Simulations of Bose Fields at Finite Temperature

M. J. Davis, S. A. Morgan, and K. Burnett

Clarendon Laboratory, Department of Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

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We introduce a time-dependent projected Gross-Pitaevskii equation to describe a partially condensed homogeneous Bose gas, and find that this equation will evolve randomized initial wave functions to equilibrium. We compare our numerical data to the predictions of a gapless, second order theory of Bose-Einstein condensation [S. A. Morgan, J. Phys. B **33**, 3847 (2000)], and find that we can determine a temperature when the theory is valid. As the Gross-Pitaevskii equation is nonperturbative, we expect that it can describe the correct thermal behavior of a Bose gas as long as all relevant modes are highly occupied. Our method could be applied to other boson fields.

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The achievement of Bose-Einstein condensation (BEC) in a dilute gas offers the possibility of studying the dynamics of a quantum field at finite temperatures in the laboratory [1,2]. However, direct numerical simulation of the full equations of motion for such systems is well beyond the capability of today's computers. Even equilibrium calculations in the region of a phase transition require nonperturbative methods, meaning that fully quantal treatments are unfeasible.

At finite temperature, when there are an appreciable number of noncondensed particles, the fully quantal second order theory of Morgan [3] (and other equivalent treatments [4,5]) should be sufficient for an accurate description of many properties of the dilute Bose gas in equilibrium and away from the region of critical fluctuations. Dynamical treatments are much harder, and in general require significant approximations. For example, calculations have been performed for small systems [6], with a restricted number of modes [7], and for the dynamics of condensate formation where the ground state is assumed to grow adiabatically [8].

The Gross-Pitaevskii equation (GPE) has been used to predict the properties of condensates near $T = 0$, when there are very few noncondensate atoms present. Both statically and dynamically it has shown excellent agreement with experiment [9–11]. It has been argued, however, that the GPE can be used to describe the dynamics of a BEC at finite temperature [12–14]. In the limit where the modes of the system are highly occupied ($N_k \gg 1$), the classical fluctuations of the field overwhelm the quantum fluctuations, and these modes may therefore be represented by a coherent wave function. This is analogous to the situation in laser physics, where the highly occupied laser modes can be well described by classical equations.

Using this argument, Damle *et al.* have performed calculations of the approach to equilibrium of a near ideal superfluid [15], and similar approximations to other quantum field equations have been successful elsewhere [16]. References [17–19] also use the GPE to represent the classical modes of a Bose-condensed system. The main advantage of this method is that realistic calculations, while still a major computational issue, are feasible—methods for solving the GPE are well developed. Also, as the GPE is nonperturbative it should be possible to study the region of the phase transition, as long as the condition $N_k \gg 1$ is satisfied.

There are, however, problems associated with the GPE. It is a classical equation, and so in equilibrium it will satisfy the equipartition theorem—all modes of the system will contain an energy $k_B T$. Thus, if we couple a system to a heat bath, and solve the equation with infinite accuracy, we will observe an ultraviolet catastrophe. Also, the higher the energy of any given mode, the lower its occupation will be in equilibrium, and eventually the criterion $N_k \gg 1$ will no longer be satisfied. For these low occupation modes a form of kinetic equation is more appropriate. The solution to both of these problems is to introduce a *cutoff* in the modes represented by the GPE.

Our theoretical approach begins with the full operator equation for the Bose field with two-body interactions

$$i\hbar \frac{\partial \hat{\Psi}(\mathbf{r})}{\partial t} = \hat{H}_0 \hat{\Psi}(\mathbf{r}) + U_0 \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}(\mathbf{r}) \hat{\Psi}(\mathbf{r}), \quad (1)$$

where $U_0 = 4\pi\hbar^2 a/m$ is the effective interaction strength at low momenta, a is the s-wave scattering length, and m is the particle mass. The route to the usual GPE is to assume that the full field operator can be replaced by a wave function $\psi(\mathbf{r})$—i.e., that *all* quantum fluctuations can be neglected. We proceed instead by defining a projection operator $\hat{\mathcal{P}}$ such that

$$\hat{\mathcal{P}} \hat{\Psi}(\mathbf{r}) = \sum_{\mathbf{k} \in C} \hat{a}_\mathbf{k} \phi_\mathbf{k}(\mathbf{r}), \quad (2)$$

where the region C is *determined* by the requirement that $\langle \hat{a}_\mathbf{k}^\dagger \hat{a}_\mathbf{k} \rangle \gg 1$, and the set $\{\phi_\mathbf{k}\}$ defines some basis in which the field operator is approximately diagonal at the boundary of C. For these modes, the quantum fluctuation part of the projected field operator can be ignored, and so we replace $\hat{a}_\mathbf{k} \rightarrow c_\mathbf{k}$ and write

$$\psi(\mathbf{r}) = \sum_{\mathbf{k} \in C} c_\mathbf{k} \phi_\mathbf{k}(\mathbf{r}). \quad (3)$$

Defining the operator $\hat{\mathcal{Q}} = \hat{\mathbb{1}} - \hat{\mathcal{P}}$ and $\hat{\mathcal{Q}} \hat{\Psi}(\mathbf{r}) = \hat{\eta}(\mathbf{r})$, operating on Eq. (1) with $\hat{\mathcal{P}}$ and taking the mean value results in what we call the finite temperature GPE

$$i\hbar\frac{\partial\psi(\mathbf{r})}{\partial t} = \hat{H}_0\psi(\mathbf{r}) + U_0\hat{\mathcal{P}}\{|\psi(\mathbf{r})|^2\psi(\mathbf{r})\} + U_0\hat{\mathcal{P}}\{2|\psi(\mathbf{r})|^2\langle\hat{\eta}(\mathbf{r})\rangle + \psi(\mathbf{r})^2\langle\hat{\eta}^\dagger(\mathbf{r})\rangle\} + U_0\hat{\mathcal{P}}\{\psi^*\langle\hat{\eta}\,\hat{\eta}\rangle + 2\psi\langle\hat{\eta}^\dagger\hat{\eta}\rangle + \langle\hat{\eta}^\dagger\hat{\eta}\,\hat{\eta}\rangle\}. \quad (4)$$

This describes the full dynamics of the region C and its coupling to an effective heat bath $\hat{\eta}(\mathbf{r})$, which in principle can be described using a form of quantum kinetic theory. The finite temperature GPE is discussed in detail in Ref. [20].

In this Letter, however, we wish to show that the GPE *alone* can describe the evolution of general configurations of the coherent region C towards an equilibrium that can be parametrized by a temperature. We therefore ignore all terms involving $\hat{\eta}(\mathbf{r})$ in Eq. (4) and concentrate on the first two terms of the first line, which we call the projected GPE. Although this equation is both unitary and reversible, we expect it to evolve general states to equilibrium, because deterministic nonlinear systems exhibit chaotic, and hence ergodic, behavior if more than a few degrees of freedom are present [21]. This is confirmed by our numerical simulations and forms the main result of this Letter.

The projected GPE describes a microcanonical system. However, if the region C is large, then fluctuations in energy and particle number in the grand canonical ensemble would be small. Hence we expect the final equilibrium state of the projected GPE to be similar to that of the finite temperature GPE coupled to a bath $\hat{\eta}(\mathbf{r})$ with the appropriate chemical potential and temperature. This does not affect the main result of this Letter, however, which is simply that equilibrium is attained. The detailed nonequilibrium dynamics of the system *will* depend on the exchange of energy and particles between C and the bath, and this will be addressed in future work.

We have performed simulations for a fully three-dimensional homogeneous Bose gas with periodic boundary conditions. This choice has been made to simplify the projection operation that must be carried out. In this case the single particle states are plane waves, and the effect of a condensate is simply to mix modes of momenta $\mathbf{p}$ and $-\mathbf{p}$. This allows us to apply the projector cleanly in momentum space, which is easily accessible by fast Fourier transform. In principle there is no barrier to performing the same computation in a trap—in practice the projection operation is much more time consuming.

The dimensionless equation we compute is

$$i\frac{\partial\psi(\tilde{\mathbf{r}})}{\partial\tau} = -\tilde{\nabla}^2\psi(\tilde{\mathbf{r}}) + C_{\mathrm{nl}}\hat{\mathcal{P}}|\psi(\tilde{\mathbf{r}})|^2\psi(\tilde{\mathbf{r}}), \quad (5)$$

where we have defined $\int d^3\tilde{\mathbf{r}}\,|\psi(\tilde{\mathbf{r}})|^2 = 1$. The nonlinear constant is $C_{\mathrm{nl}} = 2mNU_0/\hbar^2L$, where N is the total number of particles in the volume, and L is the period of the system. Our dimensionless parameters are $\tilde{\mathbf{r}} = \mathbf{r}/L$, wave vector $\tilde{\mathbf{k}} = \mathbf{k}L$, energy $\tilde{\varepsilon} = \varepsilon/\varepsilon_L$, and time $\tau = \varepsilon_L t/\hbar$, with $\varepsilon_L = \hbar^2/(2mL^2)$.

The calculations presented here have been performed with $C_{\mathrm{nl}} = 2000$, and the projector $\hat{\mathcal{P}}$ chosen such that all modes have $|\mathbf{k}| < 15 \times 2\pi/L$. This means that a large number of the states contained in the calculation are phononlike for large condensate fraction. We note that while the number of states in the problem is fixed, the nonlinear constant determines only the ratio of NU_0/L. This means that for a given value of C_{nl}, we are free to choose N, U_0, and L such that our condition $|c_{\mathbf{k}}|^2 \gg 1$ is always satisfied for a given physical situation. In particular, we can choose ^{87}Rb atoms with $N = 5 \times 10^5$ and $L \approx 17\ \mu$m to give a number density of about 10^{14} cm^{-3}—similar parameters to current experiments in traps.

We begin our simulations with wave functions far from equilibrium with a chosen total energy $\tilde{E}$. They have a flat distribution in k space out to some maximum momentum determined by $\tilde{E}$, and the phase of each momentum component is chosen at random. These initial states are then evolved for a time period of $\tau = 0.4$, by which stage equilibrium appears to have been reached. We determine the properties of the system at equilibrium by assuming that the ergodic theorem applies, and time averaging over 50 wave functions from the last $\delta\tau = 0.1$ of the simulation. We find that the equilibrium properties depend only on the total energy—they are independent of the details of the initial wave function.

Strong evidence that the simulations have reached equilibrium is given by the time dependence of the condensate population. For all energies this settles down to an average value that fluctuates by a small amount, and the results are presented in Fig. 1. Further support is provided by the distribution of the particles in momentum space. Rather than using the plane-wave basis, we transform the wave functions into the quasiparticle basis of quadratic Bogoliubov

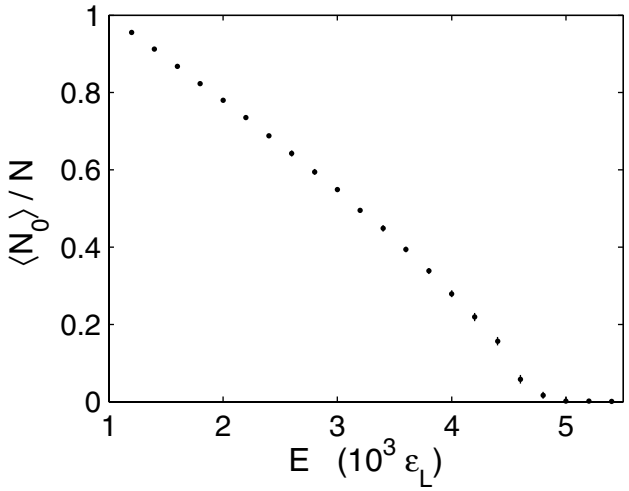

FIG. 1. Condensate fraction plotted against total energy after each individual simulation has reached equilibrium. The barely discernible vertical lines on each point indicate the magnitude of the fluctuations.

theory, the sole parameters of the transformation being the condensate fraction and the nonlinear constant $C_{\rm nl}$. We then average the populations of the quasiparticles states over time and angle to produce a one-dimensional plot, and the results are shown in Fig. 2.

The GPE is the high occupation limit of the full equation for the Bose field operator. Therefore, in equilibrium we expect the mean occupation of the quasiparticle mode k to be the classical limit of the Bose-Einstein distribution—i.e., the equipartition relation

$$\langle N_k \rangle = \frac{k_B T}{\varepsilon_k - \mu}. \tag{6}$$

Since we can determine the Bogoliubov occupation $\langle N_k \rangle$ from our simulation data, we can attempt to fit this distribution to a dispersion relation for ε_k, and hence determine the temperature.

In the limit of large condensate fraction $\langle N_0 \rangle / N \sim 1$, we expect the Bogoliubov dispersion relation to be a good estimate of the energies. The Bogoliubov transformation approximates the many-body Hamiltonian by a quadratic form, which can be diagonalized exactly. The eigenstates are quasiparticles, and in our dimensionless units the dispersion relation takes the form

$$\tilde{\varepsilon}_k = \left(\tilde{k}^4 + 2C_{\rm nl} \frac{\langle N_0 \rangle}{N} \tilde{k}^2 \right)^{1/2}. \tag{7}$$

Manipulating Eq. (6) and measuring the excitation spectrum relative to the condensate we find

$$\frac{\tilde{\varepsilon}_k}{\tilde{T}} = \left(\frac{N}{\langle N_k \rangle} - \frac{N}{\langle N_0 \rangle} \right), \tag{8}$$

where $\tilde{T} = k_B T / (N \varepsilon_L)$ is our dimensionless temperature, and the second term on the right-hand side (RHS) arises from the difference between the condensate energy and the chemical potential of the system. By comparing the curve of this relation with that of Eq. (7), a temperature can be determined. For the $\tilde{E} = 1400$ simulation we find $\tilde{T} = 0.0284$ gives an excellent fit, and this is shown in Fig. 3. At higher simulation energies, however, the shape of Eq. (8) no longer agrees with Eq. (7) and we must use a more sophisticated theory to predict the dispersion relation.

As the occupation of the quasiparticle modes becomes significant (in this case more than a few percent), the cubic and quartic terms of the many-body Hamiltonian that were neglected in the Bogoliubov transformation become important. In Ref. [3] Morgan develops a consistent extension of the Bogoliubov theory to higher order that leads to a gapless excitation spectrum. This theory treats the cubic and quartic terms of the Hamiltonian using perturbation theory in the quasiparticle basis. Expressions for the energy shifts of the excitations are given in Sec. 6.2 of Ref. [3], and we have calculated these shifts for our simulations, with typical results plotted in Fig. 4.

The energy spectrum predicted by the second order theory for the $\tilde{E} = 4000$ simulation is in good agreement with the quasiparticle populations extracted from the simulations and is a significantly better fit than the Bogoliubov theory of Eq. (7). The validity of the second order theory is constrained by the requirement [3]

$$\left(\frac{k_B T}{n_0 U_0} \right) (n_0 a^3)^{1/2} \ll 1, \tag{9}$$

where n_0 is the condensate density. For the results of Fig. 4 with $\tilde{E} = 4000$, this parameter is 0.14 and so we are beginning to probe the boundary of validity of the theory. At higher $\tilde{E}$ the shifts it predicts at low k are of the order of the unperturbed energies, and the results become unreliable. In this region higher order terms are important and the second order theory can no longer be expected to give good results.

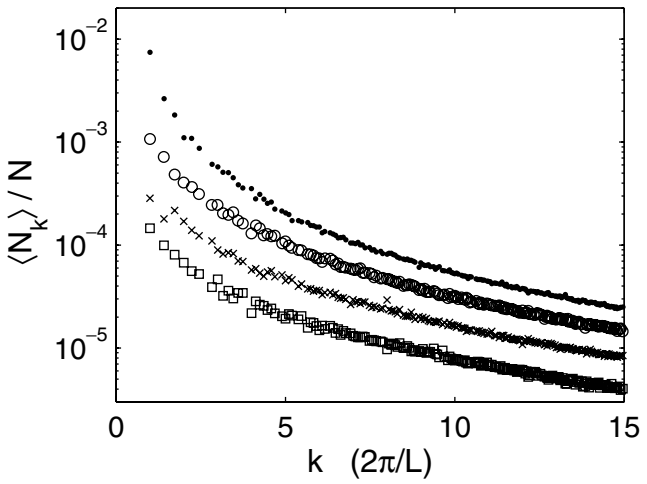

FIG. 2. Plots of the equilibrium Bogoliubov quasiparticle distributions averaged over time and angle for four different total energies. Squares, $\tilde{E} = 1600$; crosses, $\tilde{E} = 2000$; circles, $\tilde{E} = 3200$; dots, $\tilde{E} = 4600$. The mean condensate occupation for all four distributions is off axis.

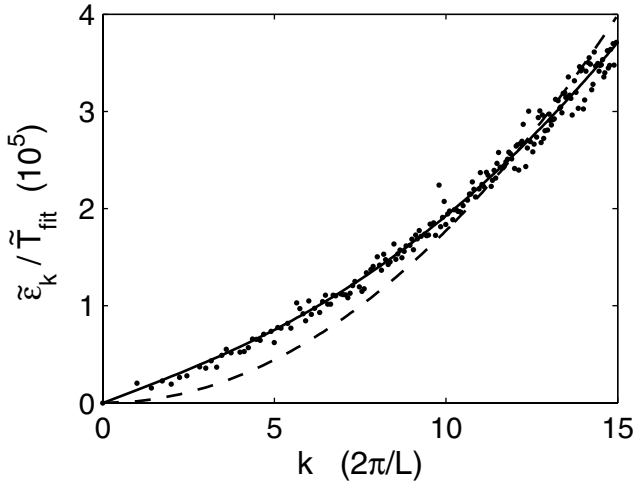

FIG. 3. Comparison of dispersion relations for $\tilde{E} = 1400$ with $\langle N_0 \rangle / N = 0.912$. The dots are a plot of the RHS of Eq. (8), and the lines plot $\tilde{\varepsilon}_k / \tilde{T}_{\rm fit}$. The solid line is for the Bogoliubov dispersion relation with $\tilde{T}_{\rm fit} = 0.0284$, while the dashed line is for the ideal gas with $\tilde{T}_{\rm fit} = 0.0223$.

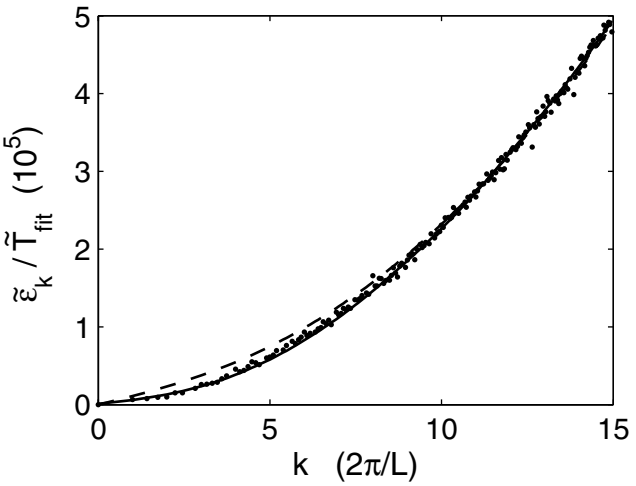

FIG. 4. Comparison of dispersion relations for $\tilde{E} = 4000$ with $\langle N_0 \rangle / N = 0.279$. The dots are a plot of the RHS of Eq. (8) and the lines plot $\tilde{\varepsilon}_k / \tilde{T}_{\rm fit}$. The dashed line is for the Bogoliubov dispersion relation with $\tilde{T}_{\rm fit} = 0.193$, and the solid line is for the second order theory of Ref. [3] with $\tilde{T}_{\rm fit} = 0.201$.

In summary for the system with $C_{\rm nl} = 2000$, Bogoliubov theory gives a good prediction of the energy spectrum for simulations with total energies $\tilde{E} \leq 1600$, while the predictions of second order theory are good up until about $\tilde{E} \approx 4000$. We would like to point out, however, that as the GPE is nonperturbative we expect it will be valid up to and beyond the transition region as long as the condition $N_k \gg 1$ is satisfied.

In addition to the results described above, we have also run simulations with $C_{\rm nl} = 10\,000$ and carried out an identical analysis. We have found that the results from evolving the GPE are qualitatively the same, and for very large condensate fractions Bogoliubov theory accurately predicts the energy spectrum accurately. However, it appears that the second order theory develops a gap in the energy spectrum in systems with a momentum cutoff. This feature is yet to be understood.

In this Letter we have presented results for some of the equilibrium properties of the homogeneous gas. Other properties such as fluctuations and coherence lengths, as well as the nonequilibrium dynamics, will be considered elsewhere. We would like to emphasize that this method relies on the lowest energy modes of the system being classical in nature, and thus cannot handle situations where strong quantum fluctuations are important.

In conclusion, we have presented evidence that the projected Gross-Pitaevskii equation is a good approximation to the classical modes of a Bose gas. We have described how to carry out the projection technique in the homogeneous case with periodic boundary conditions, and have shown that starting with a randomized wave function with a given energy, the projected GPE evolves towards an equilibrium state. We have analyzed the numerical data in terms of the gapless, finite temperature theory of Ref. [3] in the classical limit, and found that both the occupation and energies of the quasiparticles agree quantitatively with the predictions.

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