Generalized coherent state representation of Bose-Einstein condensates

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(Received 26 October 2002; published 22 May 2003)

We show that the quantum many-body state of Bose-Einstein condensates consistent with the time-dependent Hartree-Fock-Bogoliubov (TDHFB) equations is a generalized coherent state. At zero temperature, the noncondensate density and the anomalous noncondensate correlation are not independent, allowing us to eliminate one of the three variables in the TDHFB.

I. INTRODUCTION

The recent experimental realization of Bose-Einstein condensates (BEC) in supercooled trapped atoms has stimulated great interest in the theoretical description of the quantum state of BEC [1–6]. The exact quantum state and many-body wave function of this system are not known, and simple approximations such as the Hartree approximation are commonly employed. Knowing the quantum state is crucial for describing the BEC dynamics; in particular, the many-body hierarchy that leads to an infinite sequence of progressively higher-order equations may be truncated consistently by making an assumption on the quantum state of the system [7].

Despite the lack of an exact representation of the quantum state, it has been possible to make significant progress by using physically sound assumptions about how certain operator products should be factorized in order to truncate the many-body hierarchy. The Gross-Pitaevskii equation (GPE) has been used for describing the dynamics of zero-temperature trapped atomic BEC with great success [8–11]. The time-dependent Hartree-Fock-Bogoliubov (TDHFB) equations [12–15] provide the dynamics of the condensate and noncondensate atoms required for the description of finite-temperature BEC in the collisionless regime. Other finite-temperature theories include the time-dependent Bogoliubov–de Gennes equations [16], the quantum kinetic theory [17–22], and stochastic methods [23–27]. However, none of these treatments directly addresses the precise quantum state of BEC that consists of the condensate as well as the noncondensate atoms. We note that the condensate atoms are described at the mean-field level in various theories. However, the GPE is derived under the assumption that all correlations of annihilation ($\hat{c}_i$) and creation ($\hat{c}_i^\dagger$) operators for the noncondensate atoms in some basis state i vanish, e.g.,

$$\langle \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k \hat{c}_m \rangle = \langle \hat{c}_i^\dagger \hat{c}_k \rangle = \langle \hat{c}_j^\dagger \hat{c}_m \rangle = 0, \tag{1}$$

while the HFB equations are derived using a different ansatz

$$\langle \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_k \hat{c}_m \rangle = \langle \hat{c}_i^\dagger \hat{c}_k \rangle \langle \hat{c}_j^\dagger \hat{c}_m \rangle + \langle \hat{c}_j^\dagger \hat{c}_k \rangle \langle \hat{c}_i^\dagger \hat{c}_m \rangle + \langle \hat{c}_i^\dagger \hat{c}_j^\dagger \rangle \langle \hat{c}_k \hat{c}_m \rangle. \tag{2}$$

It is straightforward to show that the GPE may be derived by assuming that the quantum state of BEC at zero temperature is a coherent state [2]. This is closely related to the description of the laser by a coherent state in quantum optics [28,29]. Indeed one of the earliest stated goals in BEC research has been the development of an "atom laser," the matter-wave equivalent of laser [30–32]. It has later been argued that, owing to the presence of the intrinsic interatomic collisions, the zero-temperature BEC is more accurately represented by a squeezed state rather than a coherent state [5,6].

Equation (2) used for deriving the HFB equations is reminiscent of the Wick's theorem for a system in thermal equilibrium [7,33–37]. This implies that the thermal equilibrium state described by a statistical density matrix is clearly a possible candidate for the quantum state of BEC. However, this choice does not provide a satisfactory physical picture for the TDHFB equations that describe dynamical condensates away from equilibrium. In addition, collision-induced squeezing [5] has not been included in the current description of finite temperature BEC. The identification of a quantum state that can describe the dynamics of finite temperature BEC, consistent with the TDHFB equations is thus an open issue.

In this paper, we propose a generalized coherent state (GCS) ansatz for the many-body density matrix describing the dynamical quantum state of BEC. Such states were originally used to describe anharmonic dynamical systems such as many-body interacting fermions (or bosons) [38] while preserving some of the useful properties of the original Glauber's coherent states for the harmonic oscillator [28,29]. They encompass the Glauber coherent state as well as the squeezed state as special cases. The GCS's are particularly convenient for formulating variational dynamics because of certain algebraic structures originating from the underlying Lie group algebra [38,39]. Using this ansatz, we derive the TDHFB equations [13] via the time-dependent variational principle. The variational principle that allows the description of the many-body system in terms of a small number of parameters is intimately related to the classical Hamiltonian Poisson bracket mechanics that describes classical dynamics from the minimum action principle.

The paper is organized as follows. In Sec. II, we review the key properties of GCS relevant to variational dynamics at zero and finite temperatures. In Sec. III, we derive finite-

temperature variational equations of motion in both the real space and the trap basis. Conclusions and discussion are given in Sec. IV.

II. GENERALIZED COHERENT STATE VARIATIONAL DYNAMICS

Mathematically, a set of GCS's is determined by a Lie group G, its irreducible unitary vector representation T with the space V, and a reference state $|\Omega\rangle \in V$. The GCS's are defined as states that have a form $T(g)|\Omega\rangle$ with $g \in G$. More specifically, for a generic quadratic Hamiltonian in some operators $\hat{T}_i$,

$$\hat{H} = \sum_i c_i \hat{T}_i + \sum_{i,j} c_{ij} \hat{T}_i \hat{T}_j, \tag{3}$$

the Lie group G is characterized by the commutation relations amongst the complete set of operators $\hat{T}_i$,

$$[\hat{T}_i, \hat{T}_j] = \sum_k C_{ij}^k \hat{T}_k, \tag{4}$$

where C_{ij}^k are known as the structure constants of the set $\{\hat{T}_i\}$.

For a harmonic oscillator, $\{\hat{T}_i\} = \{\hat{a}_i, \hat{a}_j^\dagger, \hat{I}\}$, where $\hat{a}_i$, $\hat{a}_j^\dagger$ are the boson annihilation and creation operators and $\hat{I}$ is the identity operator, and $C_{ij}^k \equiv \delta_{ij}$, giving the ordinary Heisenberg-Weyl group. On the other hand, the operator set $\{\hat{T}_i\} = \{\hat{a}_i^\dagger \hat{a}_j, \hat{a}_i^\dagger \hat{a}_j^\dagger, \hat{a}_i \hat{a}_j, \hat{I}\}$ may be used to construct the following Hamiltonian that describes the system of many-body interacting bosons:

$$\hat{H} = \sum_{ij} H_{ij} \hat{a}_i^\dagger \hat{a}_j + \sum_{ijkl} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l. \tag{5}$$

An extended Heisenberg-Weyl algebra may be obtained by a repeated application of the standard boson commutators $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$. Writing $\hat{T}_{ij}^{(-)} \equiv \hat{a}_i \hat{a}_j$, $\hat{T}_{ij}^{(+)} \equiv \hat{a}_i^\dagger \hat{a}_j^\dagger$, $\hat{T}_{ij}^{(z)} \equiv \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \delta_{ij} \hat{I}$, the nonvanishing commutation relations that define the extended Heisenberg-Weyl algebra are [39]

$$[\hat{T}_{mn}^{(-)}, \hat{T}_{rs}^{(+)}] = \delta_{nr} \hat{T}_{sm}^{(z)} + \delta_{ns} \hat{T}_{rm}^{(z)} + \delta_{ms} \hat{T}_{rn}^{(z)} + \delta_{mr} \hat{T}_{sn}^{(z)}, \tag{6}$$

$$[\hat{T}_{mn}^{(z)}, \hat{T}_{rs}^{(-)}] = -\delta_{mr} \hat{T}_{ns}^{(-)} - \delta_{ms} \hat{T}_{nr}^{(-)}, \tag{7}$$

$$[\hat{T}_{mn}^{(z)}, \hat{T}_{rs}^{(+)}] = \delta_{nr} \hat{T}_{ms}^{(+)} + \delta_{ns} \hat{T}_{ms}^{(+)}, \tag{8}$$

while the mixed commutators between the linear and bilinear operators have the following form:

$$[\hat{T}_{mn}^{(+)}, \hat{a}_j] = -\delta_{mj} \hat{a}_n^\dagger - \delta_{nj} \hat{a}_m^\dagger, \tag{9}$$

$$[\hat{T}_{mn}^{(z)}, \hat{a}_j] = -\delta_{mj} \hat{a}_n, \tag{10}$$

$$[\hat{T}_{mn}^{(-)}, \hat{a}_j^\dagger] = \delta_{nj} \hat{a}_m + \delta_{mj} \hat{a}_n, \tag{11}$$

$$[\hat{T}_{mn}^{(z)}, \hat{a}_j^\dagger] = \delta_{nj} \hat{a}_m^\dagger. \tag{12}$$

At zero temperature, the unnormalized generalized coherent states that belong to such extended Heisenberg-Weyl algebra for interacting bosons have the following form [38]:

$$|\psi(\tau)\rangle = \exp\left(\sum_i \alpha_i(\tau) \hat{a}_i^\dagger + \sum_{i,j} \beta_{ij}(\tau) \hat{a}_i^\dagger \hat{a}_j^\dagger \right) |\Omega_0\rangle. \tag{13}$$

The reference state $|\Omega_0\rangle$, which can be normalized to unity $\langle \Omega_0 | \Omega_0 \rangle = 1$, may be chosen arbitrarily. However, construction of a useful set of coherent states for a given dynamic system depends crucially on the choice of $|\Omega_0\rangle$ which also determines the structure of the phase space of the dynamical system [38]. We shall take Eq. (13) to be our generalized coherent state ansatz for BEC where the reference state $|\Omega_0\rangle$ is the particle vacuum state of the ordinary Heisenberg-Weyl group, i.e., $\hat{a}_i|\Omega_0\rangle = 0$. The goal of the variational approach is to determine the time-dependent parameters $\alpha_i(\tau)$ and $\beta_{ij}(\tau)$ that represent the evolution of the state $|\psi(\tau)\rangle$. Equation (13) indicates that the GCS has a form that combines a coherent state and a squeezed state. A coherent state is given by applying a displacement operator $\hat{D}(\alpha)$ on the vacuum $|\alpha\rangle = \hat{D}(\alpha)|0\rangle$, where $\hat{D}(\alpha) \equiv \exp(\Sigma_i \alpha_i^* \hat{a}\_i - \alpha_i \hat{a}_i)$. Since $\exp(-\alpha_i^* \hat{a}_i)|0\rangle = |0\rangle$, an unnormalized coherent state may be written as $|\alpha\rangle = \exp(\Sigma_i \alpha_i \hat{a}_i^\dagger)|0\rangle$. On the other hand, a unitary squeezing operator is given by $S(\xi) = \exp(\frac{1}{2}\Sigma_{ij} \xi_{ij}^* \hat{a}_i \hat{a}_j - \xi_{ij} \hat{a}_i^\dagger \hat{a}_j^\dagger)$, where $\xi_{ij} = r_{ij} \exp(i\theta_{ij})$ is an arbitrary complex number.

GCS zero-temperature variational dynamics is obtained by implementing the dynamical variational principle, assuming that the space of trial wave functions M is represented by a set of GCS's. One possible way of formulating the variational dynamics in Hilbert space is based on projecting the vector Hx for any $x \in M$ (H being the Hamiltonian operator) into the tangent subspace to M at x. This leads to a vector field in M that determines the variational dynamics.

The variational equations at zero temperature are derived as follows: Given a Hamiltonian $\hat{H}$ and time-dependent wave functions $|\Omega(\tau)\rangle$, we minimize the action

$$S[\Omega(\tau)] = \int d\tau [i \langle \Omega(\tau)|d\Omega(\tau)/d\tau \rangle - \langle \Omega(\tau)|\hat{H}|\Omega(\tau)\rangle]. \tag{14}$$

By choosing a GCS form for $|\Omega(\tau)\rangle$, the resulting variational equations can be written in the Hamiltonian form for any set Ω_j of coordinates which parametrize $|\Omega\rangle$

$$\frac{d\Omega_j}{d\tau} = \{\mathcal{H}, \Omega_j\}, \tag{15}$$

where $\{\cdots\}$ denote Poisson brackets and $\mathcal{H}$ is the classical Hamiltonian defined by

$$\mathcal{H}(\Omega) = \langle \Omega|\hat{H}|\Omega\rangle. \tag{16}$$

The use of Poisson brackets clearly establishes the link between the variational equations and the classical dynamics. When the classical Hamiltonian is given by

$$\mathcal{H} = \sum_{n=1}^{k} \sum_{i_1,\ldots,i_n} h^{(n)}_{i_1,\ldots,i_n} \langle \hat{T}_{i_1} \rangle \cdots \langle \hat{T}_{i_n} \rangle, \qquad (17)$$

the Poisson bracket assumes a very simple form provided the wave functions $|\Omega\rangle$ are parametrized by the expectation values $\langle \Omega | \hat{T}_j | \Omega \rangle$ of the operators $\hat{T}_j$ rather than by the parameters Ω_j. These expectation values then constitute a full set of parameters that uniquely specify the quantum state $|\Omega\rangle$. In particular, if the operators $\hat{T}_j$ form a closed algebra of Eq. (4), the Poisson brackets for $\hat{T}_j$ are given by

$$\{\hat{T}_m, \hat{T}_n\} = i \sum_k C^k_{m,n} \hat{T}_k, \qquad (18)$$

and the variational equations of motion for $\hat{T}_m$ take the closed form

$$i \frac{d\langle \hat{T}_m \rangle}{d\tau} = \sum_{n=1}^{k} \sum_{j=1}^{n} \sum_{i_0,\ldots,i_n} C^k_{mi_0,\ldots,i_j} h^{(n)}_{i_1,\ldots,i_n} \langle \hat{T}_{i_1} \rangle \cdots \langle \hat{T}_{i_n} \rangle. \qquad (19)$$

For the Hamiltonian (5), it, therefore, suffices to calculate the equations of motion for the expectation values $\langle \hat{a}_i^\dagger \hat{a}_j \rangle$ and $\langle \hat{a}_i \hat{a}_j \rangle$ to uniquely specify the dynamics. In the derivation of the equations of motion we use the differential property of the Poisson brackets

$$\{f, gh\} = -\{gh, f\} = \{f, g\}h + g\{f, h\}. \qquad (20)$$

When the expectation values are for generators of the set of GCS's of some Lie group G, their Poisson brackets are given by the commutators of the underlying generators of the group. This simplifies the calculation greatly, as it gives direct correspondence between the ordinary quantum-mechanical commutators and the Poisson brackets. The variational procedure is then formally equivalent to the Heisenberg equations of motion. It should be noted that the transformation between the expectation values and the parameters may be tedious. However, the transformation is never used explicitly; suffice it to know that such transformation exists and we can then proceed to derive closed equations of motion for the expectation values.

The formulation of variational dynamics at finite temperatures constitutes a more complicated task for the following three reasons: (i) At finite temperatures, the system evolves in the *Liouville space* and a set of trial density matrices M_L rather than wave functions needs to be identified, (ii) an attempt to project $L\rho$, with $\rho \in M_L$ and L is the Liouville operator into the tangent space to our ansatz, faces a difficulty since the Liouville space does not have a natural scalar product that can be used for this projection (the scalar product inherited from Hilbert space, i.e., the overlap of two density matrices does not have a direct physical significance), (iii) the compatibility of the equilibrium and the dynamical

approaches that is straightforward at zero temperature (i.e., the state in M_L with the lowest energy must be the stationary point of the dynamical equation) is not so obvious in the Liouville space. In Appendix A, we show that all of these issues can be adequately resolved for GCS. In particular, we show that the trial density matrices may be assumed to have the form of finite-temperature equilibrium density matrices, and that the equilibrium and the dynamical approaches are compatible so that the trial density matrix that minimizes the Helmholtz free energy is, indeed, a stationary point of the dynamical equations. These results will be used in the following section.

III. VARIATIONAL EQUATIONS FOR INTERACTING BOSONS

A. GCS in real space

In this section, we apply our formalism to a system of interacting bosons described by the following Hamiltonian with a fixed chemical potential μ:

$$\hat{H} = \hat{H}_0 + \hat{H}_f(t) \qquad (21)$$

with

$$\hat{H}_0 = \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{1}{2m}\Delta + V_{trap}(\mathbf{r}) - \mu \right] \hat{\psi}(\mathbf{r})$$
$$+ \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \, \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r}-\mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}), \qquad (22)$$

$$H_f(t) = \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) V_f(\mathbf{r}) \hat{\psi}(\mathbf{r}), \qquad (23)$$

where $V_{trap}(\mathbf{r},t)$ is the magnetic potential that confines the atoms and $V_f(\mathbf{r},t)$ denotes a general time- and position-dependent external driving potential. An infinite-dimensional extended Heisenberg-Weyl algebra is generated by the operators $\hat{\psi}(\mathbf{r})$, $\hat{\psi}^\dagger$, $\hat{Y}(\mathbf{r},\mathbf{r}') \equiv \hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}')$, $\hat{Y}^\dagger(\mathbf{r},\mathbf{r}')$, $\hat{N}(\mathbf{r},\mathbf{r}')$ $\equiv \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}')$, and $\hat{I}$. The space of the representation in which the Hamiltonian [Eq. (22)] is defined can be described as the space of wave functionals $\Psi[x(\mathbf{r})]$, where the one-particle boson operators are given by

$$\hat{\psi}(\mathbf{r}) = -\frac{i}{\sqrt{2}} \left[\frac{\delta}{\delta x(\mathbf{r})} - x(\mathbf{r}) \right], \quad \hat{\psi}^\dagger(\mathbf{r}) = -\frac{i}{\sqrt{2}} \left[\frac{\delta}{\delta x(\mathbf{r})} + x(\mathbf{r}) \right]. \qquad (24)$$

$x(\mathbf{r})$ is a harmonic-oscillator coordinate associated with position $\mathbf{r}$ and Eq. (24) can be used to represent the operators $\hat{Y}$, $\hat{Y}^\dagger$, and $\hat{N}$.

At zero temperature, the set of coherent states represented by Gaussian wave functions

$$\Psi[x(\mathbf{r})] = A \exp\left\{-\frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\,\sigma(\mathbf{r},\mathbf{r}')[x(\mathbf{r})-x_0(\mathbf{r})]\right.$$

$$\left.\times[x(\mathbf{r}')-x_0(\mathbf{r}')]\right\} \tag{25}$$

are parametrized by complex-valued functions $x_0(\mathbf{r})$, and $\sigma(\mathbf{r},\mathbf{r}')$. According to the formalism developed in Sec. II and Appendix A, the coherent finite-temperature density matrices $\rho[x_j(\mathbf{r})]$ with $j=L,R$ [left (ket), right (bra)] are represented by Gaussian wave packets:

$$\rho[x_j(\mathbf{r})] = Z^{-1}\exp\left\{-\frac{1}{2}\sum_{kj}\int d\mathbf{r}d\mathbf{r}'\,\sigma_{kj}(\mathbf{r},\mathbf{r}')\right.$$

$$\left.\times[x_k(\mathbf{r})-x_k^{(0)}(\mathbf{r})][x_j(\mathbf{r}')-x_j^{(0)}(\mathbf{r}')]\right\}. \tag{26}$$

These trial density matrices are parametrized by the vector and matrix functions $x_k^{(0)}(\mathbf{r})$ and $\sigma_{kj}(\mathbf{r},\mathbf{r}')$. We note that the Gaussian wavepacket [Eq. (26)] constitutes a coordinate representation for a density matrix of the form $\rho = Z^{-1}\exp(-K)$, where K is given by a combination of linear and bilinear terms in single-particle operators.

The variational parameters of Eqs. (25) and (26) which denote the displacement and the width of the Gaussian wave packet in phase space are related to the average number of particles and the quantum mechanical squeezing of the number-phase conjugate variables in BEC. These parameters may be related to physical quantities such as the condensate fraction and the excitation energy, by transforming Eq. (25) or Eq. (26) to the quasiparticle basis; the resulting relationship between the variational parameters in different bases is not simple. However, this transformation is never used explicitly since the GCS ansatz allows us to derive equations of motion directly for the parameters of interest, the expectation values of the relevant operators.

The most convenient parametrization for trial wave functions [Eq. (25)] or density matrices [Eq. (26)] is given by the expectation values of linear and bilinear combinations of boson single-particle operators:

$$z(\mathbf{r}) \equiv \langle\hat{\psi}(\mathbf{r})\rangle, \kappa(\mathbf{r},\mathbf{r}') \equiv \langle\hat{Y}(\mathbf{r},\mathbf{r}')\rangle - z(\mathbf{r})z(\mathbf{r}'),$$

$$\rho(\mathbf{r},\mathbf{r}') \equiv \langle\hat{N}(\mathbf{r},\mathbf{r}')\rangle - z^*(\mathbf{r})z(\mathbf{r}'), \tag{27}$$

where the expectation value is taken with respect to the wave functions given by Eq. (25) or density matrices by Eq. (26). Wick's theorem [7,33–37] allows us to express the expectation value of any operator in terms of the parameters given in Eq. (27) both at zero and finite temperatures. The dynamical equations for the system of interacting bosons may therefore be derived in the same way for both zero and nonzero temperatures by starting with the Heisenberg equations of motions for linear and bilinear combinations of the single-particle operators and then evaluating the right-hand sides using the Wick's theorem. This results in closed equations for the parameters $z(\mathbf{r})$, $\kappa(\mathbf{r},\mathbf{r}')$, and $\rho(\mathbf{r},\mathbf{r}')$, which will be derived next.

B. Variational equations of motion in real space

The Heisenberg equation of motion for $\hat{\psi}(\mathbf{r})$ reads

$$i\hbar\frac{d\hat{\psi}(\mathbf{r})}{dt} = H^{sp}\hat{\psi}(\mathbf{r}) + \int d\mathbf{r}'\,\hat{\psi}^\dagger(\mathbf{r}')\bar{V}(\mathbf{r},\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}), \tag{28}$$

where

$$H^{sp}(\mathbf{r}) \equiv -\frac{1}{2m}\Delta + V_{\text{trap}}(\mathbf{r}), \tag{29}$$

$$\bar{V}(\mathbf{r},\mathbf{r}') \equiv \frac{1}{2}[V(\mathbf{r}-\mathbf{r}') + V(\mathbf{r}'-\mathbf{r})], \tag{30}$$

and we have used the commutation relations for the boson field operators

$$[\hat{\psi}(\mathbf{r}),\hat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r}-\mathbf{r}'),$$

$$[\hat{\psi}(\mathbf{r}),\hat{\psi}(\mathbf{r}')] = [\hat{\psi}^\dagger(\mathbf{r}),\hat{\psi}^\dagger(\mathbf{r}')] = 0. \tag{31}$$

Taking the expectation values of Eq. (28) and noting the definition of $\kappa(\mathbf{r},\mathbf{r}')$ and $\rho(\mathbf{r},\mathbf{r}')$ [Eq. (27)], we obtain the following equation of motion for the mean field:

$$i\hbar\frac{dz(\mathbf{r})}{dt} = H^{sp}(\mathbf{r})z(\mathbf{r}) + \int d\mathbf{r}'\,\bar{V}(\mathbf{r},\mathbf{r}')\{|z(\mathbf{r}')|^2 z(\mathbf{r})$$

$$+ z^*(\mathbf{r}')\kappa(\mathbf{r},\mathbf{r}') + z(\mathbf{r}')\rho(\mathbf{r},\mathbf{r}') + z(\mathbf{r})\rho(\mathbf{r}',\mathbf{r}')\}$$

$$+ V_f(\mathbf{r},t)z(\mathbf{r}). \tag{32}$$

The equations of motion for $\kappa(\mathbf{r},\mathbf{r}')$ and $\rho(\mathbf{r},\mathbf{r}')$ can be derived similarly by computing the time derivatives using Eqs. (27) and (28) in the product rule:

$$i\hbar\frac{d\rho(\mathbf{r},\mathbf{r}')}{dt} = H^{sp}(\mathbf{r})\rho(\mathbf{r},\mathbf{r}') + \int d\mathbf{r}''\,\bar{V}(\mathbf{r}',\mathbf{r}'')$$

$$\times\{\tilde{\xi}(\mathbf{r}'',\mathbf{r}')\rho(\mathbf{r},\mathbf{r}'') + \tilde{\xi}(\mathbf{r}'',\mathbf{r}'')\rho(\mathbf{r},\mathbf{r}')$$

$$+ \tilde{\zeta}(\mathbf{r}',\mathbf{r}'')\kappa^*(\mathbf{r}'',\mathbf{r})\} - H^{sp}(\mathbf{r}')\rho(\mathbf{r},\mathbf{r}')$$

$$- \int d\mathbf{r}''\,\bar{V}(\mathbf{r},\mathbf{r}'')\{\tilde{\xi}(\mathbf{r},\mathbf{r}'')\rho(\mathbf{r}'',\mathbf{r}')$$

$$+ \tilde{\xi}(\mathbf{r}'',\mathbf{r}'')\rho(\mathbf{r},\mathbf{r}') + \tilde{\zeta}^*(\mathbf{r},\mathbf{r}'')\kappa(\mathbf{r}'',\mathbf{r}')\}$$

$$+ V_f(\mathbf{r},t)\rho(\mathbf{r},\mathbf{r}') - V_f(\mathbf{r}',t)\rho(\mathbf{r},\mathbf{r}'), \tag{33}$$

$$i\hbar\frac{d\kappa(\mathbf{r},\mathbf{r}')}{dt} = H^{sp}(\mathbf{r})\kappa(\mathbf{r},\mathbf{r}') + \int d\mathbf{r}''\,\bar{V}(\mathbf{r}',\mathbf{r}'')$$

$$\times\{\tilde{\xi}(\mathbf{r}'',\mathbf{r}')\kappa(\mathbf{r},\mathbf{r}'') + \tilde{\xi}(\mathbf{r}'',\mathbf{r}'')\kappa(\mathbf{r},\mathbf{r}')$$

$$+ \tilde{\zeta}(\mathbf{r}',\mathbf{r}'')[\rho^*(\mathbf{r},\mathbf{r}'') + \delta(\mathbf{r}-\mathbf{r}'')]\}$$

$$+ H^{sp}(\mathbf{r}')\kappa(\mathbf{r},\mathbf{r}') + \int d\mathbf{r}''\,\bar{V}(\mathbf{r},\mathbf{r}'')$$

$$\times \{\widetilde{\xi}(\mathbf{r}'',\mathbf{r})\kappa(\mathbf{r}',\mathbf{r}'')+\widetilde{\xi}(\mathbf{r}'',\mathbf{r}'')\kappa(\mathbf{r},\mathbf{r}')$$

$$+\zeta(\mathbf{r},\mathbf{r}'')\rho(\mathbf{r}'',\mathbf{r}')\}+V_f(\mathbf{r},t)\kappa(\mathbf{r},\mathbf{r}')$$

$$+V_f(\mathbf{r}',t)\kappa(\mathbf{r},\mathbf{r}'), \qquad (34)$$

where we have introduced the auxiliary functions

$$\widetilde{\xi}(\mathbf{r},\mathbf{r}')=z^*(\mathbf{r})z(\mathbf{r}')+\rho(\mathbf{r},\mathbf{r}'), \qquad (35)$$

$$\widetilde{\zeta}(\mathbf{r},\mathbf{r}')=z(\mathbf{r})z(\mathbf{r}')+\kappa(\mathbf{r},\mathbf{r}'). \qquad (36)$$

For the commonly used special case of the contact interatomic interaction for $\bar{V}(\mathbf{r},\mathbf{r}')$, Eqs. (32)–(34) are simplified greatly; these are given in Appendix B.

   An important consequence of the GCS ansatz is that at zero temperature, the functions $\rho(\mathbf{r},\mathbf{r}')$ and $\kappa(\mathbf{r},\mathbf{r}')$ are, in fact, not independent [40]. By deriving an explicit relationship between them, it is possible to eliminate the $\rho(\mathbf{r},\mathbf{r}')$ variables. This relation is derived in the trap basis in Appendix C, and then converted into the real-space basis

$$\rho(\mathbf{r},\mathbf{r}')=\left[\sqrt{\frac{1}{4}\delta(\mathbf{r},\mathbf{r}')+\int \kappa^*(\mathbf{r},\mathbf{r}'')\kappa(\mathbf{r}'',\mathbf{r}')d\mathbf{r}''}\right.$$

$$\left.-\frac{1}{2}\delta(\mathbf{r},\mathbf{r}')\right]. \qquad (37)$$

   It can be verified by direct substitution that once Eq. (37) holds initially, it remains true throughout the dynamical evolution. The reduced set of equations are then the coupled equations (32) and (34) with $\rho(\mathbf{r},\mathbf{r}')$ replaced by the expression (37). The two independent variables $z(\mathbf{r})$ and $\kappa(\mathbf{r},\mathbf{r}')$ constitute a very convenient parametrization of squeezed states. $z(\mathbf{r})$ represents the average position, whereas $\kappa(\mathbf{r},\mathbf{r}')$ is responsible for squeezing. This can be easily understood from the fact that the coherent state is an eigenstate of the annihilation operator $\hat{\psi}(\mathbf{r})$, while a squeezed state is generated using a squeezing operator that is a function of the quadratic operator $\hat{Y}(\mathbf{r},\mathbf{r}')$ in the extended Heisenberg-Weyl algebra.

C. Variational equations of motion in the trap basis

   For completeness, we outline below the derivation of the same variational equations in the trap basis. In this basis, the Hamiltonian is written as

$$H=\sum_{ij}H_{ij}\hat{a}_i^\dagger\hat{a}_j+\sum_{ijkl}V_{ijkl}\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_k\hat{a}_l+\sum_{ij}E_{ij}a_i^\dagger\hat{a}_j. \qquad (38)$$

The matrix elements of the single-particle Hamiltonian H_{ij} are given by

$$H_{ij}=\int d^3\mathbf{r}\phi_i^*(\mathbf{r})\left[-\frac{\hbar^2}{2m}\Delta+V_{\mathrm{trap}}(\mathbf{r})\right]\phi_j(\mathbf{r}), \qquad (39)$$

where the basis state $\phi_i(\mathbf{r})$ is arbitrary; a convenient basis for trapped BEC is the eigenstates of the trap since H_{ij} is

then diagonal. The indices may also be viewed as the mode indices in a multimode quantum state. The symmetrized two-particle interaction matrix elements are

$$V_{ijkl}=\frac{1}{2}[\langle ij|V|kl\rangle+\langle ji|V|kl\rangle], \qquad (40)$$

where

$$\langle ij|V|kl\rangle=\int d^3\mathbf{r}d^3\mathbf{r}'\phi_i^*(\mathbf{r})\phi_j^*(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\phi_k(\mathbf{r}')\phi_l(\mathbf{r}), \qquad (41)$$

with $V(\mathbf{r}-\mathbf{r}')$ being a general interatomic potential. Also,

$$E_{ij}\equiv\int d\mathbf{r}\phi_i^*(\mathbf{r})V_f(\mathbf{r},t)\phi_j(\mathbf{r}), \qquad (42)$$

where $V_f(\mathbf{r},t)$ denotes a general time- and position-dependent external driving potential as defined previously. First, we proceed by establishing that our generalized coherent state (13) at zero temperature is a Gaussian in coordinate space. With the choice of the particle vacuum state of ordinary Heisenberg-Weyl algebra as our reference state $|\Omega_0\rangle$, Eq. (13) the action of the operators $\hat{a}_i$ and $\hat{a}_i^\dagger$ on the wave function $\Omega(q_1,\ldots,q_{\mathcal{N}})$ in the coordinate representation, where $\mathcal{N}$ is the total number of bosons, is

$$\hat{a}_i=-\frac{i}{\sqrt{2}}\left(\frac{\partial}{\partial q_i}-q_i\right), \quad \hat{a}_i^\dagger=-\frac{i}{\sqrt{2}}\left(\frac{\partial}{\partial q_i}+q_i\right), \quad (43)$$

and the conditions $\hat{a}_i\Omega(q_1,\ldots,q_{\mathcal{N}})=0$ for $i=1,\ldots,\mathcal{N}$ imply that the reference state $\Omega_0(q_1,\ldots,q_{\mathcal{N}})$ is a Gaussian in coordinate space:

$$\Omega_0(q_1,\ldots,q_{\mathcal{N}})=\frac{1}{\sqrt{(2\pi)^{\mathcal{N}}}}\exp\left[-\frac{1}{2}(q_1^2+\cdots+q_{\mathcal{N}}^2)\right]. \qquad (44)$$

It should be noted that, consistent with our choice of basis in Eq. (38), the index i of the coordinate variable q_i in Eqs. (43) and (44) refers to the trap basis "mode" i. In addition, although we are using the trap basis, the finite total number of particles $\mathcal{N}$ implies that the vector space used is effectively a finite-dimensional space spanned by a truncated set of trap basis states. Acting on this wave function with the generalized displacement operator [Eq. (13)] preserves its Gaussian form since the action by the operators $\hat{a}_i$ and $\hat{a}_i^\dagger$ simply shifts the origin, while the operators $\hat{a}_i\hat{a}_j$ and $\hat{a}_i^\dagger\hat{a}_j^\dagger$ change the variance. The resulting state is thus a Gaussian of the form

$$\Omega(q_1,\ldots,q_{\mathcal{N}})=A\exp\left[-\frac{1}{2}\sum_{i,j}\sigma_{ij}(q_i-\eta_i)(q_j-\eta_j)\right], \qquad (45)$$

where η_i, $i=1,\ldots,\mathcal{N}$ are the complex numbers which determine the average position while σ_{ij} is an $\mathcal{N}\times\mathcal{N}$ symmetric matrix that determines the covariances or the amount of

squeezing. For an ordinary coherent state, $\sigma_{ij} = \delta_{ij}$, i.e., a Gaussian with unit covariance.

Similarly, at finite temperatures, the trial density matrix takes the form ($k, j = L, R$)

$$\rho[q_1^j, \ldots, q_{\mathcal{N}}^j] = Z^{-1} \exp\left\{ -\frac{1}{2} \sum_{kj} \sum_{lm} \sigma_{lm}^{kj}[q_l^k - q_l^{k(0)}] \right.$$
$$\left. \times [q_m^j - q_m^{j(0)}] \right\}. \qquad (46)$$

The GCS ansatz may therefore be considered to be a ground state of some effective quadratic Hamiltonian in coordinate and momentum operators. For such a Hamiltonian, any correlation function can be represented in a path-integral form where the action only has linear and bilinear terms [41]. The resulting Wick's theorem is then identical to that for a thermal state.

The expectation values to be used in the parametrization of our state are the condensate mean field z_i, the noncondensate density ρ_{ij}, and the noncondensate correlations κ_{ij}:

$$z_i \equiv \langle \hat{a}_i \rangle, \rho_{ij} \equiv \langle \hat{a}_i^\dagger \hat{a}_j \rangle - \langle \hat{a}_i^\dagger \rangle \langle \hat{a}_j \rangle, \kappa_{ij} \equiv \langle \hat{a}_i \hat{a}_j \rangle - \langle \hat{a}_i \rangle \langle \hat{a}_j \rangle. \qquad (47)$$

Since these variables are the expectation values of the generators of the set of generalized coherent states of the extended Heisenberg-Weyl algebra, their Poisson brackets are given by the commutators of the underlying generators. This results in TDHFB equations of motion for z_i, ρ_{ij} and κ_{ij}.

At zero temperature, the relationship between ρ_{ij} and κ_{ij} [Eq. (37)] is

$$\rho_{ij} = \sqrt{\frac{1}{4} \delta_{ij} + \sum_p \kappa_{ip}^* \kappa_{pj}} - \frac{1}{2} \delta_{ij}. \qquad (48)$$

This enables us to reduce the number of equations. More details of this relation are provided in Appendix C, while the TDHFB equations in the trap basis including the simplified zero temperature form are given in Appendix D.

IV. DISCUSSION

Using the GCS ansatz, we have derived variationally the TDHFB equations of motion for BEC, which are known to be valid in the collisionless regime. This implies that the GCS ansatz should be applicable in the lower temperature, collisionless regime. It should be noted that the HFB theory has several inconsistencies such as the violation of the Hugenholtz-Pines theorem [42] that states that the excitation spectrum should be gapless in the homogeneous limit [12]. This issue has been addressed by various authors; for instance, the Popov approximation, in which the anomalous correlation is neglected, was shown to give a gapless spectrum [12]. Recently, it has been shown that by replacing the contact interaction potential with a more sophisticated pseudopotential, many of the inconsistency problems of the HFB equations including the violation of the Hugenholtz-

Pines theorem, inconsistencies with the many-body T-matrix calculations, and the ultraviolet divergences can be overcome [43]. In this paper, we have presented our HFB equations with the general interaction in both the real space and the trap basis; pseudopotentials such as those discussed in Ref. [43] can thus be accommodated.

Since the GCS is a squeezed state, the present work may be considered an extension of a previous result that demonstrated *stationary* BEC to be squeezed [5] and a more recent result that has shown that dynamically evolving BEC under the time-dependent GPE described using the Hartree approximation (i.e., pure condensate, no noncondensate atoms) is squeezed [6].

The representation of the dynamical quantum state of BEC as a GCS provides physical insight about the *total* system of condensates plus noncondensates in terms of particle annihilation and creation operators, and how it evolves as a whole in the Schrödinger picture. The interdependence of ρ and κ at zero temperature enables us to eliminate the ρ variables from these equations, reducing the size of the problem, and simplifying the solution.

The multimode squeezing, and hence the entangled state nature of BEC is clear from the form of the quantum state, Eq. (13). The study of quantum entanglement is currently gaining great interest owing to its importance in quantum information theory [44,45] as well as in the understanding of the foundations of quantum mechanics [46,47]. Experimental sources of generalized coherent states in matter-waves already exist in the form of atomic BEC. However, ways to access and manipulate this type of matter-wave entanglement remains an open challenge.

APPENDIX A: PROPERTIES OF FINITE TEMPERATURE GCS

As noted in the main text, the formulation of variational dynamics at finite temperatures requires us to address the following issues: (i) At finite temperatures, the system evolves in the Liouville space and a set of trial density matrices M_L need to be identified, (ii) an attempt to project $L\rho$, with $\rho \in M_L$ and L is the Liouville operator into the tangent space to our ansatz, faces a difficulty since the Liouville space does not have a natural scalar product that can be used for this projection, (iii) the compatibility of the equilibrium and the dynamical approaches is not so obvious in the Liouville space. In this appendix, we show how all these issues may be adequately addressed. We start by introducing the trial density matrices.

Let $\mathcal{A}$ be the real Lie algebra of the real Lie group G involved in the definition of a set of GCS's. For our case, $\mathcal{A}$ is the basic (real) algebra generated by the generators $\hat{a}_j$, $\hat{a}_j^\dagger$, and $\hat{T}_{mn}$; the elements a belonging to the algebra $\mathcal{A}$, $a \in \mathcal{A}$, are then linear combinations of these generators. In addition, let $\mathcal{A}^{(c)}$ and $G^{(c)}$ be the complexification of $\mathcal{A}$ and

G, i.e., $G^{(c)}$ is the complex Lie group that corresponds to the complex Lie algebra $\mathcal{A}^{(c)}$. Complexification of an algebra (group) gives an algebra (group) generated by the original generators for which the coefficients are allowed to be complex, rather than real numbers. More specifically, it means constructing a complex analytical algebra (group), for which the ''real'' version is the original one. For example, given a real structure that is a map $p:G \rightarrow G$, the real part of the group consists of points g so that $p(g)=g$. If one defines $p(g)=g^{\dagger}$, one has $G_{real}=\mathrm{SU}(2)$, while if one defines $p(g)=g^{*}$, one has $G_{real}=\mathrm{SL}(2,R)$. $\mathrm{SL}(2,C)$ is then a three-dimensional complex analytical group (3 is its complex dimension) that serves as a complexification for both $\mathrm{SU}(2)$ and $\mathrm{SL}(2,R)$.

The representation T of a group G associates with any $g \in G$ a linear operator $T(g)$ (acting in some complex vector space referred to as the space of the representation) so that $T(g_2 g_1)=T(g_2)T(g_1)$. T can be naturally extended to a representation of $G^{(c)}$ in the same vector space V. A representation of a group has the corresponding representation of an algebra and vice versa, and in the corresponding algebra representation, we have $T(a)$ being operators in the same space for $a \in \mathcal{A}$ with $T(a_1+a_2)=T(a_1)+T(a_2)$ and $T([a_1,a_2])=T(a_1)T(a_2)-T(a_2)T(a_1)$. The representation of $\mathcal{A}$ can also be easily extended to representation of $\mathcal{A}^{(c)}$.

We define the manifold M_L of normalized trial density matrices represented by $\rho(g)=Z^{-1}(g)T(g)$ for all elements g belonging to the complexification of G, $g \in G^{(c)}$, so that $T(g)$ is Hermitian where $Z(g)=\mathrm{Tr}[T(g)]$. The normalization condition $\mathrm{Tr}[\rho(g)]=1$ is obviously satisfied. In the GCS case, the projection that closes the dynamical equation can be formulated as follows. We define a tangent vector $v(\rho)$ that satisfies the following property:

$$\mathrm{Tr}[T(a)v(\rho)]=\mathrm{Tr}[T(a)L\rho] \qquad (A1)$$

for all $a \in \mathcal{A}^{(c)}$ and $\rho \in M_L$. For most practical applications, there is one and only one tangent vector v for any ρ that satisfies Eq. (A1). In this case, a well-defined vector field $v(\rho)$ describes the variational dynamics in the manifold M_L of trial density matrices. The physical meaning of Eq. (A1) is clear: If we refer to the operators $T(a)$ with $a \in \mathcal{A}^{(c)}$ as the fundamental operators, the variational dynamics is obtained by the requirement that the dynamical equations hold for the expectation values of the fundamental operators. This implies that, similar to the zero temperature case, the variational equation of motion at finite temperature is derived using the Heisenberg equations of motion.

We assume that the trial density matrices are represented by finite-temperature equilibrium density matrices with Hamiltonians given by the fundamental operators:

$$\rho=Z^{-1}\exp[-\beta T(a)]=Z^{-1}T(g) \qquad (A2)$$

for some $a \in \mathcal{A}^{(c)}$. This implies $g=\exp(\beta a)$, i.e., elements $g \in G$ of the Lie group G can be represented as the exponentials of the corresponding complex Lie algebra elements a

and it follows then that $g \in G^{(c)}$, because if $\mathcal{A}$ is the Lie algebra of the group G, then $\mathcal{A}^{(c)}$ is the Lie algebra that corresponds to $G^{(c)}$.

We conclude this section by demonstrating that this way of closing the dynamical equation [Eq. (A1)] guarantees the compatibility of the equilibrium and dynamical variational approaches. Using the variational approach, the equilibrium density matrix can be obtained by finding the minimum of the Helmholtz free energy

$$F(\rho)=\mathrm{Tr}(H\rho)-\beta^{-1}\mathrm{Tr}[\rho \ln(\rho)] \qquad (A3)$$

among the normalized trial density matrices $\rho \in M_L$. The requirement $\delta F=0$ yields

$$\delta F(\rho)=\mathrm{Tr}(H\delta\rho)-\beta^{-1}\mathrm{Tr}(\delta\rho\rho) \qquad (A4)$$

for any tangent $\delta\rho$. It follows from Eq. (A1) that $\delta\rho=[a,\rho]$ is a tangent for any $a \in \mathcal{A}^{(c)}$. This yields

$$\mathrm{Tr}\{T(a)L(\rho_0)\}=\mathrm{Tr}\{T(a)[H,\rho_0]\}$$
$$=\mathrm{Tr}\{H[T(a),\rho_0]\}=\beta^{-1}\mathrm{Tr}\{\ln \rho_0 [T(a),\rho_0]\}$$
$$=\beta^{-1}\mathrm{Tr}\{T(a)[\ln \rho_0,\rho_0]\}=0, \qquad (A5)$$

which implies that $v(\rho_0)=0$. Stated differently, the trial density matrix that minimizes the free energy is a stationary point of the dynamical equations.

APPENDIX B: VARIATIONAL EQUATIONS IN REAL SPACE FOR THE CONTACT POTENTIAL

For contact interatomic interaction, $\bar{V}(\mathbf{r},\mathbf{r}')\equiv U_0\delta(\mathbf{r}-\mathbf{r}')$. Here $U_0=4\pi\hbar^2 a/m$, where a is the s-wave scattering length and m is the mass of a single atom. This implies that the integrations in Eqs. (32)–(34) are removed,

$$i\hbar\frac{dz(\mathbf{r})}{dt}=H^{sp}(\mathbf{r})z(\mathbf{r})+U_0\{|z(\mathbf{r})|^2 z(\mathbf{r})+2\rho(\mathbf{r},\mathbf{r})z(\mathbf{r})$$
$$+\kappa(\mathbf{r},\mathbf{r})z^*(\mathbf{r})\}+V_f(\mathbf{r},t)z(\mathbf{r}), \qquad (B1)$$

$$i\hbar\frac{d\rho(\mathbf{r},\mathbf{r}')}{dt}=[H^{sp}(\mathbf{r})+2U_0\tilde{\xi}(\mathbf{r}',\mathbf{r}')]\rho(\mathbf{r},\mathbf{r}')$$
$$+U_0\tilde{\zeta}(\mathbf{r}',\mathbf{r}')\kappa^*(\mathbf{r},\mathbf{r}')-[H^{sp}(\mathbf{r}')$$
$$+2U_0\tilde{\xi}(\mathbf{r},\mathbf{r})]\rho(\mathbf{r},\mathbf{r}')-U_0\tilde{\zeta}^*(\mathbf{r},\mathbf{r})\kappa(\mathbf{r},\mathbf{r}')$$
$$+V_f(\mathbf{r},t)\rho(\mathbf{r},\mathbf{r}')-V_f(\mathbf{r}',t)\rho(\mathbf{r},\mathbf{r}'), \qquad (B2)$$

$$i\hbar\frac{d\kappa(\mathbf{r},\mathbf{r}')}{dt}=[H^{sp}(\mathbf{r})+2U_0\tilde{\xi}(\mathbf{r}',\mathbf{r}')]\kappa(\mathbf{r},\mathbf{r}')$$
$$+U_0\tilde{\zeta}(\mathbf{r}',\mathbf{r}')\rho^*(\mathbf{r},\mathbf{r}')+U_0\tilde{\zeta}(\mathbf{r}',\mathbf{r}')$$
$$+[H^{sp}(\mathbf{r}')+2U_0\tilde{\xi}^*(\mathbf{r},\mathbf{r})]\kappa(\mathbf{r},\mathbf{r}')$$
$$+U_0\tilde{\zeta}(\mathbf{r},\mathbf{r})\rho(\mathbf{r},\mathbf{r}')+V_f(\mathbf{r},t)\kappa(\mathbf{r},\mathbf{r}')$$
$$+V_f(\mathbf{r}',t)\kappa(\mathbf{r},\mathbf{r}'), \qquad (B3)$$

where $\widetilde{\xi}(\mathbf{r},\mathbf{r})$ and $\widetilde{\zeta}(\mathbf{r},\mathbf{r})$ are as given in Eqs. (35)–(36). The equations of motion for $\widetilde{\rho}(\mathbf{r},\mathbf{r}',t)$ and $\widetilde{\kappa}(\mathbf{r},\mathbf{r}',t)$ may be written in the compact form

$$i\hbar\frac{d\mathcal{G}}{dt}=\Sigma\mathcal{G}-\mathcal{G}\Sigma^{\dagger}, \tag{B4}$$

where we have defined 2×2 matrices

$$\Sigma(\mathbf{r},\mathbf{r}')=\begin{pmatrix}\widetilde{h}(\mathbf{r},\mathbf{r}') & \widetilde{\Delta}(\mathbf{r}',r')\\ -\widetilde{\Delta}^{*}(\mathbf{r},\mathbf{r}) & -\widetilde{h}^{*}(\mathbf{r},\mathbf{r}')\end{pmatrix},$$

$$\mathcal{G}(\mathbf{r},\mathbf{r}')=\begin{pmatrix}\rho(\mathbf{r},\mathbf{r}') & \kappa(\mathbf{r},\mathbf{r}')\\ \kappa^{*}(\mathbf{r},\mathbf{r}') & \rho^{*}(\mathbf{r},\mathbf{r}')+1\end{pmatrix}, \tag{B5}$$

and

$$\widetilde{h}(\mathbf{r},\mathbf{r}')\equiv H^{sp}(\mathbf{r})+V_{f}(\mathbf{r},t)+2U_{0}\widetilde{\xi}(\mathbf{r}',\mathbf{r}'), \tag{B6}$$

$$\widetilde{\Delta}(\mathbf{r},\mathbf{r})\equiv U_{0}\widetilde{\zeta}(\mathbf{r},\mathbf{r}). \tag{B7}$$

Equations (B1) and (B4) constitute the TDHFB equations for the contact interatomic potential approximation, in real space [12].

APPENDIX C: ZERO-TEMPERATURE RELATIONSHIP BETWEEN ρ AND κ

In order to derive the relation between ρ_{ij} and κ_{ij} at zero temperature using the GCS ansatz, we find that it suffices to consider GCS state $|\Omega\rangle$ such that $\langle\Omega|\hat{a}_{i}|\Omega\rangle=0$, i.e., Gaussian wave functions centered at $q=0$. These states form an orbit M of the group G which corresponds to the algebra generated by $\hat{T}_{mn}^{(z)}$ and $\hat{T}_{mn}^{(\pm)}$. We shall introduce a set of functions $S_{mn}^{(z)}$, $S_{mn}^{(\pm)}$ on M,

$$S_{mn}^{(z)}(\Omega)\equiv\langle\Omega|\hat{T}_{mn}^{(z)}|\Omega\rangle, \quad S_{mn}^{(\pm)}(\Omega)\equiv\langle\Omega|\hat{T}_{mn}^{(\pm)}|\Omega\rangle \tag{C1}$$

and define two sets of auxiliary functions

$$F_{mn}(\Omega)=\sum_{\alpha}[S_{m\alpha}^{(+)}S_{\alpha n}^{(-)}-S_{m\alpha}^{(z)}S_{\alpha n}^{(z)}], \tag{C2}$$

$$G_{mn}(\Omega)=\sum_{\alpha}[S_{m\alpha}^{(z)}S_{\alpha n}^{(+)}-S_{n\alpha}^{(z)}S_{\alpha m}^{(+)}]. \tag{C3}$$

Our aim is to show that $F_{mn}(\Omega)$ is a constant, i.e., its derivatives are zero. In particular, showing that $F_{mn}(\Omega)=\delta_{mn}$ and identifying the expectation values $S_{mn}^{(\pm)}$ and $S_{mn}^{(z)}$ in terms of ρ_{ij} and κ_{ij}, for our example, complete the required proof. It is found that the derivatives of $F_{mn}(\Omega)$ are linear combinations of $G_{mn}(\Omega)$, and therefore it suffices to prove that the auxiliary function $G_{mn}(\Omega)$ is zero for all m and n.

We note that since $[\hat{T}_{ij}^{(+)},\hat{T}_{ke}^{(+)}]=0$, the operators $\hat{T}_{ij}^{(+)}$ which are considered as vector fields on M determine a complex structure on M. A function f is said to be holomorphic if

it satisfies the condition $\hat{T}_{mn}^{(+)}f=0$. Operator $\hat{T}_{mn}^{(+)}$ then represents derivatives in the antiholomorphic direction.

In particular, the functions $S_{mn}^{(+)}$ constitute a set of holomorphic coordinates in the vicinity of Ω_{0} where Ω_{0}, represent states with Gaussian wave functions. It can be shown that $S_{mn}^{(+)}(\Omega_{0})=0$, while $S_{mn}^{(z)}(\Omega_{0})=\delta_{mn}$ so that

$$F_{mn}(\Omega_{0})=\delta_{mn}. \tag{C4}$$

A direct calculation yields $\hat{T}_{ij}^{(+)}G_{mn}=0$ that implies that G_{mn} is holomorphic and can therefore be written as a series in $S_{ij}^{(+)}$ in the vicinity of the point $S_{ij}^{(+)}=0$ (i.e., Ω_{0}). Since $S_{ma}^{(z)}(\Omega)=\delta_{ma}$, it follows from Eq. (C3) that the expansion of G_{mn} starts with the second-order terms:

$$G_{mn}=\sum_{j=2}^{\infty}G_{mn}^{(j)}. \tag{C5}$$

We next define the degree of a function f by $\hat{D}f=\widehat{\deg}f\equiv\frac{1}{2}\Sigma_{j}\hat{T}_{jj}^{(z)}f$. It is clear that $\widehat{\deg}S_{ij}^{(\pm)}=\pm1$, $\widehat{\deg}S_{ij}^{(z)}=0$, and $\widehat{\deg}(fg)=\widehat{\deg}f+\widehat{\deg}g$. It follows from Eq. (C3) that $\widehat{\deg}G_{mn}=1$. On the other hand, Eq. (C5) implies that $\widehat{\deg}G_{mn}^{(j)}=j$ and therefore contains the degrees of 2 and higher. This implies that $G_{mn}\equiv0$ for all m and n.

It can be verified that $\hat{T}_{mn}^{(+)}F_{mn}$ is a linear combination of G_{ab} and hence $\hat{T}_{mn}^{(+)}F_{mn}=0$. Similarly, by conjugating the relation $\hat{T}_{mn}^{(+)}F_{mn}=0$, $\hat{T}_{mn}^{(-)}F_{mn}=0$, implying that $F_{mn}(\Omega)$ is a constant. This, together with Eqs. (C2) and (C4) imply

$$F_{mn}(\Omega)=\sum_{\alpha}[S_{m\alpha}^{(+)}S_{\alpha n}^{(-)}-S_{m\alpha}^{(z)}S_{\alpha n}^{(z)}]=\delta_{mn}. \tag{C6}$$

Since $S_{mn}^{(-)}=\kappa_{mn}$ and $S_{mn}^{(z)}=\rho_{mn}+\frac{1}{2}\delta_{mn}$, Eq. (C6) gives

$$\left(\rho_{ij}+\frac{1}{2}\delta_{ij}\right)^{2}-\sum_{p}\kappa_{ip}^{*}\kappa_{pj}=\frac{1}{4}\delta_{ij}. \tag{C7}$$

Solving for ρ_{ij} finally yields

$$\rho_{ij}=\sqrt{\frac{1}{4}\delta_{ij}+\sum_{p}\kappa_{ip}^{*}\kappa_{pj}}-\frac{1}{2}\delta_{ij} \tag{C8}$$

or in matrix form

$$\rho=\sqrt{\frac{1}{4}I+\kappa^{\dagger}\kappa}-\frac{1}{2}I, \tag{C9}$$

where I is the unit operator.

Equation (C9) may also be expanded in a Taylor series as

$$\rho=\kappa^{\dagger}\kappa-(\kappa^{\dagger}\kappa)^{2}+4(\kappa^{\dagger}\kappa)^{3}-\cdots. \tag{C10}$$

It is possible to gain further insight into the nature of GCS from the fact that Eq. (C9) holds if the quantum state of the system is a quasiparticle vacuum state $|0\rangle_{qp}$ such that $\hat{\beta}_{i}(t)|0\rangle_{qp}=0$, where $\hat{\beta}_{i}(t)$ is the quasiparticle annihilation operator of the Bogoliubov transformation, $\hat{a}_{i}(t)$

$=\Sigma_{j\neq 0}U_{ji}\hat{\beta}_j(t)+V_{ji}^*\hat{\beta}_j^\dagger(t)$. For a quasiparticle vacuum state, ρ_{ij} and κ_{ij} may be written in terms of matrices U and V as follows:

$$\rho_{ij}=\sum_{p\neq 0} V_{pi}^*V_{pj} \quad \text{and} \quad \kappa_{ij}=\sum_{p\neq 0} U_{pj}V_{pi}^*, \quad \text{(C11)}$$

which implies

$$\rho^2+\rho=\kappa^\dagger\kappa \quad \text{and} \quad \rho\kappa=\kappa\rho^*, \quad \text{(C12)}$$

using the orthogonality and symmetry conditions between the matrices U and V, $UU^\dagger-VV^\dagger=1$ and $UV^T-VU^T=0$. These relations can be shown to be identical to Eq. (C9) by solving the quadratic equation in ρ. The quasiparticle vacuum state may therefore be considered a squeezed state of condensate and noncondensate atoms.

APPENDIX D: VARIATIONAL EQUATIONS IN THE TRAP BASIS

1. TDHFB Equations

The TDHFB equations in trap basis is given as follows:

$$i\hbar\frac{dz_i}{dt}=\sum_j H_{ij}z_j+\sum_{jkl} V_{ijkl}[z_j^*z_kz_l+2\rho_{jk}z_l]$$

$$+\sum_{kl} V_{ijkl}\kappa_{kl}z_j^*+\sum_j E_{ij}z_j, \quad \text{(D1)}$$

$$i\hbar\frac{d\rho_{ij}}{dt}=\sum_r \left[H_{ir}+2\sum_{kl} V_{iklr}(z_k^*z_l+\rho_{lk})+E_{ir}\right]\rho_{rj}$$

$$-\sum_r \left[H_{rj}+2\sum_{kl} V_{rjkl}(z_k^*z_l+\rho_{lk})+E_{rj}\right]\rho_{ir}$$

$$+\sum_r \left[\sum_{kl} V_{irkl}(z_kz_l+\kappa_{kl})\right]\kappa_{rj}^*$$

$$-\sum_r \left[\sum_{kl} V_{rjkl}(z_k^*z_l^*+\kappa_{kl}^*)\right]\kappa_{ir}, \quad \text{(D2)}$$

$$i\hbar\frac{d\kappa_{ij}}{dt}=\sum_r \left[H_{ir}+2\sum_{kl} V_{iklr}(z_k^*z_l+\rho_{lk})+E_{ir}\right]\kappa_{rj}$$

$$+\sum_r \left[H_{rj}+2\sum_{kl} V_{rjkl}(z_kz_l^*+\rho_{lk}^*)+E_{rj}\right]\kappa_{ir}$$

$$+\sum_r \left[\sum_{kl} V_{irkl}(z_kz_l+\kappa_{kl})\right]\rho_{rj}^*$$

$$+\sum_r \left[\sum_{kl} V_{rjkl}(z_kz_l+\kappa_{kl})\right]\rho_{ir}$$

$$+\sum_{kl} V_{ijkl}(z_kz_l+\kappa_{kl}). \quad \text{(D3)}$$

The TDHFB equations in real space derived in Sec. III, Eqs. (32)–(34), may be transformed to the corresponding trap basis, Eqs. (D1)–(D3) in a straightforward manner, using the following relations between the real-space basis and the trap basis variables:

$$z(\mathbf{r})=\sum_i z_i\phi_i(\mathbf{r}), \quad \rho(\mathbf{r},\mathbf{r}')=\sum_{ij} \rho_{ij}\phi_i^*(\mathbf{r})\phi_j(\mathbf{r}'),$$

$$\kappa(\mathbf{r},\mathbf{r}')=\sum_{ij} \kappa_{ij}\phi_i(\mathbf{r})\phi_j(\mathbf{r}'), \quad \text{(D4)}$$

along with the definition of the tetradic matrix V_{ijkl},

$$V_{ijkl}=\frac{1}{2}[\langle ij|V|kl\rangle+\langle ji|V|kl\rangle], \quad \text{(D5)}$$

where

$$\langle ij|V|kl\rangle=\int d^3\mathbf{r}d^3\mathbf{r}'\,\phi_i^*(\mathbf{r})\phi_j^*(\mathbf{r}')V(\mathbf{r}-\mathbf{r}')\phi_k(\mathbf{r}')\phi_l(\mathbf{r}),$$
$$\text{(D6)}$$

with $V(\mathbf{r}-\mathbf{r}')$ being a general interatomic potential. Under the contact interaction approximation, V_{ijkl} takes a simpler form

$$V_{ijkl}=\frac{4\pi\hbar^2 a}{m}\int d\mathbf{r}\phi_i^*(\mathbf{r})\phi_j^*(\mathbf{r})\phi_k(\mathbf{r})\phi_l(\mathbf{r}). \quad \text{(D7)}$$

2. TDHFB at zero temperature

The TDHFB equations, Eqs. (D1)–(D3), hold for all temperatures. However, we have noted that the variables ρ and κ are not independent variables for the generalized coherent-state ansatz at $T=0$. ρ_{ij} can therefore be eliminated using the following relation:

$$\rho=\left[\sqrt{\frac{1}{4}I+\kappa^\dagger\kappa}-\frac{1}{2}I\right]+\delta\rho, \quad \text{(D8)}$$

where the function $\delta\rho=0$ for $T=0$, the TDHFB equations take the following form:

$$i\hbar\frac{dz}{dt}=\mathcal{H}_z z+\mathcal{H}_{z*}z^*+Ez, \quad \text{(D9)}$$

$$i\hbar\frac{d\kappa}{dt}=(h\kappa+\kappa h^*)+\left[\sqrt{\frac{1}{4}I+\kappa^\dagger\kappa}-\frac{1}{2}I+\delta\rho\right]\Delta$$

$$+\Delta\left[\sqrt{\frac{1}{4}I+\kappa^\dagger\kappa}-\frac{1}{2}I+\delta\rho\right]+\Delta, \quad \text{(D10)}$$

$$i\hbar\frac{d\delta\rho}{dt}=\left[h,\sqrt{\frac{1}{4}I+\kappa^\dagger\kappa}-\frac{1}{2}I+\delta\rho\right]-(\kappa\Delta^*-\Delta\kappa^*)$$

$$-i\hbar\frac{1}{\sqrt{I+4\kappa^\dagger\kappa}}\left(\frac{d\kappa^\dagger}{dt}\kappa+\kappa^\dagger\frac{d\kappa}{dt}\right), \quad \text{(D11)}$$

where

$$[\mathcal{H}_z]_{ij} = H_{ij} + \sum_{kl} V_{iklj}\left[z_k^* z_l + 2\sqrt{\frac{1}{4}\delta_{lk} + \sum_m \kappa_{lm}^* \kappa_{mk}}\right.$$

$$\left. - \delta_{lk} + 2\delta\rho_{lk}\right], \tag{D12}$$

$$[\mathcal{H}_{z*}]_{ij} = \sum_{kl} V_{iklj}\kappa_{kl}, \tag{D13}$$

$$h_{ij} = H_{ij} + 2\sum_{kl} V_{iklj}\left[z_k^* z_l + \sqrt{\frac{1}{4}\delta_{lk} + \sum_m \kappa_{lm}^* \kappa_{mk}}\right.$$

$$\left. - \frac{1}{2}\delta_{lk} + \delta\rho_{lk}\right] + E_{ij}, \tag{D14}$$

$$\Delta_{ij} = \sum_{kl} V_{ijkl}[z_k z_l + \kappa_{kl}]. \tag{D15}$$

$$\tag{D16}$$

At $T=0$, $\delta\rho=0$ and $\rho = \sqrt{\frac{1}{4}I + \kappa^\dagger\kappa} - \frac{1}{2}I$. By direct differentiation of ρ, we get

$$i\hbar\frac{d\rho}{dt} = i\hbar\frac{1}{\sqrt{I+4\kappa^\dagger\kappa}}\left(\frac{d\kappa^\dagger}{dt}\kappa + \kappa^\dagger\frac{d\kappa}{dt}\right), \tag{D17}$$

while Eq. (D2) implies

$$i\hbar\frac{d\rho}{dt} = \left[h, \sqrt{\frac{1}{4}I + \kappa^\dagger\kappa} - \frac{1}{2}I\right] - (\kappa\Delta^* - \Delta\kappa^*). \tag{D18}$$

Since Eqs. (D17) and (D18) are equivalent, both the left- and the right-hand sides of Eq. (D11) are zero at $T=0$ and $\delta\rho = 0$, i.e., the only independent equations to be solved are Eqs. (D9) and (D10).

For comparison, we note that the GPE, which is a zero-temperature theory for a coherent-state ansatz, is simply obtained from Eq. (D9) by setting $\rho_{ij} = \kappa_{ij} = 0$,

$$i\hbar\frac{dz_i}{dt} = \sum_j \left[H_{ij} + \sum_{kl} V_{iklj}z_k^* z_l + E_{ij}\right]z_j. \tag{D19}$$

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