# Calculation of the microcanonical temperature for the classical Bose field

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**Abstract**
The ergodic hypothesis asserts that a classical mechanical system will in
time visit every available configuration in phase space. Thus, for an ergodic
system, an ensemble average of a thermodynamic quantity can equally well
be calculated by a time average over a sufficiently long period of dynamical
evolution. In this paper, we describe in detail how to calculate the temperature
and chemical potential from the dynamics of a microcanonical classical field,
using the particular example of the classical modes of a Bose-condensed gas.
The accurate determination of these thermodynamics quantities is essential
in measuring the shift of the critical temperature of a Bose gas due to non-
perturbative many-body effects.

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## 1. Introduction

The shift in critical temperature of the homogeneous Bose gas has been the subject of numerous
investigations over the past 50 years. As the mean density of this idealized system is constant,
the shift due to the mean-field is zero, and the first-order shift is due to long-wavelength critical
fluctuations. The first estimates were due to Lee and Yang [1, 2], who gave two different results
for the dependence on the s-wave scattering length $a$. In 1999, Baym $et\ al$ [3] determined that
the result should be

$$\Delta T_c \big/ T_c^0 = can^{1/3}, \tag{1}$$

where $n$ is the particle number density, and $c$ is a constant of order unity. Several authors
have attempted to calculate this constant, and a wide range of results have been obtained,
as summarized in figure 1 of [4]. However recent Monte Carlo calculations have apparently

settled this matter, giving a combined result of $c \approx 1.31 \pm 0.02$ [4, 5]. A useful summary and discussion of this topic is provided by Andersen [6] and Holzmann *et al* [7].

Previously we have performed numerical simulations of an equation known as the projected Gross–Pitaevskii equation (PGPE), which can be used to represent the highly occupied modes of Bose condensed gases at finite temperature [8–12]. This equation is observed to evolve randomized initial conditions to equilibrium for which it is possible to measure a temperature [13–15]. The PGPE is non-perturbative, and hence includes the effect of critical fluctuations. The only approximation made is that the modes of the gas are sufficiently highly occupied as to be well described by a classical rather than a quantum field. The occupation condition is that mode $k$ must satisfy $\langle N_k \rangle \gg 1$; however for practical simulations we may choose, for example, $\langle N_k \rangle \geqslant 5$ [16]. This method is suitable for investigating many problems of current interest in ultra-cold Bose gases, such as the shift in critical temperature due to non-perturbative effects [17].

The PGPE describes a microcanonical system, with the classical field restricted to a finite number of modes for which the occupation number condition is met. In order to study the problem of the shift in $T_c$ it is necessary to accurately determine thermodynamic quantities defined as derivatives of the entropy such as the temperature and chemical potential. In 1997 Rugh developed a new approach to statistical mechanics where he derived an expression from the Hamiltonian of a system for which the ensemble average gives the temperature within the microcanonical ensemble [18]. However, if the system is known to be ergodic then the equilibrium temperature can be determined from the system dynamics over a sufficiently long period of time.

We have applied an extension of Rugh's method to the PGPE Hamiltonian, and the appropriate expression to determine the temperature is given as equation (22) of [19]. This method was found to agree with the less rigorous methods described in [13, 14]. In [19], we made use of this method to calculate the shift in the critical temperature of the homogeneous Bose gas. Despite the calculation being performed with limited statistics and suffering from finite size effects, it gave a result of $c = 1.3 \pm 0.4$ in agreement with the Monte Carlo results [4, 5]. In [17], we applied this method to the experiment of Gerbier *et al* [20] who measured the shift in critical temperature of a trapped Bose gas, and found good agreement with experiment. In this paper, we give the details of our implementation of Rugh's method for a general mode basis for the PGPE.

## 2. Background

### 2.1. Formalism of Rugh

We consider a classical system with $M$ independent modes. The Hamiltonian can be written as $H = H(\mathbf{\Gamma})$, where $\mathbf{\Gamma} = \{\Gamma_i\} = \{Q_i, P_i\}$ is a vector of length $2M$ consisting of the canonical position and momentum coordinates. We define the gradient operator $\nabla$ in terms of its components $\nabla_i = \partial/\partial\Gamma_i$. In the notation of Rugh [21], the Hamiltonian $H$ may have a number of independent first integrals, labelled by $F = F_1, \ldots, F_m$, that are invariant under the dynamics of $H$. A particular macro-state of such a system can be specified by the values of the conserved quantities, labelled as $H = E$, $F_i = I_i$.

The usual expression for the temperature of a system in the microcanonical ensemble is given by

$$\frac{1}{k_B T} = \left(\frac{\partial S}{\partial E}\right)_{F_i}, \tag{2}$$

where all other constants of motion are held fixed, and where the entropy can be written as

$$e^{S/k_B} = \int d\Gamma \, \delta[E - H(\Gamma)] \prod_i \delta[I_i - F_i(\Gamma)]. \tag{3}$$

Using Rugh's methods, the temperature of the system can be written as

$$\frac{1}{k_B T} = \langle \mathcal{D} \cdot \mathbf{X}_T(\Gamma) \rangle, \tag{4}$$

where the angle brackets correspond to an ensemble average, and the components of the vector operator $\mathcal{D}$ are

$$\mathcal{D}_i = e_i \frac{\partial}{\partial \Gamma_i}, \tag{5}$$

where $e_i$ can be chosen to be any scalar value, including zero. The vector field $\mathbf{X}_T$ can also be chosen freely within the constraints

$$\mathcal{D}H \cdot \mathbf{X}_T = 1, \qquad \mathcal{D}F_i \cdot \mathbf{X}_T = 0, \qquad 1 \leqslant i \leqslant m. \tag{6}$$

Geometrically this means that the vector field $\mathbf{X}_T$ has a nonzero component transverse to the $H = E$ energy surface, and is parallel to the surfaces $F_i = I_i$. The expectation value in equation (4) is over all possible states in the microcanonical ensemble; however if the ergodic theorem is applicable then it can equally well be interpreted as a time average. For further details on the origin of this expression we refer the reader to Rugh's original papers [18, 21, 22], as well as derivations found in Giardinà and Livi [23], Jepps *et al* [24] and Rickayzen and Powles [25].

### 2.2. Dimensionless Hamiltonian

The classical Hamiltonian for the dilute Bose gas in dimensionless form is

$$H = \int d^3\mathbf{x} \left[ \psi^*(\mathbf{x}) H_{sp} \psi(\mathbf{x}) + V_{ad}(\mathbf{x})|\psi(\mathbf{x})|^2 + \frac{C_{nl}}{2}|\psi(\mathbf{x})|^4 \right], \tag{7}$$

where $H = \tilde{H}/(N_C \epsilon_L)$, $N_C$ is the number of particles in the system, $\mathbf{x} = \tilde{\mathbf{x}}/L$, $L$ is the unit of length, $\epsilon_L = \hbar^2/(2mL^2)$ is the unit of energy, and $m$ is the mass of the particles. The dimensionless classical Bose field operator $\psi(\mathbf{x})$ is here normalized to one, $\int d^3\mathbf{x}|\psi(\mathbf{x})|^2 = 1$, and $C_{nl}$ is the nonlinear constant defined as

$$C_{nl} = \frac{N_C U_0}{\epsilon_L L^3} = \frac{8\pi a N_C}{L}, \tag{8}$$

where $U_0 = 4\pi\hbar^2 a/m$. $H_{sp}$ is the single particle Hamiltonian with eigenbasis $H_{sp}\phi_k(\mathbf{x}) = \epsilon_k \phi_k(\mathbf{x})$, and $V_{ad}(\mathbf{x})$ is the dimensionless version of any potential *additional* to that included in the single-particle Hamiltonian.

We restrict our field $\psi(\mathbf{x})$ to be formed from the modes of the classical region $C$ defined by a high energy cutoff in the single-particle basis, such that we can write

$$\psi(\mathbf{x}) = \sum_{k \in C} c_k \phi_k(\mathbf{x}). \tag{9}$$

The equation of motion for this restricted system is the projected Gross–Pitaevskii equation

$$i\frac{\partial \psi(\mathbf{x})}{\partial \tau} = H_{sp}\psi + \mathcal{P}\{V_{ad}(\mathbf{x})\psi(\mathbf{x}) + C_{nl}|\psi(\mathbf{x})|^2\psi(\mathbf{x})\}. \tag{10}$$

The projection operator $\mathcal{P}\{F\}$ projects function $F$ onto the classical modes of the single particle Hamiltonian $H_{sp}$ via

$$\mathcal{P}\{F(\mathbf{x})\} = \sum_{k \in C} \phi_k(\mathbf{x}) \int d^3\mathbf{x}' \, \phi_k^*(\mathbf{x}') F(\mathbf{x}'). \tag{11}$$

It eliminates collisional processes which would cause the scattering of particles into higher energy single particle modes not represented by the classical field.

In the single-particle basis of $H_{sp}$ the Hamiltonian (7) can be written as

$$H = \sum_{n \in C} \epsilon_n c_n^* c_n + \sum_{mn \in C} V_{mn} c_m^* c_n + \frac{C_{nl}}{2} \sum_{mnpq \in C} c_m^* c_n^* c_p c_q \langle mn|pq \rangle, \tag{12}$$

where we have defined the matrix elements

$$V_{mn} = \int d^3\mathbf{x} \, \phi_m^*(\mathbf{x}) V_{ad}(\mathbf{x}) \phi_n(\mathbf{x}), \tag{13}$$

$$\langle mn|pq \rangle = \int d^3\mathbf{x} \, \phi_m^*(\mathbf{x}) \phi_n^*(\mathbf{x}) \phi_p(\mathbf{x}) \phi_q(\mathbf{x}). \tag{14}$$

We make use of the real, canonically-conjugate coordinates $Q_n$ and $P_n$ defined by

$$Q_n = \frac{1}{\sqrt{2\epsilon_n}} (c_n^* + c_n), \qquad P_n = i\sqrt{\frac{\epsilon_n}{2}} (c_n^* - c_n), \tag{15}$$

with the inverse transformation

$$c_n = \sqrt{\frac{\epsilon_n}{2}} Q_n + \frac{i}{\sqrt{2\epsilon_n}} P_n, \qquad c_n^* = \sqrt{\frac{\epsilon_n}{2}} Q_n - \frac{i}{\sqrt{2\epsilon_n}} P_n. \tag{16}$$

### 2.3. Choice of vector field $\mathbf{X}$

In order to satisfy conditions (6), we can choose a vector field of the form

$$\mathbf{X}_T = a\mathcal{D}H + \sum_{i=1}^{m} b_i \mathcal{D}F_i, \tag{17}$$

where the $m+1$ coefficients $\{a, b_i\}$ are determined by the $m+1$ simultaneous equations in equation (6). Due to the freedom in the choice of the vector operator $\mathcal{D}$, we can set any number of components of the length $2M$ vector $\mathbf{X}_T$ to zero. This turns out to be useful as the components corresponding to the momentum and position variables can be different orders of magnitude. Two particular choices we make use of later are $\mathbf{X}_{T,P}$ with $\mathcal{D} = \mathcal{D}_P = \{0, \partial/\partial P_i\}$ and $\mathbf{X}_{T,Q}$ with $\mathcal{D} = \mathcal{D}_Q = \{\partial/\partial Q_i, 0\}$. These lead to two different calculations for the temperature that only agree in general if the system is in thermal equilibrium. This provides a useful check that the numerical simulations have indeed reached thermal equilibrium, as well as giving two independent values for the temperature.

For the classical Bose gas Hamiltonian (7), there can be several constants of motion that must be taken into account. These depend on the details of the single-particle Hamiltonian $H_{sp}$—examples include components of the angular and/or linear momentum. The effect of including these additional first integrals in the definition of the vector field $\mathbf{X}_T$ is to account for the energy that is associated with a conserved quantity and hence is unavailable for thermalization. This ensures that only the appropriate free energy is used to calculate the

temperature. We conjecture that the same result can be achieved by first transforming to a coordinate system where the total angular and linear momenta, etc, are all zero and therefore do not contribute to the energy of the system. Rugh demonstrated this explicitly in [21] for a system of particles with a conserved centre-of-mass motion, and our numerical results support this conjecture.

An exception to this, however, is the conservation of normalization $N = \sum_n c_n^* c_n$. This must be considered explicitly because there is no coordinate system in which it can be made to vanish. The constraint on $N$ means that the ground-state of the system will, in general, have a finite energy that is not accessible for thermalization. We note that the effect of this constraint is in general more complicated than a simple subtraction of the ground-state energy (which could be achieved by hand) and depends on the definition of the operator $\mathcal{D}$ used to calculate the temperature, as shown below.

We need to choose a vector field $\mathbf{X}_T$ which satisfies equations (6) with $F_1 = N = \sum_n c_n^* c_n$. The result is

$$\mathbf{X}_T = \frac{\mathcal{D}H - \lambda_N \mathcal{D}N}{|\mathcal{D}H|^2 - \lambda_N \mathcal{D}N \cdot \mathcal{D}H}, \tag{18}$$

where the parameter

$$\lambda_N = \frac{\mathcal{D}N \cdot \mathcal{D}H}{|\mathcal{D}N|^2}, \tag{19}$$

looks similar to a chemical potential. Substituting equation (18) into equation (4) we find that our full expression for the dimensionless temperature $\tilde{T} = k_B T / N_C \epsilon_L$ is

$$\frac{1}{\tilde{T}} = \left\langle \frac{\mathcal{D}^2 H - \lambda_N \mathcal{D}^2 N - \mathcal{D}\lambda_N \cdot \mathcal{D}N}{|\mathcal{D}H|^2 - \lambda_N (\mathcal{D}H \cdot \mathcal{D}N)} \right\rangle$$
$$- \left\langle \frac{(\mathcal{D}H - \lambda_N \mathcal{D}N) \cdot [\mathcal{D}|\mathcal{D}H|^2 - (\mathcal{D}H \cdot \mathcal{D}N)\mathcal{D}\lambda_N - \lambda_N \mathcal{D}(\mathcal{D}H \cdot \mathcal{D}N)]}{[|\mathcal{D}H|^2 - \lambda_N (\mathcal{D}H \cdot \mathcal{D}N)]^2} \right\rangle, \tag{20}$$

where

$$\mathcal{D}\lambda_N = \frac{\mathcal{D}(\mathcal{D}N \cdot \mathcal{D}H)}{|\mathcal{D}N|^2} + \frac{\mathcal{D}N \cdot \mathcal{D}H}{|\mathcal{D}N|^4} \mathcal{D}(|\mathcal{D}N|^2). \tag{21}$$

The chemical potential of the system can be determined in a similar manner using a different choice of vector field. In particular we wish to calculate

$$\frac{\mu}{k_B T} = -\left( \frac{\partial S}{\partial N} \right)_E = \langle \mathcal{D} \cdot \mathbf{X}_\mu(\mathbf{\Gamma}) \rangle, \tag{22}$$

where the conditions on the vector field are

$$\mathcal{D}H \cdot \mathbf{X}_\mu = 0, \qquad \mathcal{D}N \cdot \mathbf{X}_\mu = 1. \tag{23}$$

This results in expressions identical to the RHS of equations (18)–(20) but with $H$ and $N$ interchanged, and so we will not write them out in full.

The technique outlined above has been described previously by one of us in [19], and in particular the result of equation (20) was given in that work. The numerical method has also been applied by the current authors in [15, 17]. The purpose of this paper is to outline in detail the procedure for calculating the terms in equations (20) and (21). This is not a trivial exercise, and the proliferation of terms can make it difficult to avoid errors in both the analytical and numerical implementation. By discussing our approach to evaluating

equations (20) and (21) we hope to facilitate other researchers wanting to make use of the method. The basic numerical requirement is an efficient and accurate numerical transform from real space to basis space and vice versa. This may be provided, for example, by fast Fourier transforms using a basis of plane waves appropriate for a homogeneous system [13, 14], or an efficient quadrature for trapped systems [15].

## 3. Formulae

In this section we give explicit analytic expressions for all quantities required in the evaluation of equations (20) and (21). As we are using the canonical coordinates defined in equation (15) it is easiest to evaluate the derivatives of the Hamiltonian using the mode expansion of the Hamiltonian (12). However, this leaves us with expressions involving inner products of vector quantities with summations that would be computationally expensive to evaluate directly for any sizeable basis. We show how to define auxiliary field functions that can be used to simplify these terms for implementation with an efficient numerical transform.

### 3.1. Derivatives

We begin by writing out the necessary derivatives of the Hamiltonian using the two choices of vector operator defined earlier, $\mathcal{D}_Q$ and $\mathcal{D}_P$. In component form the first derivatives of the Hamiltonian are

$$
(\mathcal{D}_Q H)_i = \epsilon_i^2 Q_i + \sqrt{\frac{\epsilon_i}{2}} \sum_n [V_{ni} c_n^* + V_{in} c_n] + C_{\mathrm{nl}} \sqrt{\frac{\epsilon_i}{2}} \sum_{pqm} [c_p^* c_q^* c_m \langle pq|mi \rangle + c_m^* c_p c_q \langle mi|pq \rangle],
\tag{24}
$$

$$
(\mathcal{D}_P H)_i = P_i + \frac{\mathrm{i}}{\sqrt{2\epsilon_i}} \sum_n [V_{ni} c_n^* - V_{in} c_n] + \mathrm{i} \frac{C_{\mathrm{nl}}}{\sqrt{2\epsilon_i}} \sum_{pqm} [c_p^* c_q^* c_m \langle pq|mi \rangle - c_m^* c_p c_q \langle mi|pq \rangle],
\tag{25}
$$

and the second derivatives are

$$
(\mathcal{D}_Q^2 H)_{ij} = \delta_{ij} \epsilon_i^2 + \frac{\sqrt{\epsilon_i \epsilon_j}}{2} [V_{ij} + V_{ji}] + \frac{C_{\mathrm{nl}}}{2} \sqrt{\epsilon_i \epsilon_j} \sum_{pq} [4 c_p^* c_q \langle pi|qj \rangle
$$
$$
+ c_p c_q \langle ij|pq \rangle + c_p^* c_q^* \langle pq|ij \rangle],
\tag{26}
$$

$$
(\mathcal{D}_P^2 H)_{ij} = \delta_{ij} + \frac{1}{2\sqrt{\epsilon_i \epsilon_j}} [V_{ij} + V_{ji}] + \frac{C_{\mathrm{nl}}}{2\sqrt{\epsilon_i \epsilon_j}} \sum_{pq} [4 c_p^* c_q \langle pi|qj \rangle
$$
$$
- c_p c_q \langle ij|pq \rangle - c_p^* c_q^* \langle pq|ij \rangle].
\tag{27}
$$

We also need the derivatives of the other first integral of the Hamiltonian—the normalization given by $N = \sum_{k \in C} |c_k|^2$. These are

$$
(\mathcal{D}_Q N)_i = \epsilon_i Q_i, \qquad (\mathcal{D}_P N)_i = \frac{P_i}{\epsilon_i},
\tag{28}
$$

$$
(\mathcal{D}_Q^2 N)_{ij} = \epsilon_i \delta_{ij}, \qquad (\mathcal{D}_P^2 N)_{ij} = \frac{\delta_{ij}}{\epsilon_i}.
\tag{29}
$$

From equation (20) we can see that we need the terms,

$$\mathcal{D}(|\mathcal{D}H|^2)_i = 2\sum_j (\mathcal{D}H)_j (\mathcal{D}^2 H)_{ij}, \qquad \mathcal{D}(|\mathcal{D}N|^2)_i = 2\sum_j (\mathcal{D}N)_j (\mathcal{D}^2 N)_{ij}, \qquad (30)$$

$$\mathcal{D}(\mathcal{D}N \cdot \mathcal{D}H)_i = \sum_j [(\mathcal{D}N)_j (\mathcal{D}^2 H)_{ij} + (\mathcal{D}H)_j (\mathcal{D}^2 N)_{ij}]. \qquad (31)$$

Some of these expressions are simple to calculate e.g.

$$\mathcal{D}_Q(|\mathcal{D}_Q N|^2)_i = 2\sum_j (\mathcal{D}_Q N)_j (\mathcal{D}_Q^2 N)_{ij} \qquad (32)$$

$$= 2\sum_j (\epsilon_j Q_j)(\epsilon_i \delta_{ij}) = 2\epsilon_i^2 Q_i, \qquad (33)$$

$$\mathcal{D}_P(|\mathcal{D}_P N|^2)_i = 2\sum_j (\mathcal{D}_P N)_j (\mathcal{D}_P^2 N)_{ij} \qquad (34)$$

$$= 2\sum_j \left(\frac{P_i}{\epsilon_i}\right) \left(\frac{\delta_{ij}}{\epsilon_i}\right) = 2\frac{P_i}{\epsilon_i^2}, \qquad (35)$$

$$\sum_j (\mathcal{D}_Q H)_j (\mathcal{D}_Q^2 N)_{ij} = \sum_j (\mathcal{D}_Q H)_j \epsilon_i \delta_{ij} = \epsilon_i (\mathcal{D}_Q H)_i, \qquad (36)$$

$$\sum_j (\mathcal{D}_P H)_j (\mathcal{D}_P^2 N)_{ij} = \frac{\delta_{ij}}{\epsilon_i} = \frac{(\mathcal{D}_P H)_i}{\epsilon_i}. \qquad (37)$$

However, the remainder are more complicated. To calculate them efficiently we make the following vector definitions:

$$a_j = \sqrt{\epsilon_j}(\mathcal{D}_Q H)_j, \qquad b_j = \frac{(\mathcal{D}_P H)_j}{\sqrt{\epsilon_j}}, \qquad (38)$$

$$f_j = \sqrt{\epsilon_j}(\mathcal{D}_Q N)_j, \qquad g_j = \frac{(\mathcal{D}_P N)_j}{\sqrt{\epsilon_j}}, \qquad (39)$$

with the corresponding auxiliary field functions

$$A(\mathbf{x}) = \sum_j a_j \phi_j(\mathbf{x}), \qquad B(\mathbf{x}) = \sum_j b_j \phi_j(\mathbf{x}), \qquad (40)$$

$$F(\mathbf{x}) = \sum_j f_j \phi_j(\mathbf{x}), \qquad G(\mathbf{x}) = \sum_j g_j \phi_j(\mathbf{x}). \qquad (41)$$

Making use of these definitions we find

$$\mathcal{D}_Q(|\mathcal{D}_Q H|^2)_i = 2\sum_j (\mathcal{D}_Q H)_j (\mathcal{D}_Q^2 H)_{ij},$$

$$= 2\sum_j \frac{a_j}{\sqrt{\epsilon_j}} \left(\delta_{ij}\epsilon_i^2 + \frac{\sqrt{\epsilon_i \epsilon_j}}{2}[V_{ij} + V_{ji}] + \frac{C_{\text{nl}}}{2}\sqrt{\epsilon_i \epsilon_j}\sum_{pq}[4c_p^* c_q \langle pi|qj\rangle \right.$$

$$+ c_p c_q \langle ij|pq\rangle + c_p^* c_q^* \langle pq|ij\rangle] \Big),$$

$$= 2a_i \epsilon_i^{3/2} + \sqrt{\epsilon_i} \sum_j a_j [V_{ij} + V_{ji}] + C_{\mathrm{nl}} \sqrt{\epsilon_i} \sum_{pqj} a_j [4c_p^* c_q \langle pi|qj\rangle$$

$$+ c_p c_q \langle ij|pq\rangle + c_p^* c_q^* \langle pq|ij\rangle], \tag{42}$$

$$\mathcal{D}_P (|\mathcal{D}_P H|^2)_i = 2 \sum_j (\mathcal{D}_P H)_j (\mathcal{D}_P^2 H)_{ij},$$

$$= 2 \sum_j \sqrt{\epsilon_j} b_j \Big( \delta_{ij} + \frac{1}{2\sqrt{\epsilon_i \epsilon_j}} [V_{ij} + V_{ji}] + \frac{C_{\mathrm{nl}}}{2\sqrt{\epsilon_i \epsilon_j}} \sum_{pq} [4c_p^* c_q \langle pi|qj\rangle$$

$$- c_p c_q \langle ij|pq\rangle - c_p^* c_q^* \langle pq|ij\rangle] \Big),$$

$$= 2\sqrt{\epsilon_i} b_i + \frac{1}{\sqrt{\epsilon_i}} \sum_j b_j [V_{ij} + V_{ji}] + \frac{C_{\mathrm{nl}}}{\sqrt{\epsilon_i}} \sum_{pqj} b_j [4c_p^* c_q \langle pi|qj\rangle$$

$$- c_p c_q \langle ij|pq\rangle - c_p^* c_q^* \langle pq|ij\rangle], \tag{43}$$

and

$$\sum_j (\mathcal{D}_Q N)_j (\mathcal{D}_Q^2 H)_{ij} = \sum_j \frac{f_j}{\sqrt{\epsilon_j}} \Big( \delta_{ij} \epsilon_i^2 + \frac{\sqrt{\epsilon_i \epsilon_j}}{2} [V_{ij} + V_{ji}]$$

$$+ \frac{C_{\mathrm{nl}}}{2} \sqrt{\epsilon_i \epsilon_j} \sum_{pq} [4c_p^* c_q \langle pi|qj\rangle + c_p c_q \langle ij|pq\rangle + c_p^* c_q^* \langle pq|ij\rangle] \Big),$$

$$= f_i \epsilon_i^{3/2} + \frac{\sqrt{\epsilon_i}}{2} \sum_j f_j [V_{ij} + V_{ji}] + \frac{C_{\mathrm{nl}}}{2} \sqrt{\epsilon_i} \sum_{pqj} f_j [4c_p^* c_q \langle pi|qj\rangle$$

$$+ c_p c_q \langle ij|pq\rangle + c_p^* c_q^* \langle pq|ij\rangle], \tag{44}$$

$$\sum_j (\mathcal{D}_P N)_j (\mathcal{D}_P^2 H)_{ij} = \sum_j \sqrt{\epsilon_j} g_j \Big( \delta_{ij} + \frac{1}{2\sqrt{\epsilon_i \epsilon_j}} [V_{ij} + V_{ji}] + \frac{C_{\mathrm{nl}}}{2\sqrt{\epsilon_i \epsilon_j}} \sum_{pq} [4c_p^* c_q \langle pi|qj\rangle$$

$$- c_p c_q \langle ij|pq\rangle - c_p^* c_q^* \langle pq|ij\rangle] \Big),$$

$$= \sqrt{\epsilon_i} g_i + \frac{1}{2\sqrt{\epsilon_i}} \sum_j g_j [V_{ij} + V_{ji}] + \frac{C_{\mathrm{nl}}}{2\sqrt{\epsilon_i}} \sum_{pqj} g_j [4c_p^* c_q \langle pi|qj\rangle$$

$$- c_p c_q \langle ij|pq\rangle - c_p^* c_q^* \langle pq|ij\rangle]. \tag{45}$$

### 3.2. Evaluation of terms with auxiliary fields

The above expressions are written in a form that they can be easily calculated using efficient quadratures in real space. We outline in detail how to calculate all of these terms, and write them in the most efficient form we have found. We make the definitions,

$$\sum_n V_{in} c_n = \int \mathrm{d}^3 \mathbf{x}\, \phi_i^*(\mathbf{x}) V_{\mathrm{ad}}(\mathbf{x}) \psi(\mathbf{x}) \equiv W_i, \tag{46}$$

$$\sum_n V_{ni} c_n^* = \int \mathrm{d}^3 \mathbf{x}\, \psi^*(\mathbf{x}) V_{\mathrm{ad}}(\mathbf{x}) \phi_i(\mathbf{x}) \equiv W_i^*, \tag{47}$$

where we have assumed that the potential $V_{ad}(\mathbf{x})$ is real. We can therefore write the appropriate parts of equations (24) and (25) as

$$\sum_n [V_{ni}c_n^* + V_{in}c_n] = 2\,\mathrm{Re}(W_i), \tag{48}$$

$$\sum_n [V_{ni}c_n^* - V_{in}c_n] = -2\mathrm{i}\,\mathrm{Im}(W_i). \tag{49}$$

The next set of terms are

$$\sum_{pqm} c_m^* c_p c_q \langle mi|pq\rangle = \int \mathrm{d}^3\mathbf{x}\,\phi_i^*(\mathbf{x})|\psi(\mathbf{x})|^2\psi(\mathbf{x}) \equiv K_i, \tag{50}$$

$$\sum_{pqm} c_p^* c_q^* c_m \langle pq|mi\rangle = \int \mathrm{d}^3\mathbf{x}|\psi(\mathbf{x})|^2\psi^*(\mathbf{x})\phi_i(\mathbf{x}) \equiv K_i^*. \tag{51}$$

Hence, parts of equations (24) and (25) can be written as

$$\sum_{pqm} [c_p^* c_q^* c_m \langle pq|mi\rangle + c_m^* c_p c_q \langle mi|pq\rangle] = 2\,\mathrm{Re}(K_i), \tag{52}$$

$$\sum_{pqm} [c_p^* c_q^* c_m \langle pq|mi\rangle - c_m^* c_p c_q \langle mi|pq\rangle] = -2\mathrm{i}\,\mathrm{Im}(K_i). \tag{53}$$

For the terms involving the auxiliary fields we have expressions like

$$\sum_{pqj} a_j c_p^* c_q \langle pi|qj\rangle = \int \mathrm{d}^3\mathbf{x}\phi_i^*(\mathbf{x})|\psi(\mathbf{x})|^2 A(\mathbf{x}) \equiv (A_1)_i, \tag{54}$$

$$\sum_{pqj} a_j c_p c_q \langle ij|pq\rangle = \int \mathrm{d}^3\mathbf{x}\,\phi_i^*(\mathbf{x})A^*(\mathbf{x})\psi(\mathbf{x})^2 \equiv (A_2)_i, \tag{55}$$

$$\sum_{pqj} a_j c_p^* c_q^* \langle pq|ij\rangle = \int \mathrm{d}^3\mathbf{x}\psi^*(\mathbf{x})^2\phi_i(\mathbf{x})A(\mathbf{x}) \equiv (A_2)_i^*, \tag{56}$$

$$\sum_j a_j V_{ij} = \int \mathrm{d}^3\mathbf{x}\,\phi_i^*(\mathbf{x})V_{ad}(\mathbf{x})A(\mathbf{x}) \equiv (A_3)_i, \tag{57}$$

$$\sum_j a_j V_{ji} = \int \mathrm{d}^3\mathbf{x}\,A^*(\mathbf{x})V_{ad}(\mathbf{x})\phi_i(\mathbf{x}) \equiv (A_3)_i^*, \tag{58}$$

where we have made use of the fact that $a_j = a_j^*$. We have similar expression for all the other auxiliary vector fields $b$, $f$ and $g$ and will refrain from writing these all out. We can write parts of equations (42), (43), (44) and (45) as

$$\sum_{pqj} a_j[4c_p^* c_q \langle pi|qj\rangle + c_p c_q \langle ij|pq\rangle + c_p^* c_q^* \langle pq|ij\rangle] = 4(A_1)_i + 2\,\mathrm{Re}(A_2)_i, \tag{59}$$

$$\sum_{pqj} b_j[4c_p^* c_q \langle pi|qj\rangle - c_p c_q \langle ij|pq\rangle - c_p^* c_q^* \langle pq|ij\rangle] = 4(B_1)_i - 2\,\mathrm{Re}(B_2)_i, \tag{60}$$

$$\sum_{pqj} f_j[4c_p^* c_q \langle pi|qj\rangle + c_p c_q \langle ij|pq\rangle + c_p^* c_q^* \langle pq|ij\rangle] = 4(F_1)_i + 2\,\mathrm{Re}(F_2)_i, \tag{61}$$

$$\sum_{pqj} g_j[4c_p^*c_q\langle pi|qj\rangle - c_pc_q\langle ij|pq\rangle - c_p^*c_q^*\langle pq|ij\rangle] = 4(G_1)_i - 2\,\mathrm{Re}(G_2)_i, \tag{62}$$

$$\sum_{j} a_j[V_{ij} + V_{ji}] = 2\,\mathrm{Re}(A_3)_i, \qquad \sum_{j} b_j[V_{ij} + V_{ji}] = 2\,\mathrm{Re}(B_3)_i, \tag{63}$$

$$\sum_{j} f_j[V_{ij} + V_{ji}] = 2\,\mathrm{Re}(F_3)_i, \qquad \sum_{j} g_j[V_{ij} + V_{ji}] = 2\,\mathrm{Re}(G_3)_i. \tag{64}$$

The remaining terms are diagonal second derivatives of the form $\mathcal{D}^2 H = \sum_i(\mathcal{D}^2 H)_{ii}$, in which we have matrix elements

$$\sum_{pq} c_p^*c_q\langle pi|qi\rangle = \int \mathrm{d}^3\mathbf{x}|\phi_i(\mathbf{x})|^2|\psi(\mathbf{x})|^2 \equiv (M_1)_i, \tag{65}$$

$$\sum_{pq} c_pc_q\langle ii|pq\rangle = \int \mathrm{d}^3\mathbf{x}\phi_i^*(\mathbf{x})^2\psi(\mathbf{x})^2 \equiv (M_2)_i, \tag{66}$$

$$\sum_{pq} c_p^*c_q^*\langle pq|ii\rangle = \int \mathrm{d}^3\mathbf{x}\psi^*(\mathbf{x})\phi_i(\mathbf{x})^2 \equiv (M_2)_i^*, \tag{67}$$

and thus the appropriate parts of equations (26) and (27) are

$$\sum_{pq}[4c_p^*c_q\langle pi|qi\rangle + c_pc_q\langle ii|pq\rangle + c_p^*c_q^*\langle pq|ii\rangle] = 4(M_1)_i + 2\,\mathrm{Re}(M_2)_i, \tag{68}$$

$$\sum_{pq}[4c_p^*c_q\langle pi|qi\rangle - c_pc_q\langle ii|pq\rangle - c_p^*c_q^*\langle pq|ii\rangle] = 4(M_1)_i - 2\,\mathrm{Re}(M_2)_i. \tag{69}$$

We have now explicitly outlined the calculation of all terms necessary to calculate the temperature and chemical potential of the equilibrium dynamical evolution of a microcanonical PGPE system.

### 3.3. Summary

Here we summarize all the components of the vector quantities required for the evaluation of the temperature according to equation (20) making use of the definitions made in the previous section for both choices of vector operator $\mathcal{D}_Q$ and $\mathcal{D}_P$. The inner products between these vectors found in equation (20) can be easily evaluated numerically. In addition, these are all the terms required for calculating the chemical potential as well.

$$(\mathcal{D}_Q H)_i = \epsilon_i^2 Q_i + \sqrt{2\epsilon_i}\,\mathrm{Re}(W_i) + C_{\mathrm{nl}}\sqrt{2\epsilon_i}\,\mathrm{Re}(K_i), \tag{70}$$

$$(\mathcal{D}_P H)_i = P_i + \frac{2}{\sqrt{\epsilon_i}}\,\mathrm{Im}(W_i) + C_{\mathrm{nl}}\sqrt{\frac{2}{\epsilon_i}}\,\mathrm{Im}(K_i), \tag{71}$$

$$\left(\mathcal{D}_Q^2 H\right)_{ii} = \epsilon_i^2 + \epsilon_i V_{ii} + C_{\mathrm{nl}}\epsilon_i[2(M_1)_i + \mathrm{Re}(M_2)_i], \tag{72}$$

$$\left(\mathcal{D}_P^2 H\right)_{ii} = 1 + \frac{V_{ii}}{\epsilon_i} + \frac{C_{\mathrm{nl}}}{\epsilon_i}[2(M_1)_i - \mathrm{Re}(M_2)_i]. \tag{73}$$

$$\mathcal{D}_Q(|\mathcal{D}_Q N|^2)_i = 2\epsilon_i^2 Q_i, \tag{74}$$

$$\mathcal{D}_P(|\mathcal{D}_P N|^2)_i = 2\frac{P_i}{\epsilon_i^2}, \tag{75}$$

$$\sum_j (\mathcal{D}_Q H)_j (\mathcal{D}_Q^2 N)_{ij} = \epsilon_i (\mathcal{D}_Q H)_i, \tag{76}$$

$$\sum_j (\mathcal{D}_P H)_j (\mathcal{D}_P^2 N)_{ij} = \frac{(\mathcal{D}_P H)_i}{\epsilon_i}. \tag{77}$$

$$\mathcal{D}_Q(|\mathcal{D}_Q H|^2)_i = 2a_i \epsilon_i^{3/2} + 2\sqrt{\epsilon_i}\,\mathrm{Re}(A_3)_i + C_{\mathrm{nl}}\sqrt{\epsilon_i}[4(A_1)_i + 2\,\mathrm{Re}(A_2)_i], \tag{78}$$

$$\mathcal{D}_P(|\mathcal{D}_P H|^2)_i = 2\sqrt{\epsilon_i}\,b_i + \frac{2}{\sqrt{\epsilon_i}}\,\mathrm{Re}(B_3)_i + \frac{C_{\mathrm{nl}}}{\sqrt{\epsilon_i}}[4(B_1)_i - 2\,\mathrm{Re}(B_2)_i], \tag{79}$$

$$\sum_j (\mathcal{D}_Q N)_j (\mathcal{D}_Q^2 H)_{ij} = f_i \epsilon_i^{3/2} + \sqrt{\epsilon_i}\,\mathrm{Re}(F_3)_i + C_{\mathrm{nl}}\sqrt{\epsilon_i}[2(F_1)_i + \mathrm{Re}(F_2)_i], \tag{80}$$

$$\sum_j (\mathcal{D}_P N)_j (\mathcal{D}_P^2 H)_{ij} = \sqrt{\epsilon_i}\,g_i + \frac{1}{\sqrt{\epsilon_i}}\,\mathrm{Re}(G_3)_i + \frac{C_{\mathrm{nl}}}{\sqrt{\epsilon_i}}[2(G_1)_i - \mathrm{Re}(G_2)_i]. \tag{81}$$

## 4. Numerical results

In this section, we outline the algorithm for applying the formulae of the previous section to simulation results, and give examples of the results obtained for the PGPE for trapped Bose gas systems.

We have previously demonstrated in [13–15] that the PGPE will evolve any randomized initial field function to an equilibrium that can be characterized by a temperature, and have made use of this in the beyond mean-field calculation of the critical temperature of a trapped Bose gas in [17].

The basic requirement to determine the temperature in such calculations is to evaluate equation (20) over a sufficiently long period of simulation time for the ergodic averaging to be effective. Our procedure is as follows. Beginning with an initial random field configuration with a predetermined energy, we run our simulation for sufficiently long such that we can be reasonably sure that equilibrium has been reached (this can be checked as described below). This is typically for 100 or more trap periods for simulations of Bose gases in a harmonic potential. We usually save 1000 or more field configurations at equally spaced times throughout the evolution, which are sufficiently separated in time that there is little correlation between samples.

The temperature analysis is performed after the simulation is completed. The field configurations are stored as vectors of basis coefficients, and we make use of efficient computational routines that avoid numerical aliasing to transform to and from a real space representation. For each saved field configuration we calculate the vector components $P_i$ and $Q_i$, the derivatives in equations (28)–(31), the auxillary fields given by equations (40) and (41), and then their overlaps with the various functions of the field $\psi(\mathbf{x})$ as in equations (54)–(58). This allows us to calculate the vector quantities defined in equations (70)–(81) that appear in equation (20). We then form the appropriate dot products of these quantities to give a single sample of $\mathcal{D}_Q \cdot \mathbf{X}_T$ and $\mathcal{D}_P \cdot \mathbf{X}_T$.

These values are calculated for every saved field configuration. These can then be plotted versus time, and any initial transients before the field has settled into equilibrium can be identified (typically this a very small fraction of the total simulation time). The quantities $\mathcal{D}_Q \cdot \mathbf{X}_T$ and $\mathcal{D}_P \cdot \mathbf{X}_T$ are numerically distinct from one another before equilibrium is reached, however they can be quite noisy and so sometimes it is difficult to tell when they are in agreement. We exclude the transients from the final averaging to determine the temperature— typically we discard at least the first quarter of the time evolution to ensure accuracy.
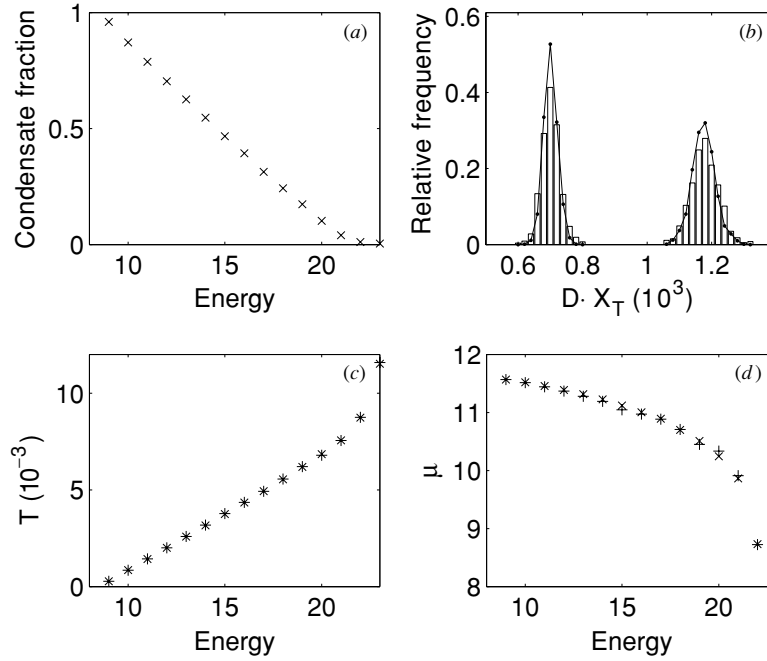
**Figure 1.** Data extracted from PGPE simulations in equilibrium. (*a*) Condensate fraction versus energy of simulation. (*b*) Histograms of the quantity $\mathcal{D} \cdot \mathbf{X}_T$ on the RHS of equation (4) for the simulations with $E = 10$ and $E = 11$. The bars are for the operator $\mathcal{D}_Q$, and the dots connected by solid lines for $\mathcal{D}_P$. (*c*) Temperature versus energy. Plusses: $T_Q$, crosses: $T_P$. (*d*) Chemical potential versus energy. Plusses: $\mu_Q$, crosses: $\mu_P$. All quantities are in dimensionless units as defined in the text.

We now illustrate with a set of typical numerical results from applying the method described in this paper to the PGPE for trapped Bose gas systems. We solve the PGPE (10) for a harmonic trapping potential $V(\mathbf{x}) = (x^2 + y^2 + 8z^2)/4$ and no additional potential $V_{\mathrm{ad}}(\mathbf{x})$. The unit of length is $L = (\hbar/2m\omega_x)^{1/2}$ and energy $\epsilon_L = \hbar\omega_x$. We have a dimensionless energy cutoff of $E_{\mathrm{cut}} = 31$ such that there are 1739 classical modes, and the data shown are for $C_{\mathrm{nl}} = 2000$. We begin individual simulations with a randomized initial condition with fixed energy, and evolve in dimensionless time until $\tau = 1200$, which is slightly more than 190 radial trap periods. We find that these simulations equilibrate very quickly, and use 1000 field samples over the last two-thirds of the evolution for the ergodic averaging. The results are shown in figure 1, some of which have previously been reported in [15].

Figure 1(*a*) shows the condensate fraction versus energy for the PGPE system (we remind the reader that energy given by equation (12) is a conserved quantity in these calculations). The condensate fraction is determined by the Penrose–Onsager criterion: it is the largest eigenvalue found by diagonalizing the single-particle density matrix formed by ergodic averaging as described in [15]. It looks somewhat different to the result for the full three-dimensional system due to the basis cutoff that is present in these simulations. Figure 1(*b*) shows the distribution of the function $\mathcal{D} \cdot \mathbf{X}_T$ for two different simulations, using the formulae for both $\mathcal{D}_Q$ and $\mathcal{D}_P$. The temperature is found by the inverse of the mean value of these distributions, and is shown for all simulations in figure 1(*c*). We can see that the results of both calculations agree very well, and so we can be confident that firstly the simulations have reached equilibrium, and secondly that the numerical implementation of these calculations are free from errors. Figure 1(*d*) shows the similar calculation for the chemical potential.

One interesting point is that the width of the distributions in figure 1(*b*) calculated using the operator $\mathcal{D}_P$ are slightly narrower than those for $\mathcal{D}_Q$. While this is of no consequence conceptually, in practice the narrower the distribution the fewer samples are required for an estimate of the mean to a required accuracy. Given the large amount of freedom in the choice of the operator $\mathcal{D}$, it seems quite possible that for particular problems that some choices will be better than others. We have found situations where one of these distributions is significantly narrower than the other. This has also been pointed out by Rugh [21]. However, with no *a priori* way to estimate the width of the distributions, finding the most accurate method of determining the temperature is a matter of trial and error.

## 5. Conclusions

To investigate the effect of critical fluctuations in Bose gases using the PGPE in the microcanonical ensemble it is necessary to have accurate methods of determining the thermodynamic temperature and chemical potential. In this paper, we have explicitly outlined a method of how to do so using the assumption of ergodicity and the dynamical evolution of the PGPE. The method could potentially be applied to other nonlinear classical field Hamiltonians.

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