-well potential as in Fig. 1: The result of our theory (solid curve) is similar to the results of the semiclassical approximation [15] (circles) over most of the range where that approximation is applicable, namely, a symmetric potential with two minima. The theory based on eigenmodes of the GPE (dashed curve) coincides with the last two methods at the deep tunneling limit, while the HF calculation (dots) produces different results in both the deep tunneling regime and the low barrier regime.

might be necessary to calculate it with a model that can bare asymmetric modes, as provided by our theory.

B. Semiclassical functional theory

Reference [15] presented a calculation of the tunneling rate in a double-well potential using a semiclassical functional theory and suggested an expression in the form of an integral based on the particle density calculated using the GPE. This method of calculation, which is unambiguous for the case of a one-dimensional potential, was used in Fig. 8 for a symmetric potential. It shows good agreement with the results of our method over most of the regime where it is valid, namely, when

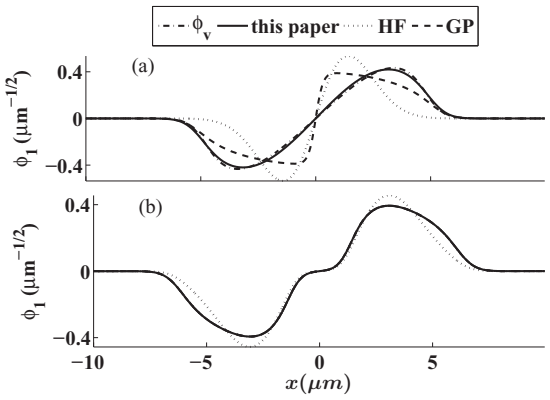

FIG. 9. Comparison between the shape of the first excited mode ϕ_1 within different theories in two regimes: (a) no barrier and (b) high barrier. (a) In a harmonic potential, our theory yields a mode function ϕ_1 fairly close to the normalized Bogoliubov quasiparticle function $v_1(\mathbf{r})$, while the eigenmode of the GPE and the Hartree-Fock mode are different. (b) For a high barrier, the eigenmode of the GPE coincides with our theory and v_1, whereas the HF mode is still different.

the potential has two distinct minima. However, the full shape of the modes and the solution for asymmetric potentials was not provided in Ref. [15]; the method appears to be appropriate only for symmetric or nearly symmetric potentials.

C. Two-mode Hartree-Fock method

A two-mode Hartree-Fock method for bosons, which was termed the multiconfigurational time-dependent Hartree method (MCTDH) was developed several years ago [27–29,31,32] and applied to several steady-state and time-dependent situations [30,33]. This approach is derived in a straightforward manner from the assumption that the multi-particle wave function can be written as a superposition of Fock states of particles in one of two modes ϕ_1 and ϕ_2,

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)=\sum_n c_n\Phi_{n,N-n}(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N), \tag{68}$$

where

$$\Phi_{n,N-n}=\hat{\mathcal{S}}\phi_1(\mathbf{r}_1),\ldots,\phi_1(\mathbf{r}_n)\,\phi_2(\mathbf{r}_{n+1}),\ldots,\phi_2(\mathbf{r}_N) \tag{69}$$

is the state with n particles in mode ϕ_1 and $N-n$ particles in mode ϕ_2, and $\hat{\mathcal{S}}$ denotes the symmetrization over all permutations of $\{\mathbf{r}_j\}$. This is equivalent to assuming that the field operator in Eq. (3) is written as

$$\hat{\Psi}(\mathbf{r})=\phi_1(\mathbf{r})\hat{a}_1+\phi_2(\mathbf{r})\hat{a}_2, \tag{70}$$

where, in contrast to Eq. (1), both ϕ_i and $\hat{a}_i$ are time dependent or subject to variation. This ansatz is used in the Heisenberg equations of motion for the field operator. Upon multiplying this equation by either $\hat{a}_1^\dagger$ or $\hat{a}_2^\dagger$ from the left and taking the expectation value $\langle\hat{a}_i^\dagger\partial\hat{\Psi}/\partial t\rangle$, the following equations of motion for the spatial modes are obtained:

$$i\hbar\frac{\partial\phi_i}{\partial t}=\mathcal{P}\left[H_0\phi_i+g\sum_{mjkl}(\rho^{-1})_{im}\rho_{mjkl}\phi_j^*\phi_k\phi_l\right], \tag{71}$$

where $\mathcal{P}\equiv 1-\sum_j|\phi_j\rangle\langle\phi_j|$ is a projection operator that ensures the orthogonality of the mode functions. $\rho_{ij}=\langle\hat{a}_i^\dagger\hat{a}_j\rangle$ and $\rho_{ijkl}=\langle\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_k\hat{a}_l\rangle$ are the one-particle and two-particle reduced density matrices.

For two modes, the tensor ρ_{ijkl} has $2^4=16$ components, so that in general the equation of motion for each mode function involves 6 different combinations of $\phi_j^*\phi_k\phi_l$ and the 16 components of ρ_{ijkl}.

The two-mode Hartree-Fock theory has been demonstrated to give physical results in some of the situations examined so far. However, it is not able to obtain splitting into a fully separated double well that leads to full fragmentation where coherence is totally lost even when the splitting time is very long and the barrier height very large [27,33]. Here we suggest that this result might be due to a fundamental problem that occurs in the two-mode HF method when the interaction strength is large, as we explain below. This problem is demonstrated in Fig. 8, where we show the tunneling rate predicted by the two-mode HF theory using imaginary time propagation of the self-consistent equations for converging into a steady-state solution [43]. It is clear that these results are not comparable with the physically reasonable results

provided by the other theories, and indicate that the two-mode HF method cannot predict full fragmentation under these circumstances even when the barrier separation is large.

In order to explain the origin of this failure, we first note that Eq. (71) is invariant under a SU(2) transformation of the modes, as in Eq. (36). Let us now examine the case of a symmetric potential and choose the symmetric-antisymmetric mode representation. When the separation between the wells is not too large (or the number of particles is high enough), most of the particles will occupy the symmetric mode (the "condensate" ϕ_0), while only a small number of particles occupy the first excited mode ϕ_1. Within the ground state, the density matrix components with odd number of antisymmetric field operators must vanish. We then obtain the following equations for the modes:

$$i\hbar\frac{\partial\phi_0}{\partial t}=(H_0-\mu)\phi_0+g[(\bar{n}_0|\phi_0|^2+2\bar{n}_1|\phi_1|^2)\phi_0+\bar{m}_1\phi_1^2\phi_0^*], \tag{72}$$

$$i\hbar\frac{\partial\phi_1}{\partial t}=(H_0-\mu-E_1)\phi_1+g\frac{N_0}{N_1}(2\bar{n}_1|\phi_0|^2\phi_1+\bar{m}_1^*\phi_0^2\phi_1^*). \tag{73}$$

Here N_0 and N_1 ($N_0+N_1=N$) are the expectation values of the number of particles in the two modes, $\bar{n}_0\equiv\rho_{0000}/N_0\approx N_0$, $\bar{n}_1=\rho_{0110}/N_0\approx N_1$ and $\bar{m}_1=\rho_{0011}/N_0$, and we have omitted the term proportional to ρ_{1111}, which is third order in ϕ_1. The chemical potential μ and excited-mode frequency follow from the action of the projection operator $\mathcal{P}$.

When the well separation is not too large, so $N_1\ll N_0$, the terms proportional to $\bar{n}_1$ and $\bar{m}_1$ can be omitted from Eq. (72), and the GPE is recovered. Equation (73) takes the form of a Schrödinger equation for a single particle in a potential,

$$V_{\rm eff}=V+g\frac{N_0}{N_1}(2\bar{n}_1+\bar{m}_1^*)|\phi_0|^2. \tag{74}$$

Note that in terms of the $\hat{b}$ operators defined just before Eq. (10), the coefficients $\bar{n}_1$ and $\bar{m}_1$ are given by $\bar{n}_1=\langle\hat{b}_1^\dagger\hat{b}_1\rangle$ and $\bar{m}_1=\langle\hat{b}_1\hat{b}_1\rangle$, respectively. According to the two-mode reduction of the Bogoliubov theory in Sec. III, these coefficients are given by

$$\bar{n}_1=|\tilde{v}_1|^2=N_1, \tag{75}$$

$$\bar{m}_1=-\tilde{u}_1\tilde{v}_1=-\sqrt{N_1(N_1+1)}. \tag{76}$$

It follows that $V_{\rm eff}\approx V+gN|\phi_0|^2[2-\sqrt{(N_1+1)/N_1}]$. Unless $N_1\gg1$, as expected in the limit where $J/U\to0$ [see Eq. (64)], the effective potential turns out to be more attractive than the effective potential $V+gN|\phi_0|^2$ that is experienced by the condensate mode ϕ_0. This leads to a considerable difference between the mode ϕ_1 calculated by the HF method compared with calculations using the other methods, as demonstrated in Fig. 9. When the two wells are separated by a high barrier, the shapes of ϕ_0 and ϕ_1 in the two wells are significantly different, as demonstrated in Fig. 10. In the left-right basis, this yields that the mode ϕ_L retains a nonvanishing tail in the right well, and vice versa. This effect, in turn, is responsible for keeping the tunneling rate high even when the separation between the wells is large,

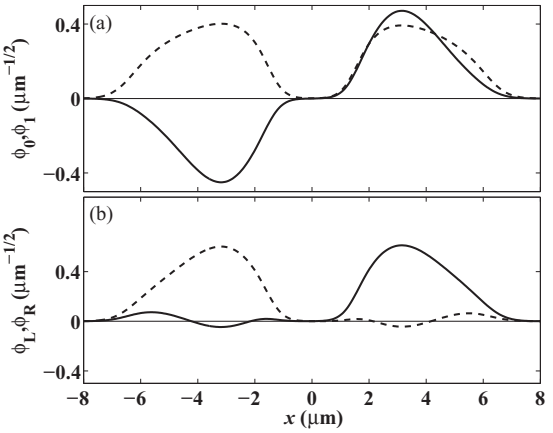

FIG. 10. Spatial modes obtained with the two-mode HF method for a strongly separated double-well potential with a slight asymmetry as in Fig. 1. (a) In the condensate-excitation representation, the excitation has a narrower profile compared to the condensate mode at each well, due to an effective attractive potential [Eq. (74)]. (b) This gives rise to considerable tails of the left mode ϕ_L in the right well, and vice versa, so that even in the limit of complete separation, the overlap between ϕ_L and ϕ_R does not vanish.

so that, in a self-consistent manner, N_1 does not grow with growing separation and fragmentation is not achieved. This is clearly an unphysical result which violates requirement (b) in Sec. II B. For similar reasons, requirement (a) is violated as well.

Equations (72) and (73) are calculated self-consistently with the solution of the many-body Hamiltonian (5). This self-consistent calculation yields the shape of the modes and the values of $\bar{n}_1$ and $\bar{m}_1$. Because of the self-consistency requirement, it is difficult to derive an analytic estimate of these values for a given shape of the potential and interaction strength. However, our numerical calculations show that when the barrier height is increased to form a potential with large well separation, the tunneling rate hangs up at a certain value and does not decrease further when the barrier height is further increased. This problem occurs only at very high barrier heights and low tunneling rates when the interaction is relatively weak. However, when the interaction strength is comparable to that used in our example, the problem appears at relatively low levels of separation: the left-right overlap remains large and the tunneling rate hangs up at a high value, as in Fig. 8.

It is interesting to note that the quantities $\bar{n}_1$ and $\bar{m}_1$ are equivalent to the normal and the anomalous densities of the noncondensate single-particle excitations in the Bogoliubov theory [11]. A self-consistent theory that fully takes these quantities into account leads to an unphysical theory of the Bogoliubov excitations, which predicts an excitation gap. In order to overcome this problem, it is essential to use an approximation such as the Popov approximation which neglects the anomalous density, thereby obtaining a physically reasonable theory at the price of losing full self-consistency. Here, as well, we have shown that a fully self-consistent theory, which assumes the existence of only two modes, leads to unphysical results and therefore it is essential to

abandon self-consistency for the sake of gaining an improved approximation.

VII. SUMMARY AND DISCUSSION

We developed a theory of many interacting bosonic particles in a double-well potential which is valid over the whole range of barrier heights, from a harmonic (single-well) potential to a double-well potential with large separation between the two wells. In the two limits of high and low (or no) barrier, this theory provides correct predictions for fundamental physical properties; in the high barrier regime, our theory coincides with the two-site Bose-Hubbard model with standard values of its parameters, and in the low barrier regime, it provides satisfactory agreement with the GPE and Bogoliubov theory for a single excitation above the condensate.

Our theory provides a continuous description of adiabatic splitting of a condensate all the way from a single well with a coherent condensate to a well-separated double well with a fragmented state of two nonoverlapping modes. In a harmonic potential with no barrier at zero temperature, most of the atoms are in the condensate state, while a small fraction of particles occupy pairs of single-particle excited states. The noncondensate fraction grows with increased particle-particle interaction and this reflects squeezing in the system. While the lowest single-particle excitation energy decreases with growing interaction energy, the lowest collective (Bogoliubov) excitation energy in a harmonic trap stays equal to $\hbar\omega$ and reflects a collective motion of the center of mass in the trap. When the barrier grows and separates the BEC into two well-separated wells, the fraction of noncondensate particles grows together with the squeezing, while the lowest single-particle excitation energy and collective excitation energy decrease. When the barrier grows to a level where the noncondensate fraction is macroscopic, the standard Bogoliubov approximation ceases to be valid, while our generalized two-mode theory is better interpreted in the left-right mode representation rather than the condensate-excitation representation. We have also shown that a coherence measure may be defined for the two-mode system, such that the drop of coherence is closely related to the increase of squeezing and the growth of noncondensate population. At finite temperatures, the coherence further decreases due to the thermal occupation of collective excitations. With growing barrier and decrease of the collective excitation energy, the coherence drastically drops when the excitation energy becomes comparable to or smaller than the temperature.

A two-mode basis that can be used for the theory presented here is the condensate-mode function, which is the lowest energy solution of the GPE, and the lowest first excited solution of the Schrödinger equation with an effective repulsive potential due to the condensate. We have shown that there is good agreement between the spatial shape of this first excited mode and the quasiparticle wave functions $u_1(\mathbf{r})$ and $v_1(\mathbf{r})$. This agreement improves with growing barrier height. This mode basis is suitable even for highly asymmetric potentials and may be extended into a many-mode basis.

A crucial step in our derivation was the neglect of terms in the Hamiltonian proportional to the parameter G [see Eq. (27)], which measures the overlap between the spatial densities of the left and right modes. In the low tunneling regime, this step is justified because G drops to zero much faster than other parameters, such as the tunneling rate. The neglect of G in the high tunneling regime yields good agreement with the excitation energy given by the Bogoliubov theory. We conjecture that in a full multimode Hamiltonian treatment, a multimode cancellation effect may cancel with this term, and this is responsible for the fact that a two-mode theory without this term in the Hamiltonian provides better predictions than a theory that keeps all the two-mode terms but still neglects terms involving other modes.

We compared our theory to previous two-mode theories with predictions both for the spatial shape of the modes and the many-body structure of the ground state and excitations. We showed that while the semiclassical functional theory [15] recovers our parameters fairly well over most of the range of barrier height, the method based on eigenstates of the GPE gives comparable predictions only in the regime of weak coupling between the left and right modes. The two-mode Hartree-Fock method does not provide comparable predictions for the tunneling rate when the interaction is relatively strong and does not show fragmentation at large barrier separations. This result, together with the above observation that led to the neglect of the factor G, indicates that a self-consistent theory does not always lead to physical results, and needs to be fixed, similar to self-consistent theories of a Bose gas at finite temperature, which led to a nonphysical gap in the excitation spectrum [11].

The insight provided by this work may help to better understand matter-wave splitting for atom interferometry. Improved quantitative predictions for low barriers and higher temperature may be achieved by a high-temperature Bogoliubov theory, which uses a multimode description of the excitations. However, we believe that our theory is unique in that it provides a clear connection of this regime with the high barrier regime, where two-mode theories can provide appropriate predictions.

We are currently working on the extension of this work into a time-dependent two-mode theory, which will also be valid along the whole range of coupling between the modes. Such a theory, together with the current steady-state foundation, may enable a more general understanding of both the spatial and many-body aspects of matter-wave dynamics in multiple-well structures.

ACKNOWLEDGMENTS

This work was supported in part by the US-Israel Binational Science Foundation (Grants No. 2006212 and No. 2011295) and the James Franck German-Israel Binational Program.

APPENDIX: ESTIMATE OF THE FUNCTIONAL FORM OF QUASIPARTICLE WAVE FUNCTIONS

Here we estimate the deviation of the spatial form of the quasiparticle wave functions $u_1(\mathbf{r})$ and $v_1(\mathbf{r})$ of the first Bogoliubov excitation from the mode function ϕ_1 satisfying Eq. (7). We use an equivalent form of the Bogoliubov

de-Gennes equations (13), which is based on the functions $\psi_k^{(\pm)}(\mathbf{r}) = u_k(\mathbf{r}) \pm v_k(\mathbf{r})$. These functions satisfy [12]

$$(h_0 + 2gN|\phi_0|^2)h_0\psi_k^{(+)} = E_k^2\psi_k^{(+)}, \tag{A1}$$

$$h_0(h_0 + 2gN|\phi_0|^2)\psi_k^{(-)} = E_k^2\psi_k^{(-)}, \tag{A2}$$

with $h_0 \equiv H_0 + gN|\phi_0|^2 - \mu$, such that $h_0\phi_k = \epsilon_k\phi_k$. From Eq. (13), it also follows that

$$h_0\psi_k^{(-)} = E_k\psi_k^{(+)}. \tag{A3}$$

We now use the expansion of $\psi_1^{(+)}$ in terms of the mode functions $\psi_1^{(+)} = \sum_{k=1}^{\infty} c_k\phi_k$ to obtain

$$\sum_{k'}\left[\epsilon_{k'}(\epsilon_k\delta_{kk'} + 2NU_{kk'}) - E_1^2\delta_{kk'}\right]c_{k'} = 0. \tag{A4}$$

Using perturbation theory, namely, assuming that $c_1 \gg c_k$ for all $k > 1$, we obtain, to the lowest order in c_k,

$$c_k \approx \frac{2NU_{k1}\epsilon_1}{\epsilon_k(\epsilon_k + 2NU_{kk}) - E_1^2}c_1. \tag{A5}$$

If we expand u_1 and v_1 in terms of the mode functions as $u_1 = \sum_k c_{uk}\phi_k$ and $v_1 = \sum_k c_{v1}\phi_k$, it follows from Eq. (A3) that

$$c_{uk} = \tfrac{1}{2}(1 + E_1/\epsilon_k)c_k, \tag{A6}$$

$$c_{vk} = \tfrac{1}{2}(1 - E_1/\epsilon_k)c_k, \tag{A7}$$

so that the ratio between the coefficients with $k > 1$ and those of $k = 1$ is

$$\frac{c_{uk}}{c_{u1}} = \frac{U_{k1}}{U_{11}}\frac{\epsilon_1^2(E_1/\epsilon_1 - 1)(E_1/\epsilon_k + 1)}{E_k^2 - E_1^2}, \tag{A8}$$

$$\frac{c_{vk}}{c_{v1}} = \frac{U_{k1}}{U_{11}}\frac{\epsilon_1^2(E_1/\epsilon_1 + 1)(E_1/\epsilon_k - 1)}{E_k^2 - E_1^2}, \tag{A9}$$

where $E_k^2 = \epsilon_k(\epsilon_k + 2NU_{kk})$. In a shallow potential, where $|\phi_0|^2$ is flat in most of the trap region, the integrals U_{k1} for $k \neq 1$ are small due to the orthogonality of the modes, so that $|U_{k1}/U_{11}| \ll 1$. This ratio may become higher when the trap is tighter, but it is always much smaller than unity. In a symmetric or slightly asymmetric potential, the main contribution from higher modes comes from the third excited mode ($k = 3$) or higher modes with odd index. The factor $\epsilon_1^2/(E_k^2 - E_1^2)$ is then always smaller than $1/(k^2 - 1) < 1/8$. For a harmonic trap, it follows that the magnitude of the coefficients c_{uk} is on the order of $1/k^2$ and it is even smaller for c_{vk}. However, for a double-well potential where ϵ_1, as well as E_1, significantly decrease, while ϵ_k and E_k stay large as in a harmonic trap, these higher mode contributions significantly decrease, and the spatial shape of the quasiparticle wave functions u_1 and v_1 become more and more similar to the first excited single-particle mode ϕ_1.

[1] M. R. Andrews, C. G. Townsend, H.-J. Miesner, D. S. Durfee, D. M. Kurn, and W. Ketterle, Science **275**, 637 (1997).

[2] Y. Shin, M. Saba, T. A. Pasquini, W. Ketterle, D. E. Pritchard, and A. E. Leanhardt, Phys. Rev. Lett. **92**, 050405 (2004).

[3] T. Schumm, S. Hofferberth, L. M. Andersson, S. Wildermuth, S. Groth, I. Bar-Joseph, J. Schmiedmayer, and P. Krüger, Nature Phys. **1**, 57 (2005).

[4] G.-B. Jo, Y. Shin, S. Will, T. A. Pasquini, M. Saba, W. Ketterle, and D. E. Pritchard, M. Vengalattore, and M. Prentiss, Phys. Rev. Lett. **98**, 030407 (2007).

[5] S. Fölling, S. Trotzky, P. Cheinet, M. Feld, R. Saers, A. Widera, T. Müller, and I. Bloch, Nature (London) **448**, 1029 (2007).

[6] J. Esteve, C. Gross, A. Weller, S. Giovanazzi, and M. K. Oberthaler, Nature (London) **445**, 1216 (2008).

[7] K. Maussang, G. E. Marti, T. Schneider, P. Treutlein, Y. Li, A. Sinatra, R. Long, J. Esteve, and J. Reichel, Phys. Rev. Lett. **105**, 080403 (2010).

[8] M. Albiez, R. Gati, J. Fölling, S. Hunsmann, M. Cristiani, and M. K. Oberthaler, Phys. Rev. Lett. **95**, 10402 (2005).

[9] S. Levy, E. Lahoud, I. Shomroni, and J. Steinhauer, Nature (London) **449**, 579 (2007).

[10] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **71**, 463 (1999), and references therein.

[11] A. Griffin, Phys. Rev. B **53**, 9341 (1996).

[12] D. A. W. Hutchinson, K. Burnett, R. J. Dodd, S. A. Morgan, M. Rusch, E. Zaremba, N. P. Proukakis, M. Edwards, and C. W. Clark, J. Phys. B **33**, 3825 (2000).

[13] L. Salasnich, A. Parola, and L. Reatto, Phys. Rev. A **60**, 4171 (1999).

[14] A. Smerzi, S. Fantoni, S. Giovanazzi, and S. R. Shenoy, Phys. Rev. Lett. **79**, 4950 (1997).

[15] I. Zapata, F. Sols, and A. J. Leggett, Phys. Rev. A **57**, R28 (1998).

[16] S. Raghavan, A. Smerzi, S. Fantoni, and S. R. Shenoy, Phys. Rev. A **59**, 620 (1999).

[17] E. A. Ostrovskaya, Y. S. Kivshar, M. Lisak, B. Hall, F. Cattani, and D. Anderson, Phys. Rev. A **61**, 031601 (2000).

[18] L. Pitaevskii and S. Stringari, Phys. Rev. Lett. **87**, 180402 (2001).

[19] J. R. Anglin, P. Drummond, and A. Smerzi, Phys. Rev. A **64**, 063605 (2001).

[20] R. Gati and M. K. Oberthaler, J. Phys. B **40**, R61 (2007); S. Giovanazzi, J. Esteve, and M. K. Oberthaler, New J. Phys. **10**, 045009 (2008).

[21] E. Boukobza, M. Chuchem, D. Cohen, and A. Vardi, Phys. Rev. Lett. **102**, 180403 (2009).

[22] G. Ferrini, A. Minguzzi, and F. W. J. Hekking, Phys. Rev. A **78**, 023606 (2008).

[23] J. Javanainen and S. M. Yoo, Phys. Rev. Lett. **76**, 161 (1996).

[24] Y. Castin and J. Dalibard, Phys. Rev. A **55**, 4330 (1997).

[25] M. Greiner, O. Mandel, T. W. Hänsch, and I. Bloch, Nature (London) **419**, 51 (2002).

[26] D. Ananikian and T. Bergeman, Phys. Rev. A **73**, 013604 (2006); **74**, 039905(E) (2006).

[27] A. I. Streltsov, O. E. Alon, and L. S. Cederbaum, Phys. Rev. Lett. **99**, 030402 (2007).

[28] O. E. Alon, A. I. Streltsov, and L. S. Cederbaum, Phys. Rev. A **77**, 033613 (2008).

[29] K. Sakmann, A. I. Streltsov, O. E. Alon, and L. S. Cederbaum, Phys. Rev. A **78**, 023615 (2008).

[30] O. E. Alon, A. I. Streltsov, and L. S. Cederbaum, Phys. Lett. A **373**, 301 (2009).
[31] D. Masiello, S. B. McKagan, and W. P. Reinhardt, Phys. Rev. A **72**, 063624 (2005).
[32] D. J. Masiello and W. P. Reinhardt, Phys. Rev. A **76**, 043612 (2007).
[33] D. K. Faust and W. P. Reinhardt, Phys. Rev. Lett. **105**, 240404 (2010).
[34] D. S. Murphy and J. F. McCann, Phys. Rev. A **77**, 063413 (2008).
[35] Ch. Lee, E. A. Ostrovskaya, and Y. S. Kivshar, J. Phys. B **40**, 4235 (2007).
[36] S. Zöllner, H.-D. Meyer, and P. Schmelcher, Phys. Rev. A **75**, 043608 (2007).
[37] P. I. Schneider, S. Grishkevich, and A. Saenz, Phys. Rev. A **80**, 013404 (2009).
[38] Y. Japha and Y. B. Band, J. Phys. B **35**, 2383 (2002).
[39] Y. Castin and R. Dum, Phys. Rev. A **57**, 3008 (1998).
[40] L. J. LeBlanc, A. B. Bardon, J. McKeever, M. H. T. Extavour, D. Jervis, J. H. Thywissen, F. Piazza, and A. Smerzi, Phys. Rev. Lett. **106**, 025302 (2011).
[41] J. M. Vogels, K. Xu, C. Raman, J. R. Abo-Shaeer, and W. Ketterle, Phys. Rev. Lett. **88**, 060402 (2002).
[42] A. Stern, Y. Aharonov, and Y. Imry, Phys. Rev. A **41**, 3436 (1990).
[43] Y. Japha and Y. B. Band, e-print arXiv:1010.4918v1.