Nonlinear mixing of quasiparticles in an inhomogeneous Bose condensate

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We use a one-dimensional time-dependent nonlinear Schrödinger equation (NLSE) to study the temporal evolution of excited-state populations of an inhomogeneous Bose condensate. We show how one can decompose an arbitrary single-particle wave function into a condensate and a collection of quasiparticles and we use this method to analyze simulations in which the initial wave function contains a finite amount of excitation in a single mode. The nonlinear mixing of the quasiparticles is dominated by processes that approximately conserve energy and we see the reversible transfer of excitation between energetically matched modes. We show analytically how the time scale for nonlinear mixing depends on the amount of initial excitation and the size of the nonlinearity. We propose that, by averaging over the phase of the excitations, the NLSE can be used as a simple tool for the simulation of incoherent excitations. This will allow the techniques presented here to be used to explore finite-temperature mixing effects. [S1050-2947(98)00105-X]

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I. INTRODUCTION

Recent experiments [1,2] on the excitation spectrum of Bose-condensed trapped alkali gases have provided striking agreement with theory [3,4] based on the nonlinear Schrödinger equation (NLSE) of Ginzburg and Pitaevskii, and Gross [5]. As well as measuring the energies of the excitations, however, the experiments can also probe their damping and observe decay rates that vary strongly with temperature [6]. Theoretical predictions for these decay rates exist for homogeneous gases (see, for example, Refs. [7,8]) and recently some predictions for the inhomogeneous condensates of current experiments have appeared [9,10]. As part of an approach to this problem we have been looking at the nonlinear mixing of the excitations (quasiparticles) on the condensate and we present some of the results from this work in this paper. Although we concentrate here on simple processes at zero temperature, we believe that the techniques used can be extended to estimate finite-temperature mixing processes using only the NLSE.

In Sec. II we briefly review the theory of the zero-temperature excitations on the condensate. Conventionally, the shapes and frequencies of the excitations are given by the Bogoliubov–de Gennes equations and are not orthogonal to the condensate. It is possible to modify them, however, to produce orthogonal excitations and we show how this can be achieved. In Sec. III we present a technique that allows one to decompose a single-particle wave function into a condensate and a collection of quasiparticles, even if one uses the conventional excitations that are not orthogonal to the condensate. We use this decomposition technique in Sec. IV to analyze the results of simulations in which we propagate the NLSE with a finite initial population in a single-quasiparticle mode. As the amount of excitation is increased we observe nonlinear mixing into other quasiparticle modes. The evolution is dominated by processes that approximately conserve

energy and we observe the reversible transfer of population between energetically matched modes. In Sec. V we take an analytical approach and derive a result for how the time scale for nonlinear mixing depends on the amount of initial excitation and the size of the nonlinearity. Finally, in Sec. VI we argue that the NLSE can be used to approximately simulate the evolution of the full quantum field and that therefore the techniques presented here for the analysis of nonlinear mixing can be extended to study finite-temperature effects such as the decay of excitations.

II. REVIEW OF THE THEORY OF QUASIPARTICLES

A number of authors have considered the problem of finding the shapes and frequencies of the excitations on an inhomogeneous condensate (see, for example, Refs. [3,4,11,12]). The fundamental excitations, or normal modes, are termed ''quasiparticles'' and at low temperatures the system may be considered to consist of a condensate and a thermal population of weakly interacting quasiparticles. The shapes and energies of the quasiparticles can be obtained either by considering linear deviations around the condensate or by describing the system using an approximate quadratic Hamiltonian that can be diagonalized using standard methods. The details of these two approaches can be found in Ref. [12] and we give a brief review of the relevant theory below.

At very low temperatures a dilute gas of identical bosons can form a Bose-Einstein condensate (BEC) in which all the atoms are described by the same wave function $\Psi(\mathbf{r},t)$. The equation of motion for this wave function is given by the time-dependent NLSE

$$\iota\hbar \frac{\partial \Psi}{\partial t} = \hat{H}_0 \Psi + U_0 |\Psi|^2 \Psi, \tag{1}$$

where Ψ is normalized to the number of particles in the trap, i.e., $\int d^3\mathbf{r}\,|\Psi|^2 = N$. $\hat{H}_0$ is the noninteracting single-particle Hamiltonian given by

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\nabla_r^2 + V_{\text{trap}}(\mathbf{r}), \qquad (2)$$

where $V_{\text{trap}}(\mathbf{r})$ is the magnetic potential that confines the atoms. In accordance with the current experimental configurations, we will take this to be harmonic. In Eq. (1) the particle interactions are modeled by a local potential. In three dimensions (3D) this is achieved using the Fermi pseudopotential [13,14]

$$V_{\text{int}}(\mathbf{r}-\mathbf{r}') = U_0\delta(\mathbf{r}-\mathbf{r}'), \qquad (3)$$

where U_0 is related to the s-wave scattering length a by

$$U_0 = \frac{4\pi\hbar^2 a}{m}. \qquad (4)$$

This is a common approximation in the theoretical approach to BEC and should be valid for the dilute gases under consideration. A detailed discussion of the validity of this replacement can be found in Ref. [15].[1]

Equation (1) has a lowest-energy eigenstate solution of the form

$$\Psi(\mathbf{r},t) = \psi_g(\mathbf{r})e^{-\iota\mu t}, \qquad (5)$$

where μ is the chemical potential of the system. Thus ψ_g satisfies the time-independent NLSE

$$\mu\psi_g = \hat{H}_0\psi_g + U_0|\psi_g|^2\psi_g. \qquad (6)$$

We can find the excitations on top of this ground-state, or condensate, wave function by considering a small disturbance and linearizing with respect to it. Since the nonlinear term in Eq. (1) couples waves traveling in opposite directions we look for a solution of the form

$$\Psi(\mathbf{r},t) = e^{-\iota\mu t}\left[\psi_g(\mathbf{r}) + \sum_i \{u_i(\mathbf{r})c_i e^{-\iota\omega_i t}\right.$$
$$\left. + v_i^*(\mathbf{r})c_i^* e^{+\iota\omega_i t}\}\right], \qquad (7)$$

where the c_i's are constants. If we substitute this into Eq. (1), linearize with respect to the c_i's, and equate coefficients of $e^{\pm\iota\omega t}$, then we find the so-called Bogoliubov–de Gennes (BdG) equations

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[1]In our one-dimensional simulations we can still use Eq. (3), but the parameter U_0 can no longer be directly related to the s-wave scattering length as in Eq. (4), since this equation is only valid in 3D. In our simulations, therefore, U_0 is an input parameter describing the importance of the nonlinear term, but is not directly related to physical quantities.

$$\mathcal{L}u_i + U_0\psi_g^2 v_i = \omega_i u_i,$$
$$\mathcal{L}v_i + U_0\psi_g^{*2}u_i = -\omega_i v_i, \qquad (8)$$

where

$$\mathcal{L} \equiv \hat{H}_0 - \mu + 2U_0|\psi_g|^2. \qquad (9)$$

Equations (8) imply that the u_i's and v_i's satisfy the orthogonality and symmetry relations

$$\int d^3\mathbf{r}\,\{u_i u_j^* - v_i v_j^*\} = \delta_{ij}, \qquad (10)$$

$$\int d^3\mathbf{r}\,\{u_i v_j - v_i u_j\} = 0. \qquad (11)$$

In this approach, the normalization when $i=j$ in Eq. (10) can be freely chosen since Eqs. (8) are linear. However, the above relations have a deeper significance in the fact that the quantum quasiparticle operators obey Bose commutation relations and this forces the normalization to 1. Equations (6) and (8) completely determine the shapes and frequencies of the linear excitations on the condensate. Analytical solutions can be obtained in the homogeneous case and for the trapped gas in the noninteracting and strong-coupling (Thomas-Fermi) limits [4], but otherwise they must be solved numerically. This is achieved by converting to a basis set and the method is described in detail in Ref. [12].

One feature of the BdG equations that is particularly important later in this paper is the existence of an exact solution with $\omega=0$, $u_0(\mathbf{r})=\psi_g(\mathbf{r})$, and $v_0(\mathbf{r})=-\psi_g^*(\mathbf{r})$. This "condensate" mode has zero norm, but otherwise satisfies the orthogonality and symmetry relations of Eqs. (10) and (11), which both take the form

$$\int d^3\mathbf{r}\,\{\psi_g^* u_i + \psi_g v_i\} = 0. \qquad (12)$$

However, $\int d^3\mathbf{r}\,\{\psi_g^* u_i\}$ and $\int d^3\mathbf{r}\,\{\psi_g v_i\}$ are not separately zero, so the excitations defined by Eqs. (8) are not orthogonal to the condensate. This point is discussed further below, but it is shown in Sec. III that the partial orthogonality of Eq. (12) is sufficient to allow one to project out the condensate and quasiparticle contributions to any single-particle wave function.

The second approach to finding the excitations of the system involves working with the many-body Hamiltonian, which in the field operator formalism is given by

$$\hat{H} = \int d^3\mathbf{r}\left\{\hat{\Psi}^\dagger(\mathbf{r},t)\hat{H}_0\hat{\Psi}(\mathbf{r},t)\right.$$
$$\left. + \frac{1}{2}U_0\hat{\Psi}^\dagger(\mathbf{r},t)\hat{\Psi}^\dagger(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\right\}, \qquad (13)$$

where $\hat{\Psi}(\mathbf{r},t)$ is the usual Bose field operator. We follow Refs. [16,17] and write the field operator as

$$\hat{\Psi}(\mathbf{r},t) = e^{-\iota\mu t}[\psi_g(\mathbf{r}) + \hat{\delta}(\mathbf{r},t)], \qquad (14)$$

where $\psi_g(\mathbf{r})$ satisfies Eq. (6) and the operator $\hat{\delta}(\mathbf{r},t)$ represents quantum and thermal fluctuations above the condensate. If we substitute Eq. (14) into the Hamiltonian and dis-

card terms that contain three or four $\hat{\delta}(\mathbf{r},t)$ operators then we are left with a quadratic Hamiltonian that can be diagonalized exactly. This is achieved by the Bogoliubov transformation

$$\hat{\delta}(\mathbf{r},t) = \sum_i \{u_i(\mathbf{r})\hat{\beta}_i + v_i^*(\mathbf{r})\hat{\beta}_i^\dagger\} \tag{15}$$

if the functions u_i and v_i are chosen to satisfy the equations

$$\int d^3\mathbf{r} \{u_i^*[\mathcal{L}u_j + U_0\psi_g^2 v_j] + v_i^*[\mathcal{L}v_j + U_0\psi_g^{*2}u_j]\} = \omega_i\delta_{ij}, \tag{16}$$

$$\int d^3\mathbf{r} \{u_i[\mathcal{L}v_j + U_0\psi_g^{*2}u_j] + v_i[\mathcal{L}u_j + U_0\psi_g^2 v_j]\} = 0. \tag{17}$$

In addition, since the operators $\hat{\delta}(\mathbf{r},t)$ and $\{\hat{\beta}_i\}$ satisfy the usual Bose commutation relations, there are further restrictions on the possible values of u_i and v_i, which are the orthonormality and symmetry conditions of Eqs. (10) and (11) [18].

It is clear by inspection that the BdG relations of Eqs. (8) satisfy Eqs. (16) and (17) and are therefore sufficient to diagonalize the Hamiltonian. However, it has been pointed out by Gardiner that they are not necessary conditions [the necessary conditions are given by Eqs. (16) and (17)] and that this allows one to choose the excitations to be orthogonal to the condensate [19]. This is achieved by projecting out the overlap with the condensate from the solutions to the BdG equations. Thus we define new u and v functions by

$$\widetilde{u}_i = u_i - a_i\psi_g/N_0,$$

$$\widetilde{v}_i^* = v_i^* + a_i^*\psi_g/N_0, \tag{18}$$

where $a_i = \int d^3\mathbf{r} \{\psi_g^* u_i\} = -\int d^3\mathbf{r} \{\psi_g v_i\}$ [the equality of these two projections follows from Eq. (12)] and $\int d^3\mathbf{r} |\psi_g|^2 = N_0$. The new excitations satisfy the modified BdG equations

$$\mathcal{L}\widetilde{u}_i + U_0\psi_g^2\widetilde{v}_i = \omega_i(\widetilde{u}_i + a_i\psi_g/N_0),$$

$$\mathcal{L}\widetilde{v}_i + U_0\psi_g^{*2}\widetilde{u}_i = -\omega_i(\widetilde{v}_i - a_i\psi_g^*/N_0) \tag{19}$$

and still diagonalize the quasiparticle Hamiltonian, giving the same eigenvalues as before. The orthogonality and symmetry relations of Eqs. (10) and (11) are still satisfied, as they must be since they are required by the Bose commutation relations. Further discussion of the nature of these excitations (with particular emphasis on the conservation of the number of particles) can be found in Refs. [20,21]. In the rest of this paper we will refer to the excitations that obey Eq. (19) as the orthogonal excitations and the ones that obey Eq. (8) as the linear excitations.

After the Bogoliubov transformation the Hamiltonian takes the form

$$\hat{H} = E_0 + \sum_i \omega_i\hat{\beta}_i^\dagger\hat{\beta}_i, \tag{20}$$

where E_0 is some constant. Thus the evolution of the quasiparticle operators is given to this order by

$$\hat{\beta}_i(t) = \hat{\beta}_i(0)e^{-\iota\omega_i t}. \tag{21}$$

If we now allow the quasiparticles to become coherent so that they have nonvanishing quantum expectation values $\langle\hat{\beta}_i(0)\rangle = b_i(0) \neq 0$, then we find that the expectation value of the field operator becomes

$$\langle\hat{\Psi}(\mathbf{r},t)\rangle = \Psi(\mathbf{r},t) = e^{-\iota\mu t}\left[\psi_g(\mathbf{r}) + \sum_i \{u_i(\mathbf{r})b_i(0)e^{-\iota\omega_i t} + v_i^*(\mathbf{r})b_i^*(0)e^{+\iota\omega_i t}\}\right], \tag{22}$$

which has the same form as Eq. (7). This provides the connection between the two approaches to finding the excitations of the system. It is of course unsurprising that the two methods lead to the same result since in the first case we linearize around a classical field and in the second we define a quantum field of noninteracting oscillators, which we then allow to become classical. One would not expect the order in which we carried out these procedures to affect any physical predictions.

III. QUASIPARTICLE PROJECTION METHOD

We have shown in Sec. II that the quasiparticles are the linear excitations on the condensate. In the limit of infinitesimal excitation, they are therefore the eigenstates of the system. In general, however, finite amounts of excitation will be present and this will result in nonlinear effects owing to the higher-order terms neglected in the linearization procedure. In order to be able to follow the evolution of the quasiparticles, we require a method of decomposing an arbitrary single-particle wave function into a condensate and a collection of excitations. This is achieved using the orthogonality and symmetry relations that the quasiparticles satisfy and we describe the method we use in this section.

In the linear regime the quasiparticles do not interact with the condensate. Once there is a finite amount of excitation, however, we must consider the change in the condensate due to the excitations and we therefore write the wave function as

$$\Psi(\mathbf{r},t) = e^{-\iota\mu t}\left[(1+b_g)\psi_g(\mathbf{r}) + \sum_{i>0} \{\widetilde{u}_i(\mathbf{r})b_i(t) + \widetilde{v}_i^*(\mathbf{r})b_i^*(t)\}\right]. \tag{23}$$

This expansion is a simple extension of that in Eq. (7) that allows the condensate and quasiparticle populations to vary with time. Any single-particle wave function can be written in this way since ψ_g and its excitations form a complete set. The summation excludes the zero-frequency mode since its effect is contained in the imaginary part of the condensate coefficient (see the discussion at the end of this section). For convenience we normalize the condensate wave function to 1 and change the parameter U_0 in Eq. (1) to N_0U_0, where N_0 is the number of particles in the condensate. The functions $\widetilde{u}_i$

and $\widetilde{v}_i$ are normalized according to Eq. (10) and the total wave function of Eq. (23) is therefore normalized as

$$\int d^3\mathbf{r}\,|\Psi|^2 = |1+b_g|^2 + \sum_{i,j} \int d^3\mathbf{r}\,\{(\widetilde{u}_i^*\widetilde{u}_j + \widetilde{v}_i^*\widetilde{v}_j)b_i^*b_j$$

$$+ (\widetilde{u}_i\widetilde{v}_j)b_ib_j + (\widetilde{u}_i^*\widetilde{v}_j^*)b_i^*b_j^*\}. \qquad (24)$$

The interpretation of the coefficients is therefore that $N_0|1 + b_g|^2$ gives the condensate population and $N_0|b_i|^2$ gives the number of quasiparticles in level i.

To determine the coefficients b_i, we need to apply the quasiparticle orthogonality and symmetry conditions. This is simplest if we work with the orthogonal excitations that were introduced in Eq. (18). The quasiparticle coefficients can then be obtained by calculating the quantities

$$\int d^3\mathbf{r}\,\{\widetilde{u}_j^*\Psi e^{+\iota\mu t} - \widetilde{v}_j^*\Psi^* e^{-\iota\mu t}\}$$

$$= \sum_i \left[b_i \int d^3\mathbf{r}\,\{\widetilde{u}_j^*\widetilde{u}_i - \widetilde{v}_j^*\widetilde{v}_i\} \right.$$

$$\left. + b_i^* \int d^3\mathbf{r}\,\{\widetilde{u}_j^*\widetilde{v}_i^* - \widetilde{v}_j^*\widetilde{u}_i^*\} \right] = b_j, \qquad (25)$$

where we have used Eqs. (10) and (11) in the final step. The condensate coefficient is obtained from the expression

$$\int d^3\mathbf{r}\,\{\psi_g^*\Psi e^{+\iota\mu t}\} = 1 + b_g. \qquad (26)$$

In practice, we carry out this projection procedure within a basis set description since this is more convenient numerically.

Since the linear excitations are the ones conventionally defined, it is interesting to note that the above decomposition is still possible (although somewhat more complicated) even if we do not use orthogonal excitations. This is because only the partial orthogonality of Eq. (12) is actually necessary for the decomposition. We consider the same expressions as in Eqs. (25) and (26), which now become

$$\int d^3\mathbf{r}\,\{u_j^*\Psi e^{+\iota\mu t} - v_j^*\Psi^* e^{-\iota\mu t}\} = (2 + b_g + b_g^*)a_j^* + b_j, \qquad (27)$$

$$\int d^3\mathbf{r}\,\{\psi_g^*\Psi e^{+\iota\mu t}\} = 1 + b_g + \sum_i \{b_ia_i - b_i^*a_i^*\}, \qquad (28)$$

where the a_i's are the overlap coefficients defined as in Eq. (18), but with N_0 set equal to 1, i.e., $a_i = \int d^3\mathbf{r}\,\{\psi_g^*u_i\} = -\int d^3\mathbf{r}\,\{\psi_g v_i\}$ with $\int d^3\mathbf{r}\,|\psi_g|^2 = 1$. These equations are no longer sufficient to determine all the coefficients and we must also consider the quantity

$$\int d^3\mathbf{r}\,\{\psi_g^*\Psi e^{+\iota\mu t} + \psi_g\Psi^* e^{-\iota\mu t}\} = 2 + b_g + b_g^*, \qquad (29)$$

where we have used Eq. (12) in obtaining the right-hand side. Since the coefficients a_i are all known, the combination

of this equation with Eq. (27) leads to the values of all the coefficients b_j, which can then be used in Eq. (28) to determine the coefficient b_g.

Thus, whether or not one uses excitations defined to be orthogonal to the condensate, one can uniquely decompose an arbitrary single-particle wave function into a condensate and a collection of excitations. The relationship between the coefficients found in the two methods is easily deduced from Eqs. (18) to be

$$\widetilde{b}_i = b_i, \quad i \neq g$$

$$\widetilde{b}_g = b_g + 2\iota \sum_{i\neq 0} \text{Im}\,[a_ib_i], \qquad (30)$$

where Im means "the imaginary part of" and the tilde indicates quantities in the basis of orthogonal excitations. Thus the two descriptions differ only in the imaginary part of the condensate coefficient. In fact, this corresponds to the zero mode discussed earlier, as we can see by writing out the change in the wave function which that mode produces:

$$\delta\Psi(\mathbf{r},t) = \psi_g b_0 - \psi_g^*b_0^* = \iota\psi_g\text{Im}\,[b_0], \qquad (31)$$

where we have used the fact that ψ_g can be chosen to be real. In the linear limit we have $b_0 \sim e^{-\iota\omega_0 t}$, which is a constant since $\omega_0 = 0$. Thus $\delta\Psi(\mathbf{r},t)$ is proportional to the condensate and independent of time and can therefore be absorbed into the original definition of the condensate wave function. However, in the nonlinear limit it is no longer true that $\text{Im}\,[b_0]$ is independent of time and so in general this mode corresponds to a change in the imaginary part of the condensate coefficient. In the limit of small excitation (or short times) this is equivalent to a rotation of the condensate phase. We would expect to find such a mode because the Hamiltonian of Eq. (13) is invariant with respect to changes in the phase of the field operator. This symmetry was broken in Eq. (14) where a specific phase was assigned to the condensate. The remnant of the original symmetry appears in the existence of a mode at zero energy corresponding to a change in this phase and this is the so-called Goldstone mode that appears in theories involving spontaneous symmetry breaking.

The quasiparticle projection technique described in this section allows one to analyze in detail the results of any simulations performed using the NLSE. We shall use it in the next section to study the nonlinear mixing of quasiparticles, but it can also be used in a variety of other simulations such as a study of the efficiency with which various perturbations produce excitations.

IV. NONLINEAR MIXING: NUMERICAL RESULTS

The quasiparticle projection method described above allows one to determine the populations of the quasiparticle modes (by which we mean the coefficients $|b_i|^2$) for an arbitrary wave function. The combination of this with a time evolver for the NLSE allows one to perform a wide range of simulations to explore the effects of nonlinear mixing of the

excitations. The simplest such simulation is one in which the wave function is allowed to evolve freely and initially consists of a condensate and an excitation in a single-quasiparticle mode. This is the kind of simulation we shall discuss in the rest of this paper, although more complicated initial configurations containing many excited modes will be the subject of future work. All our simulations are performed in 1D, although the theoretical analysis of Sec. V applies in any dimension.

A. Description of method

Our numerical procedure is as follows. First we solve the time-independent problem formulated in Eqs. (6) and (8), taking as the input the chemical potential μ of the system. This provides us with the condensate population N_0 and the functional forms of ψ_g and the u_i's and v_i's. Using these we construct an initial wave function that consists of a condensate and a certain amount of excitation in a single mode (mode k say).[2] This is achieved by writing the wave function in the form of Eq. (23) and setting $b_k(0)$ equal to the required value and all the other b_i coefficients (including b_g) to zero. The total condensate coefficient is therefore 1 initially. This procedure changes the overall normalization of the wave function to a value that is greater than 1 by an amount of order $b_k^2(0)$. We then propagate this wave function in the time-dependent NLSE of Eq. (1) (with U_0 replaced by $N_0 U_0$) and save the result at various times to produce a set of stored wave functions that sample the evolution. Each of these wave functions is analyzed using the quasiparticle projection method to obtain all the coefficients b_i as a function of time.

Since we are more interested in the quasiparticle populations than in their phases, we construct a number of initial wave functions that differ only in the phase of the initial excitation $b_k(0)$. Each of these wave functions is separately evolved and the evolutions of the quasiparticle populations are obtained by averaging over all these simulations. Thus we consider $\langle |b_i|^2 \rangle = (1/N_S) \Sigma_S |b_i|^2$, where angular brackets denote the mean value and Σ_S denotes a sum over the N_S simulations. The results quoted in this paper come from averaging over eight simulations with the initial phase uniformly distributed around the unit circle. Although not directly relevant to the results we shall discuss here, this phase averaging may be seen as an attempt to recover the evolution of incoherent quasiparticles from the coherent evolution given by the NLSE (this is the subject of Sec. VI).

We should briefly discuss the question of which basis should be used to analyze the simulations. The initial wave function is constructed using the solutions to the time-independent NLSE and the BdG equations for some particular value of the chemical potential μ, so we could describe the evolution using that same basis. However, the addition of a finite amount of excitation changes the chemical potential of the system and so a better basis to use is one that corresponds to its new value. This can be found by observing the rotation rate of the condensate phase since this varies as

$e^{-i\mu t}$. Unfortunately, this requires a knowledge of the condensate coefficient as a function of time, which itself necessitates a basis decomposition. Consequently, we first analyze the simulations using the original basis (from which the initial wave function was constructed) and from this determine the rate of rotation of the condensate phase. This provides us with the value of the new chemical potential, which we then use in Eqs. (6) and (8) to find the new wave functions u_i and v_i. The simulations are then reanalyzed using this basis. We observe that the evolution of the quasiparticle populations is much smoother when analyzed in this basis than in the original one and thus the results are more easily interpreted. The choice of basis is a matter of finding the simplest description, in which the evolution can be most easily interpreted in terms of physical processes involving well-defined quasiparticles.

B. Results and interpretation

In this section we will describe the results of our numerical simulations. In interpreting these results we will speak loosely of the collision of quasiparticles and their creation and annihilation since these are the physical processes occurring in the gas. We actually observe a smooth evolution of the quasiparticle populations $|b_i|^2$, however, and the results may equally well be interpreted in terms of harmonic generation produced by the nonlinearity.

The simplest simulation we can perform is to start with a very small amount of excitation in a single mode and confirm that its evolution is $b_i \sim e^{i\omega_i t}$ as predicted from the linear response analysis of Sec. II. We did this using a condensate with $\mu = 1$ and an initial excitation in mode 2 given by $|b_2(0)| = 0.01$. Mode 2 is the lowest-lying nontrivial excitation (mode 1 is a simple displacement of the center of mass) and corresponds to a ''breathing mode'' of the condensate. The population in the mode did not change significantly during an evolution of length 30 trap periods, which corresponds to a time of the order of a few tenths of a second for trap frequencies of order 100 Hz as in current experiments. In addition, the phase of the excitation evolved at the constant rate expected from the linear analysis.

As the amount of excitation in the initial mode is increased, nonlinear mixing processes into other modes become important. We performed simulations with $|b_2(0)| = 0.05$, 0.1, 0.2, and 0.5, again on top of a condensate with $\mu = 1$. Results from the last two of these simulations are shown in Figs. 1 and 2. The effect of the nonlinear mixing is predominantly a transfer of the quasiparticle population between modes 2 and 4. Since mode 4 is at roughly twice the energy of mode 2, this is just the frequency-doubling process that we would expect from the form of the nonlinearity. In the case of the simulation with $|b_2(0)| = 0.5$ (Fig. 2), we can see that the process is reversible. This is a consequence of the fact that in a trap there is a discrete set of states rather than the continuum required for an irreversible decay of an excitation.

A number of features of Figs. 1 and 2 are of interest. First, the rate at which the quasiparticle population is transferred between modes is seen to depend on the amount of initial excitation. This is a consequence of the process being nonlinear. Second, we can see that the change in population of

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[2] In our simulations we worked with the linear excitations, i.e., the ones that satisfy the BdG relations of Eqs. (8) rather than Eqs. (19).
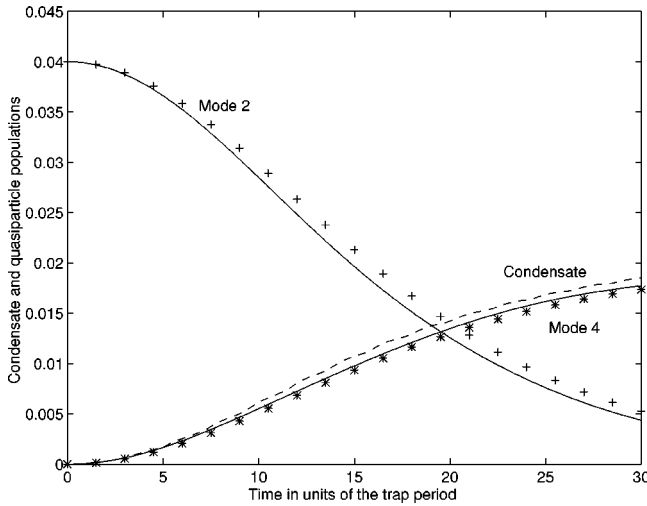
FIG. 1. Evolution of the average quasiparticle populations and the change in the condensate population ($|1+b_g|^2-1$) for $\mu=1$ and $|b_2(0)|=0.2$. The pluses and asterisks are the predictions of Eq. (37) for modes 2 and 4, respectively.

mode 2 is roughly twice that of mode 4. This is a consequence of the requirement that energy be conserved. When mode 2 is populated, the mechanism for the transfer of population is the mutual annihilation of two quasiparticles in that mode, followed by the formation of a single quasiparticle at twice the energy, i.e., in mode 4 (note that quasiparticle number is not conserved). Transfer of population from mode 4 to mode 2 is achieved via the reverse process, namely, the decay of a single quasiparticle into two of half the energy. In each case two quasiparticles in mode 2 are involved for each one in mode 4. A third feature of the figures is that the change in the condensate population follows that in mode 4. A physical explanation for this is that a three-quasiparticle process as described above is composed of the scattering of two real particles, in which one particle either enters or leaves the condensate. It can also be viewed as a consequence of the fact that the normalization of the wave function is conserved, as is discussed in Sec. V.

We can also observe the effect of nonlinear mixing on the population of mode 2 by plotting the width of the condensate as a function of time. This is because mode 2 is a breathing mode in which the width of the condensate oscillates in time (this can be seen by looking at its functional form, for example, in the Thomas-Fermi limit). As such, it is readily excited experimentally as one only needs to vary the currents in the trapping coils symmetrically. In fact, observation of the width of the condensate mimics the technique used experimentally to measure the frequencies and decay rates of the excitations [1,2,6]. Figure 3 shows the behavior of the condensate width for the simulation with $\mu=1$ and $|b_2(0)|=0.5$. As expected, the width oscillates at a frequency of 1.9 (in units of the trap spacing), which is the frequency of mode 2 for this condensate. Furthermore, the amplitude of oscillation does indeed closely follow the population in mode 2 as given in Fig. 2. The fact that the reversible transfer of population into and out of mode 2 can be seen in the amplitude of the oscillations in the condensate width leads us to hope that it will be possible to observe it experimentally.

So far we have focused on results for a condensate with $\mu=1$, as the amount of excitation in mode 2 is increased. The next thing to consider is what happens when we increase μ, i.e., the number of particles in the condensate, while fixing the amount of excitation in the mode. Since an increase in μ involves an increase in the nonlinearity responsible for the mixing effects we would naively expect to see much the same behavior as before, but on a shorter time scale. Although this is observed, we also notice that the magnitude of the mixing decreases and modes other than mode 4 can play an important role. Figures 4 and 5 shows plots of the quasiparticle populations for condensates with $\mu=2$ and 4, respectively, with an initial excitation of $|b_2(0)|=0.2$. A comparison with Fig. 1 shows that the transfer of excitation does indeed occur faster than for $\mu=1$, but with a smaller amplitude. This is a consequence of the fact that the energy matching between modes 2 and 4 (characterized by the energy difference $\Delta\omega_{24}=\omega_4-2\omega_2$) is less good for the larger values of μ, resulting in a suppression of the nonlinear mixing. This effect is discussed further in Sec. V.

As $\Delta\omega_{24}$ increases, the quasiparticle evolution becomes less dominated by the coupling between modes 2 and 4 and the presence of other modes becomes increasingly important. In particular, once we have a significant population in both mode 2 and mode 4, we can observe the effect of the annihilation of a single quasiparticle from each of these modes to form one in mode 6, which is approximately an energy-conserving process. The effect of this can clearly be seen in Fig. 4 as a growth and decay in the population in mode 6. One consequence of the transfer of population to mode 6 is the absence of one of the repopulation peaks in mode 2, the remnant of which can just be seen in Fig. 4 between $t=5$ and 10. The three main processes occurring during this time are the decay of mode 4 to mode 2, frequency doubling of mode 2 to mode 4, and the collision of a quasiparticle in mode 4 with one in mode 2 to give one in mode 6. The net effect is a depletion of mode 4, a growth in mode 6, and a small growth in mode 2. Subsequently, mode 6 decays back to modes 4 and 2 and almost all the original population eventually returns to mode 2. Processes of this kind provide the
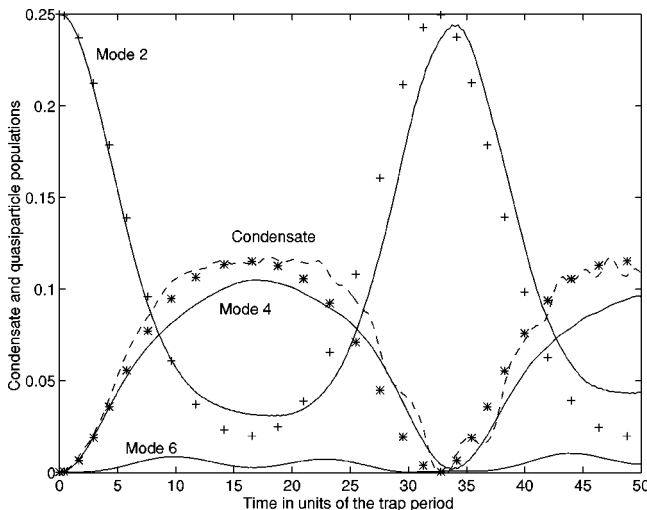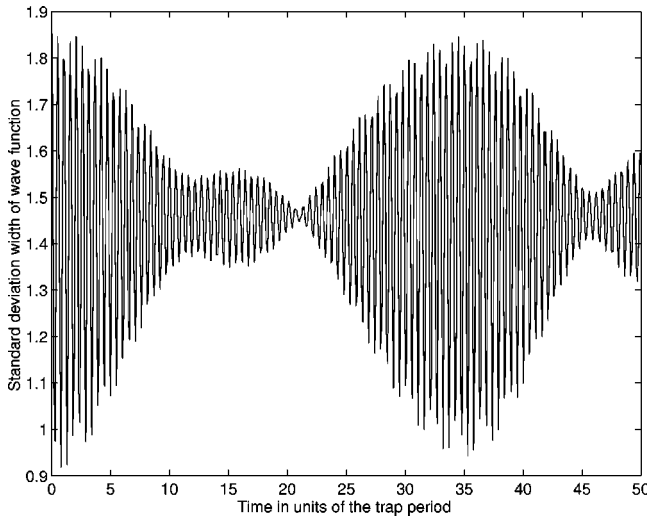

FIG. 2. Evolution of the average quasiparticle populations and the change in the condensate population for $\mu=1$ and $|b_2(0)|=0.5$. The pluses and asterisks are results from the numerical simulation of Eq. (35) for modes 2 and 4, respectively.

FIG. 3. Evolution of the standard deviation width of the wave function for a condensate with $\mu = 1$ and $b_2(0) = 0.5$.

mechanism by which the energy, initially in a single mode, is ultimately dissipated among a large number of modes. Consequently, they limit the number of times the population returns to the initial state and control how the system relaxes to equilibrium. Since they rely on the presence of excitation in more than a single mode they are not the dominant mixing processes if we start with only one excited mode. At finite temperatures, however, when many modes are excited, these processes can be expected to play a more significant role and may lead to an effectively irreversible decay of the initial excitation.

So far we have only considered the case that mode 2 is excited initially and we should briefly mention the behavior of other modes. For comparison, we looked at mode 5 since it is significantly more energetic and has opposite (odd) parity. For a condensate with $\mu = 1$, this mode is much more stable than mode 2 and there is very little mixing even for an initial excitation of $|b_2(0)| = 0.2$. The reason for this is that the dominant mixing should be into mode 10 since this is at roughly twice the energy. However, the energy gap $\Delta\omega_{5\,10} = \omega_{10} - 2\omega_5$ is rather large for this condensate and so the nonlinear mixing is strongly suppressed.

It is also instructive to consider the case that mode 4 is initially populated. For a condensate with $\mu = 1$ we have seen that this mode is energetically very well matched to mode 2 and we might therefore expect to see it decay strongly into this mode, just as we saw the repopulation of mode 2 from mode 4 in Fig. 2. In fact, this does not happen and the excitation, like that in mode 5, is very stable. The reason for this can be seen from a perturbative argument. If the initial mode has a frequency ω_λ then the dominant nonlinear terms at $t = 0$ have frequency components at 0 and $\pm 2\omega_\lambda$. Thus there is a strong coupling to the condensate and to the mode nearest $2\omega_\lambda$. There is only a weak coupling, however, to the other modes including the one with energy closest to $\frac{1}{2}\omega_\lambda$. This is a consequence of using the NLSE to simulate the quasiparticle evolution. Quantum mechanically we would expect the rate for a boson scattering process into some state to be proportional to $n + 1$, where n is the number of bosons already occupying that state. Thus there is a rate for the process even if $n = 0$. In the NLSE, however, the

quasiparticles operators are replaced by complex numbers, so there is no spontaneous emission term. Thus mode 4 does not decay to mode 2 in the absence of a population in that mode and this explains its stability. In reality spontaneous decay processes will occur and in principle one could put them into the NLSE by hand using a quantum jump approach, although this would greatly slow down the computation. However, one can easily infer the rate for such processes by considering the corresponding stimulated rate and replacing its dependence on the quasiparticle populations $|b_i|^2$ with $|b_i|^2 + 1$.

Finally, we should discuss how much the evolution of the quasiparticle populations depend on the phase of the initial excitation. Since the leading-order term in the evolution of the quasiparticles is just a phase rotation (corresponding to the energy of the quasiparticle), two simulations that start with a phase difference of ϕ should have the same evolution but with the origin of time displaced by an amount ϕ/ω_i, as long as any nonlinear effects are negligible in this time period. Thus any fast oscillations in the evolution of the populations will cancel out when we average over phases and only processes that produce slow changes will have an effect. It is shown in Sec. V that such processes are ones that conserve energy, so that any variation from the mean evolution is a consequence of energy-nonconserving processes. These should be negligible if the nonlinear mixing rates are small so that the quasiparticles provide a good basis. Figure 6 shows the same results as Fig. 1 except that instead of plotting the quasiparticle populations averaged over eight simulations, the results from each simulation separately are plotted and superimposed. Each of these simulations corresponds to a particular choice of phase for the initial excitation and Fig. 6 clearly shows that the variation in the quasiparticle populations from the mean value at any time is indeed very small. The variation in the condensate population is larger, however, and is comparable to the amount it has changed, although this is still a small fraction of the total condensate population. This is a result of the fact that the condensate has a large response at zero frequency.
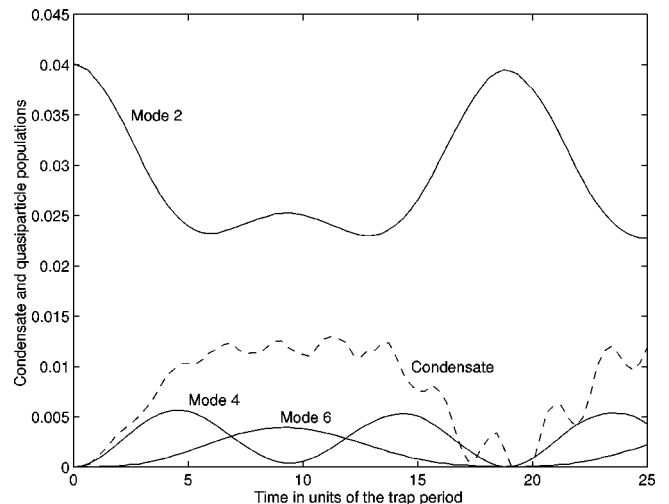

FIG. 4. Evolution of the average quasiparticle populations and the change in the condensate population for $\mu = 2$ and $|b_2(0)| = 0.2$.
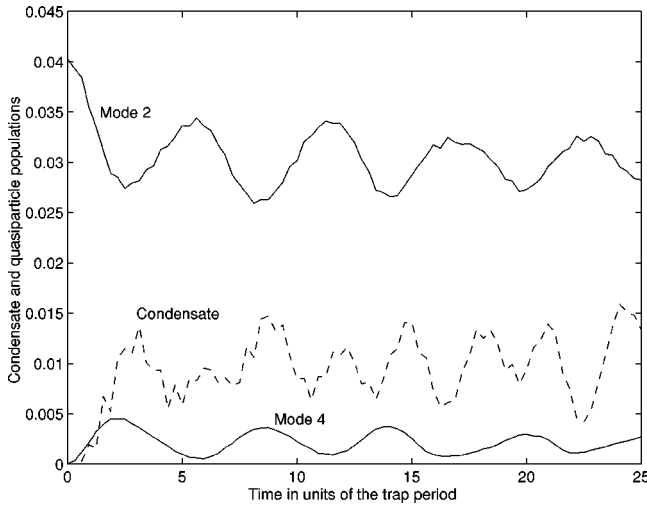
FIG. 5. Evolution of the average quasiparticle populations and the change in the condensate population for $\mu=4$ and $|b_2(0)| =0.2$.

As we increase the nonlinearity or the amount of initial excitation then we see a stronger dependence on the initial phase of the excitation as expected. Eventually we will reach a regime where the evolution depends so strongly on the initial phase that we cannot meaningfully interpret the results of the simulations in terms of the evolution of well-defined quasiparticles. This is the regime where the amount of excitation is so large that a description of the system in terms of a basis provided by the linear excitations ceases to be useful. We can use the phase dependence of the evolution as a test to see whether or not a description in terms of quasiparticles is meaningful. For the simulations presented here the quasiparticle description is applicable, but is beginning to break down for the simulation depicted in Fig. 5 where the evolution is strongly dependent on the initial phase. This explains why the average over phases produces a less smooth plot in this case than for the other simulations.

V. NONLINEAR MIXING: ANALYTICAL RESULTS

We can make further progress towards understanding the nonlinear mixing processes discussed above by using an ana-
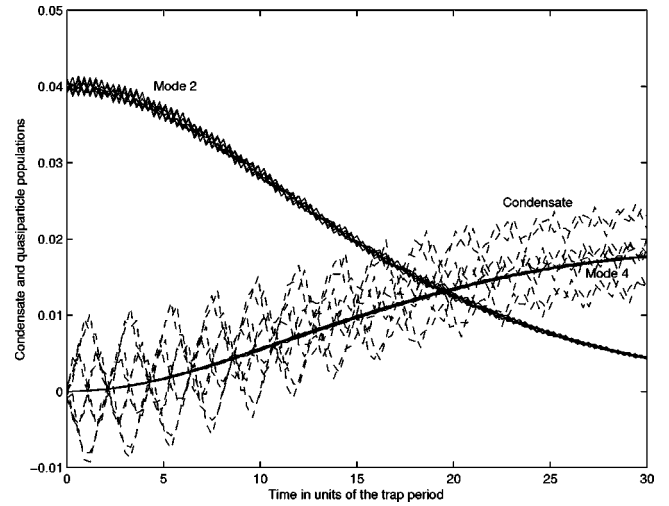

FIG. 6. Evolution of the quasiparticle populations and the change in the condensate population for $\mu=1$. The results from eight simulations are shown superimposed. These simulations correspond to the initial condition $b_2(0)=0.2e^{\iota\phi}$ with $\phi=0$, $\pi/4$, $\pi/2,\ldots,7\pi/4$.

lytical approach in which we explicitly obtain the equations of motion for the condensate and quasiparticle coefficients. This is achieved most simply if we use the excitations that are orthogonal to the condensate as defined in Eq. (19) and all equations in this section are written in terms of these excitations. Using these equations we can see what processes dominate the evolution and what parameters affect the time scales for nonlinear mixing. We have been able to solve an approximate form of the equations in one special case and obtain an expression for the rate of nonlinear mixing in terms of the nonlinearity and the amount of initial excitation.

The equations of motion for the coefficients b_i are obtained by substituting the expansion of Eq. (23) into the time-dependent NLSE and carrying out the projection procedure described in Sec. III analytically. This leads to the following equations of motion for the quasiparticle and condensate coefficients (using units $\hbar=1$)

$$\iota\frac{db_i}{dt}=\omega_i b_i+N_0U_0\int d^3\mathbf{r}\,\{\widetilde{u}_i^*[2\,\mathrm{Re}\,(b_g)|\psi_g|^2\psi_g+\psi_g^*\Delta^2+2\psi_g|\Delta|^2+|\Delta|^2\Delta]$$

$$+\widetilde{v}_i^*[2\,\mathrm{Re}\,(b_g)|\psi_g|^2\psi_g^*+\psi_g^*\Delta^2+2\psi_g^*|\Delta|^2+|\Delta|^2\Delta^*]\},\tag{32}$$

$$\iota\frac{db_g}{dt}=2\sum_i\omega_i\,\mathrm{Re}\,[a_ib_i]+N_0U_0\int d^3\mathbf{r}\,\{2\,\mathrm{Re}\,(b_g)|\psi_g|^4$$

$$+\psi_g^{*2}\Delta^2+2|\psi_g\Delta|^2+\psi_g^*|\Delta|^2\Delta\},\tag{33}$$

where

$$\Delta=b_g\psi_g+\sum_j\{\widetilde{u}_jb_j+\widetilde{v}_j^*b_j^*\}\tag{34}$$

and Re means ''the real part of.'' The above equations can be simplified somewhat if one uses the fact that ψ_g can be chosen to be real. The normalization has been chosen as

discussed in Sec. III below Eq. (23) and the coefficients a_i are the same quantities that appear in Eqs. (18), but with N_0 set equal to 1.

The linear terms in the above equations merit a brief discussion. The leading-order term in Eq. (32) describes the energy of the quasiparticle mode and in the linear regime is the only important contribution to the equation of motion. The term proportional to Re (b_g) is quadratic in effect if not appearance since Eq. (33) shows that if Re (b_g) is zero initially, it can only change as a result of quadratic terms in the equation of motion. In addition, we see from Eq. (33) that the excited states affect the imaginary part of the ground-state coefficient at linear order. This is because the equations are written using excitations orthogonal to the condensate and these are not the linear excitations of the system [they satisfy Eq. (19) rather than Eq. (8)]. The form of this linear term is exactly what we would expect as a result of the relation between the coefficients of the orthogonal and linear excitations given in Eq. (30).

The fast motion given by the energy of the excitations in Eq. (32) can be removed by defining slowly varying quantities b_i^s by $b_i^s = b_i e^{\iota \omega_i t}$. Substituting this into Eqs. (32) and (33) and expanding Δ produces a large number of terms, all of which contain oscillating factors of the form $e^{\iota(\omega_i \pm \omega_j)t}$. At this stage some approximation is required to reduce the complexity of the equations and this is provided by the rotating-wave approximation (RWA), in which one considers only terms for which this oscillating factor is close to zero. These terms correspond to processes for which energy is (nearly) conserved and produce a smooth time evolution. The neglected terms cause rapid oscillations around the mean and have little effect on the long-term motion. In addition, since they are rapidly varying, their effect tends to cancel if we average over the phase of the excitations. For the case that mode 2 is initially populated, we have seen that the dominant coupling is to mode 4. If we neglect any variation in the population of the condensate and consider only these modes, then we obtain the equations of motion

$$\iota \frac{db_2^s}{dt} = N_0 U_0 M_{24} b_2^{s*} b_4^s e^{-\iota \Delta \omega_{24} t},$$

$$\iota \frac{db_4^s}{dt} = \frac{1}{2} N_0 U_0 M_{24}^* b_2^{s2} e^{+\iota \Delta \omega_{24} t}, \quad (35)$$

where M_{24} is a matrix element given by

$$M_{24} = 2 \int d^3\mathbf{r} \{ \psi_g^* [2\tilde{u}_2^* \tilde{v}_2^* \tilde{u}_4 + \tilde{v}_2^* \tilde{v}_2^* \tilde{v}_4]$$

$$+ \psi_g [2\tilde{u}_2^* \tilde{v}_2^* \tilde{v}_4 + \tilde{u}_2^* \tilde{u}_2^* \tilde{u}_4] \} \quad (36)$$

and $\Delta \omega_{24} = \omega_4 - 2\omega_2$. These equations show that the change of population in mode 4 is half that of mode 2 (as required by energy conservation) and therefore that $|b_2|^2 + 2|b_4|^2$ is a constant of the motion. They can be extended readily to deal with the more general case that a large number of modes are strongly coupled.

Equations of precisely this form have been studied in the context of harmonic generation in nonlinear optics [22], where it is shown that a general solution can be written in the form of elliptic integrals. In the case that $\Delta \omega_{24} = 0$ and mode 4 is initially unpopulated, the solution is particularly simple and is given by

$$b_2^s(t) = b_2^s(0) \text{sech} \left(\left| \frac{N_0 U_0 M_{24} b_2^s(0)}{\sqrt{2}} \right| t \right),$$

$$b_4^s(t) = \pm \iota \frac{b_2^{s2}(0)}{\sqrt{2}|b_2^s(0)|} \tanh \left(\left| \frac{N_0 U_0 M_{24} b_2^s(0)}{\sqrt{2}} \right| t \right), \quad (37)$$

where the sign $\pm$ corresponds to $N_0 U_0 M_{24} \lessgtr 0$, respectively, and we have taken the matrix element M_{24} to be real (this is not a significant restriction). The relative phase of b_2^{s2} and b_4^s in this solution is always $\pm \pi/2$ and the equations are particularly simple in this case precisely because there is no evolution of the relative phase. Equations (37) show that the time scale for nonlinear mixing is set by the quantity $|\sqrt{2}/N_0 U_0 M_{24} b_2^s(0)|$. Evaluation of this parameter [23] using data appropriate to recent experiments of Jin *et al.* [1,6] gives a time scale for the decay of mode 2 of 120 ms, which is close to the observed value. We do not believe that the present analysis applies in that situation, however, as $\Delta \omega_{24}$ is large compared to this time scale.

The solution of Eq. (37) predicts that the transfer of quasiparticle population from mode 2 to mode 4 is complete and irreversible, which is not what is seen in the simulations. The reason for this is that it applies only to the special case that $\Delta \omega_{24} = 0$. In the more general case where $\Delta \omega_{24} \neq 0$, numerical simulation of Eqs. (35) shows that the population transfer is no longer complete and is periodic with a period that decreases as $N_0 U_0$ and $\Delta \omega_{24}$ increase. This is a result of the fact that the $e^{\iota \Delta \omega_{24} t}$ term can introduce a sign change into the equations on a time of order $1/\Delta \omega_{24}$, thereby turning the depletion of a mode into a growth and vice versa. The period also depends on $N_0 U_0$, however, because once the relative phase of b_2^{s2} and b_4^s differs from $\pm \pi/2$, the nonlinearity can cause phase evolution and so also introduce sign changes into the equations.[3] As $\Delta \omega_{24}$ increases, the time available for population transfer to occur decreases, leading to a reduction in the net amount of transfer that is achieved. This was discussed in Sec. IV B and can be seen clearly from a comparison of Figs. 1 and 5. The solution of Eq. (37) and a result from the simulation of Eq. (35) are compared with the results from the simulations in Figs. 1 and 2. The agreement is quite good, demonstrating that the evolution is dominated by processes that approximately conserve energy (corresponding to the terms we kept when we made the RWA), and the differences can be attributed largely to the neglect of the variation in the condensate population.

The evolution of the condensate as given by Eq. (33) is rather more complicated. One feature of the simulations is that its phase rotates at a rate greater than the original chemical potential (we discussed this issue in Sec. IV A when deciding what basis to use to analyze the simulations). The additional rotation describes the shift in the energy of the

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[3]Simulation of Eqs. (35) shows that if $b_4^s(0)$ is nonzero and has a phase that is not at $\pm \pi/2$ to that of $b_2^{s2}(0)$ then the population transfer is periodic even if $\Delta \omega_{24} = 0$.

condensate caused by the presence of a finite amount of excitation and is observed numerically to be independent of any mixing between excited states that may occur.[4] Although the frequency shift is small, its effect is cumulative and we must take it into account if we are to be able to treat the change in the condensate coefficient b_g as a small parameter. This means that we must describe the wave function using a basis set corresponding to the new chemical potential. The analytical predictions give the best fit to the results of the simulations if we use this basis.

Once the rotation of the condensate phase has been removed, we observe that the change in its population is roughly proportional to the population in mode 4 for the case that only modes 2 and 4 need be considered (see Figs. 1 and 2). We can understand this from the fact that the evolution preserves the normalization of the wave function. The normalization is given by $\int d^3\mathbf{r}\,|\Psi|^2$, so substitution of Eq. (23) leads [as in Eq. (24)] to

$$\int d^3\mathbf{r}\,|\Psi|^2 = |1+b_g|^2 + \sum_{i,j} \int d^3\mathbf{r}\,\{(\widetilde{u}_i^*\widetilde{u}_j + \widetilde{v}_i^*\widetilde{v}_j)b_i^*b_j$$
$$+ (\widetilde{u}_i\widetilde{v}_j)b_ib_j + (\widetilde{u}_i^*\widetilde{v}_j^*)b_i^*b_j^*\} = c, \qquad (38)$$

where c is a constant of order 1. This contains terms that oscillate on a fast time scale so b_g must also have fast oscillations if the normalization is to be conserved. However, we are only interested in the slowly varying terms that describe the long-time evolution. Consideration of these terms alone gives

$$|1+b_g|^2 + \sum_i \int d^3\mathbf{r}\,\{|\widetilde{u}_i|^2 + |\widetilde{v}_i|^2\}|b_i|^2 = c \sim 1. \quad (39)$$

For the case that only modes 2 and 4 are significantly occupied, we also know that $|b_2|^2 + 2|b_4|^2$ is a constant of the motion from energy conservation arguments. Using this in Eq. (39) gives

$$|1+b_g|^2 - 1 \sim \int d^3\mathbf{r}\,\{2(|\widetilde{u}_2|^2 + |\widetilde{v}_2|^2)$$
$$- (|\widetilde{u}_4|^2 + |\widetilde{v}_4|^2)\}|b_4|^2, \qquad (40)$$

which shows that the change in the condensate population follows that in mode 4. When more modes are involved this result will no longer hold (see Fig. 4, for example), although extensions of it can readily be derived from Eq. (39) and the new energy conservation condition.

VI. EXTENSION TO FINITE TEMPERATURES

The NLSE simulates the evolution of coherent quasiparticles since at all times the coefficients b_i in Eq. (23) have a well-defined phase in addition to a well-defined amplitude. If one is interested in extending the techniques presented here to study finite-temperature mixing effects then one would need to simulate incoherent quasiparticles. Although a time-

dependent formalism at finite temperatures does exist [17], it is computationally prohibitive, especially in more than one dimension. Thus, if the NLSE can be used to estimate the evolution of incoherent quasiparticles, then it will provide a useful tool to attack the problem of finite-temperature damping. In fact, the NLSE has recently been used to simulate the experimental procedure for determining the damping of excitations on the condensate and gave a decay rate for the breathing mode that was in good agreement with the low-temperature experimental results [24]. This provides additional motivation for attempts to extend the use of the NLSE to finite temperatures.

Use of the NLSE at finite temperatures represents an attempt to simulate the quantum field using a classical one. We saw in Sec. II that a classical approach (linearization on the NLSE) and a quantum approach (diagonalization of a quadratic Hamiltonian) gave the same results for the excitations of the system. This was because the two approaches could be related by allowing the quasiparticle operators to become coherent. We wish to extend this idea to consider the dynamics of the system and this involves using the time-dependent NLSE to describe the evolution of the quantum field. The quantum-mechanical evolution can be obtained from the many-body Hamiltonian of Eq. (13) and is given by

$$\imath\hbar\,\frac{\partial\hat{\Psi}(\mathbf{r},t)}{\partial t} = \hat{H}_0\hat{\Psi}(\mathbf{r},t) + U_0\hat{\Psi}^\dagger(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t),$$
$$(41)$$

where $\hat{\Psi}(\mathbf{r},t)$ is normalized to N. This has exactly the same form as the NLSE if we replace the field operator $\hat{\Psi}(\mathbf{r},t)$ by its expectation value in a coherent state, i.e., the function Ψ that appears in Eq. (1). This is precisely the procedure used in the linear analysis and motivates the use of the NLSE in the nonlinear regime.

In a recent paper Kagan and Svistunov [25] give a justification for the use of the NLSE in this context and argue that it is valid even when no condensate is present and the system is far from equilibrium, provided that the single-particle modes are highly occupied. They show that if the single-particle density matrix is diagonal in the number-state representation then it is also approximately diagonal in a coherent-state representation, with no correlation between the phases of the various coherent states in the ensemble. In addition, each coherent state evolves independently to a good approximation. Thus, to represent the evolution of the density matrix we can perform many classical simulations with various initial phases and then average over these phases. We might expect this representation to be approximately valid as long as the evolution is not strongly dependent on the phase and indeed it is argued in Ref. [25] that for all practical purposes it is sufficient to consider the evolution of a coherent state with one particular phase.

Applying the arguments above in a quasiparticle basis means that an incoherent quasiparticle with no well-defined phase can be described by a collection of coherent quasiparticles with phases distributed evenly around the unit circle.

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[4]This energy shift is largely (but not entirely) due to the change in the normalization of the wave function.

We saw in Sec. IV B and Fig. 6 that the quasiparticle evolution does not strongly depend on the phase of the initial excitation when the amount of excitation and the nonlinearity are not too large. This confirms our expectations for the case that the quasiparticles are well defined and form a meaningful basis. Eventually a description of the evolution in terms of quasiparticles involves a strong dependence on their phase, but this represents a breakdown in the quasiparticle description of the system and does not imply that the NLSE can no longer be used to simulate the quantum field.

Thus we propose that the NLSE can be used to approximately simulate the full quantum field over a wide range of temperatures. At very low temperatures the justification comes from the fact that it can be derived from a product wave function in which all the atoms are in the same single-particle state. At high temperatures the justification is that the relevant excited states (single particle or quasiparticle) are highly occupied so that a classical approximation is expected to be valid. Of course a classical simulation cannot reproduce all aspects of the quantum evolution and one consequence of this that was observed in the numerical simulations of Sec. IV B is the absence of spontaneous emission terms in the quasiparticle evolution. Nonetheless, the use of a classical field to represent a quantum one is a common approximation in a wide range of physical contexts as it is often the only approach that is computationally feasible and it is expected to be accurate enough for practical purposes [26].

VII. CONCLUSION

In this paper we have shown how to determine the contribution of a condensate and its excitations to any wave function appearing in the NLSE. We have used this method to study the nonlinear mixing of quasiparticles for simulations in which we start from an initial wave function that contains a finite amount of excitation in a single mode. We have observed that the evolution is dominated by processes that conserve energy and that the initial population can be reversibly transferred to an energetically matched mode. This is a result of the fact that in an inhomogeneous system there are only discrete states rather than a continuum. We have shown analytically that the time scale for the transfer of population is inversely dependent on the nonlinearity and the amount of initial excitation and is generally of the order of tens of trap cycles (between 0.01 and 0.1 s for the current experimental traps). We do not see the exponential decay of the initial population reported in a recent experiment [6], but this was performed at temperatures that were significant fractions of the critical temperature. We believe that the reversible transfer of population between modes should be observable at low temperatures and it would be interesting if this could be seen experimentally.

Finally, we have argued that the NLSE can be used to approximately simulate the full quantum field and that therefore the techniques presented here can be extended to study the evolution of incoherent quasiparticles in the presence of a thermal component. This means that one can estimate finite-temperature mixing effects without the need to apply computationally more demanding approaches such as simulating the full time-dependent Hartree-Fock-Bogoliubov equations.

[1] D. S. Jin, J. R. Enscher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Phys. Rev. Lett. **77**, 420 (1996).

[2] M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. M. Kurn, D. S. Durfee, C. G. Townsend, and W. Ketterle, Phys. Rev. Lett. **77**, 988 (1996).

[3] M. Edwards, P. A. Ruprecht, K. Burnett, R. J. Dodd, and C. W. Clark, Phys. Rev. Lett. **77**, 1671 (1996).

[4] S. Stringari, Phys. Rev. Lett. **77**, 2360 (1996).

[5] V. L. Ginzburg and L. P. Pitaevskii, Zh. Éksp. Teor. Fiz. **34**, 1240 (1958) [Sov. Phys. JETP **7**, 858 (1958)]; E. P. Gross, J. Math. Phys. **4**, 195 (1963).

[6] D. S. Jin, M. R. Matthews, J. R. Enscher, C. E. Wieman, and E. A. Cornell, Phys. Rev. Lett. **78**, 764 (1997).

[7] E. M. Lifshitz and L. P. Pitaevskii, *Statistical Physics Part 2*, Landau and Lifshitz Course of Theoretical Physics Vol. 9 (Pergamon, Oxford, 1980).

[8] F. Mohling and A. Sirlin, Phys. Rev. **118**, 370 (1960).

[9] P. O. Fedichev, G. V. Shlyapnikov, and J. T. M. Walraven, e-print cond-mat/9710128.

[10] S. Giorgini, e-print cond-mat/9709259.

[11] A. L. Fetter, Ann. Phys. (N.Y.) **70**, 67 (1972).

[12] M. Edwards, R. J. Dodd, C. W. Clark, and K. Burnett, J. Res. Natl. Inst. Stand. Technol. **101**, 553 (1996), special issue on Bose-Einstein condensation, edited by K. Burnett, M. Edwards, and C. W. Clark.

[13] E. Fermi, Riv. Sci. **7**, 13 (1936).

[14] K. Huang, *Statistical Mechanics*, 2nd ed. (Wiley, New York, 1987).

[15] N. Proukakis, K. Burnett, and H. Stoof, Phys. Rev. A **57**, 1230 (1998).

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

[17] N. Proukakis and K. Burnett, J. Res. Natl. Inst. Stand. Technol. **101**, 457 (1996), special issue on Bose-Einstein condensation, edited by K. Burnett, M. Edwards, and C. W. Clark.

[18] J.-P. Blaizot and G. Ripka, *Quantum Theory of Finite Systems* (MIT Press, Cambridge, MA, 1986).

[19] C. W. Gardiner (private communication). The discussion of excitations orthogonal to the condensate is due to Gardiner.

[20] C. W. Gardiner, Phys. Rev. A **56**, 1414 (1997).

[21] Y. Castin and R. Dum, Phys. Rev. A (to be published).

[22] J. A. Armstrong, N. Bloembergen, J. Ducuing, and P. S. Pershan, Phys. Rev. **127**, 1918 (1962).

[23] R. Dodd (private communication).

[24] A. Smerzi and S. Fantoni, Phys. Rev. Lett. **78**, 3589 (1997).

[25] Yu. Kagan and B. V. Svistunov, Phys. Rev. Lett. **79**, 3331 (1997).

[26] G. D. Moore and N. Turok, Phys. Rev. D **55**, 6538 (1997).