

Quantum dynamics of Bose-Hubbard Hamiltonians beyond the Hartree-Fock-Bogoliubov approximation: The Bogoliubov back-reaction approximation

I. Tikhonenkov,¹ J. R. Anglin,² and A. Vardi¹

¹Department of Chemistry, Ben-Gurion University of the Negev, P.O.B. 653, Beer-Sheva 84105, Israel

²Fachbereich Physik, Technische Universität Kaiserslautern, D67663, Kaiserslautern, Germany

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We formulate a method for studying the quantum field dynamics of ultracold Bose gases confined within optical lattice potentials, within the lowest Bloch-band Bose-Hubbard model. Our formalism extends the two-sites results of Vardi and Anglin [Phys. Rev. Lett. **86**, 568 (2001)] to the general case of M lattice sites. The methodology is based on mapping the Bose-Hubbard Hamiltonian to an $SU(M)$ pseudospin problem and truncating the resulting hierarchy of dynamical equations for correlation functions, up to pair correlations between $SU(M)$ generators. Agreement with few-site exact many-particle calculations is consistently better than the corresponding Hartree-Fock-Bogoliubov approximation. Moreover, our approximation compares favorably with a more elaborate two-particle irreducible effective action formalism, at a fraction of the analytic and numerical effort.

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I. INTRODUCTION

Strong correlation effects, which imply enhanced quantum fluctuations around mean field order parameters, are playing an increasingly important role in recent experiments on dilute quantum gases. One strategy for boosting the importance of correlations and fluctuations involves the control of coupling parameters. Interatomic interactions can be effectively tuned by means of magnetic Feshbach resonances [1–6], allowing for a controlled transition into the nonunitary regime $n^{1/3}a_s > 1$, where the effective s -wave scattering length a_s is larger than the average distance between particles $n^{1/3}$ with n being the number density of the gas. Quantum fluctuations also dominate quasi-one-dimensional systems [7–15] where transverse confinement may be used to increase the effective coupling strength $g_{1D} = 2\hbar^2 a_s / (ml_\perp^2)$ without explicit control of the three-dimensional s -wave scattering length. In the extreme Tonks-Girardeau strong-coupling regime $g_{1D}m/(\hbar^2 n) \gg 1$, spatial correlations dictate the impenetrability of bosons, leading to ideal fermion-like density distributions [8,9].

An alternative to increasing effective interaction strengths, is to decrease other (e.g., kinetic) terms in the many-body Hamiltonian. In a Bose gas confined by an optical lattice, an effective momentum cutoff is introduced by controlling the barrier heights, thus suppressing the hopping frequency J between adjacent sites. Given N particles interacting with strength U , the strong-interaction regime is achieved for $UN/J > 1$, as manifested in the quantum transition from a superfluid to a Mott-insulator phase [16–18].

Considerable theoretical effort is currently aimed at developing efficient methods for the description of correlated quantum gases, far from equilibrium but over time scales long enough for equilibration to occur, so that the dynamical onset of interesting quantum correlations may be studied. Exact many-body solutions may be found numerically via stochastic phase-space methods [19]. Another approach relies on perturbations of the lowest-order mean-field theory given by the Gross-Pitaevskii (GP) equation. The result is a

family of mean-field pairing theories. The standard zero-temperature Bogoliubov prescription [20] gives the natural small-oscillation modes by linearization about the GP ground state. However, this linear response theory does not account for the back-reaction of excitations on the condensate order-parameter and is thus limited to small perturbations and short time scales.

Back-reaction is accounted for within the Hartree-Fock-Bogoliubov (HFB) theory, which prescribes a set of coupled equations for the condensate order-parameter and pair correlation functions [21–24]. Since both normal and anomalous correlations are included, this approach comes at the cost of ultraviolet divergences of anomalous quantities. While this problem is relatively easy to deal with by renormalization of the coupling parameters, a more serious issue, also related to the inclusion of anomalous correlations, is the HFB spectral gap [21]. This unphysical gap in the excitation spectrum results in from the breaking of $U(1)$ gauge symmetry. Formally, both the GP and the Bogoliubov theories break $U(1)$ in selecting an arbitrary phase for the condensate order parameter. Consequently, the ground state of these effective theories is degenerate [as opposed to the true nondegenerate and $U(1)$ invariant ground state], resulting in the appearance of spurious, zero-energy excitations, known as Goldstone modes. While several methods have been proposed to carry out the Bogoliubov treatment in a particle-number-conserving fashion [25,26], symmetry breaking in GP and Bogoliubov is relatively mild, in that the dynamical equations remain $U(1)$ invariant. In comparison, the inclusion of the anomalous terms in the HFB formalism, completely removes $U(1)$ invariance, thus eliminating the Goldstone modes associated with gauge transformations of the broken symmetry solution and opening the spectral gap. An intermediate form between Bogoliubov and HFB is the HFB-Popov (HFB-P) approximation [21,27] where $U(1)$ symmetry is restored by elimination of noncondensate anomalous terms only. While the resulting theory is gapless, it does not conserve the total number of particles and is thus inadequate for describing dynamical condensate depletion. Finally, if all

anomalous quantities are neglected, one obtains the bosonic Hartree Fock (HF) theory [21] which is both gapless and conserving, but does not allow for any dynamical depletion, since the populations of condensed and noncondensed particles are conserved separately. It is thus highly desirable to develop a theoretical description that (a) is U(1) invariant and hence gapless, (b) conserves the total number of particles, yet (c) allows for dynamical depletion of the condensate.

Recently, a perturbative approximation scheme based on a two-particle irreducible (2PI) effective action expansion, has been used to study the nonequilibrium dynamics of condensates in optical lattices [24] within the lowest Bloch-band Bose-Hubbard model. Within the 2PI effective action expansion, the Bogoliubov and HFB theories emerge as one-loop and a single two-loop correction respectively, to the classical GP action. Higher-order approximations, obtained by including two-vertex terms in the diagrammatic expansion of the effective action (denoted as in Ref. [24] by “2nd”) and by a $1/\mathcal{N}$ expansion up to second order in the coupling strength (denoted henceforth by “ $1/\mathcal{N}$ ”) with \mathcal{N} being the number of auxiliary classical fields used to approximate the quantum field, have been compared with HFB and exact few-sites numerical calculations. The results demonstrate some improvement of the higher-order approximations over HFB in predicting the exact many-body dynamics. However, at sufficiently long times all approximations fail due to interaction effects. A nonperturbative $1/\mathcal{N}$ 2PI effective action expansion approach have also been developed and applied to the equilibration of a homogeneous Bose gas in 1D [28].

In this work we develop a mean-field theory for the description of quantum dynamics in the Bose-Hubbard model. The technique, referred to here as Bogoliubov back-reaction (BBR), is a many-site extension of previous work on a two-site model [29,30], based on the perturbation of equations of motion for the reduced single-particle density operator, instead of the usual field operator approach. The resulting equations involve the two-point reduced single-particle density matrix (SPDM) and the four-point correlation functions. They contain only normal (i.e., number conserving) quantities, and are thus U(1) symmetric. The approximation conserves the total number of particles, yet it allows for population transfer from the condensate to the excitations, thus accounting for condensate depletion during the evolution. We compare BBR calculations with full many-body numerical results for up to a hundred particles and five lattice sites, as well as with HFB and 2PI effective action results. The BBR results give better, longer-time predictions than current rival approximations, at a small fraction of the theoretical effort.

In Sec. II we present the Bose-Hubbard model and the standard HFB approach. In Sec. III we transform the Bose-Hubbard Hamiltonian with M lattice sites into an SU(M) pseudospin problem, derive dynamical equations for the SU(M) generators spanning the single-particle density operator, and truncate the resulting hierarchy of dynamical equations for correlation functions to obtain the BBR equations of motion. Section IV contains numerical few-sites results and comparison with HFB as well as 2PI effective action approximation methods. Discussion, conclusions and prospects for future research are presented in Sec. V.

II. CONVENTIONAL MEAN-FIELD THEORIES: GROSS-PITAEVSKII AND HARTREE-FOCK-BOGOLIUBOV

We begin with the standard Bose-Hubbard model Hamiltonian for an ultracold gas in a one-dimensional periodic optical lattice

$$\hat{H} = J \sum_i (\hat{a}_{i+1}^\dagger \hat{a}_i + \hat{a}_i^\dagger \hat{a}_{i+1}) + \frac{U}{2} \sum_i \hat{a}_i^\dagger \hat{a}_i^\dagger \hat{a}_i \hat{a}_i, \quad (1)$$

where \hat{a}_i and \hat{a}_i^\dagger are annihilation and creation operators, respectively, for a particle in site i . We consider only on-site interactions with strength U and nearest-neighbor tunneling with hopping rate J . These approximations are justified because adjacent site interactions and next-to-nearest-neighbor tunneling amplitudes are characteristically at least two orders of magnitude smaller than on-site interactions and nearest-neighbor hopping [16]. The Bose-Hubbard model is viable as long as there are no transitions into excited Bloch bands.

Using the Hamiltonian (1) we write the Heisenberg equations of motion for the field-operators \hat{a}_j ,

$$i \frac{d}{dt} \hat{a}_j = J(\hat{a}_{j-1} + \hat{a}_{j+1}) + U \hat{a}_j^\dagger \hat{a}_j \hat{a}_j. \quad (2)$$

The lowest order mean field theory for Bose-Hubbard model is obtained by replacing the field operators \hat{a}_j , and \hat{a}_j^\dagger the by c numbers a_j and a_j^* . This approximation is tantamount to assuming coherent many-body states with a well-defined phase between sites. Rescaling $a \rightarrow \sqrt{Na}$ and $\tau = Jt$ we arrive at the discrete GP equation

$$i \frac{d}{d\tau} a_j = (a_{j-1} + a_{j+1}) + L |a_j|^2 a_j, \quad (3)$$

where $L = UN/J$ is the characteristic coupling parameter. Within the GP mean field theory (3) fluctuations are completely neglected and the system is always assumed to be described by a single, coherent order parameter. Therefore an accurate description of the superfluid to Mott insulator quantum phase transition is not possible. Nevertheless, qualitative differences exist between mean field dynamics in the weak-coupling regime $L < 2$, where the system exhibits full-amplitude Rabi-like oscillations, and the strong coupling case $L > 2$, where self-trapped motion is observed [24,29–32].

To go beyond the GP approximation, a higher-order mean field theory may be formulated by adding to Eq. (2) additional equations of motion for the normal density operators $\hat{a}_j^\dagger \hat{a}_k$, and the anomalous density operators $\hat{a}_j \hat{a}_k$,

$$\begin{aligned} i \frac{d}{dt} \hat{a}_j \hat{a}_k &= J(\hat{a}_k \hat{a}_{j-1} + \hat{a}_k \hat{a}_{j+1} + \hat{a}_j \hat{a}_{k-1} + \hat{a}_j \hat{a}_{k+1}) \\ &+ U(\hat{a}_j^\dagger \hat{a}_k \hat{a}_j \hat{a}_k + \hat{a}_k^\dagger \hat{a}_j \hat{a}_k \hat{a}_k) + \frac{U}{2} (\hat{a}_j \hat{a}_j + \hat{a}_k \hat{a}_k) \delta_{jk}, \end{aligned} \quad (4)$$

$$\begin{aligned} i\frac{d}{dt}\hat{a}_j^\dagger\hat{a}_k = & J(\hat{a}_j^\dagger\hat{a}_{k-1} + \hat{a}_j^\dagger\hat{a}_{k+1} - \hat{a}_{j-1}^\dagger\hat{a}_k - \hat{a}_{j+1}^\dagger\hat{a}_k) \\ & + U(\hat{a}_j^\dagger\hat{a}_k^\dagger\hat{a}_k\hat{a}_k - \hat{a}_j^\dagger\hat{a}_j^\dagger\hat{a}_k\hat{a}_k). \end{aligned} \quad (5)$$

Taking the expectation values of Eq. (2) and Eqs. (4) and (5), and using the HFB Gaussian ansatz, we truncate third- and fourth-order moments as

$$\langle\hat{A}\hat{B}\hat{C}\rangle \approx \langle\hat{A}\rangle\langle\hat{B}\hat{C}\rangle + \langle\hat{B}\rangle\langle\hat{A}\hat{C}\rangle + \langle\hat{C}\rangle\langle\hat{A}\hat{B}\rangle - 2\langle\hat{A}\rangle\langle\hat{B}\rangle\langle\hat{C}\rangle, \quad (6)$$

$$\begin{aligned} \langle\hat{A}\hat{B}\hat{C}\hat{D}\rangle \approx & \langle\hat{A}\hat{B}\rangle\langle\hat{C}\hat{D}\rangle + \langle\hat{A}\hat{C}\rangle\langle\hat{B}\hat{D}\rangle + \langle\hat{A}\hat{D}\rangle\langle\hat{B}\hat{C}\rangle \\ & - 2\langle\hat{A}\rangle\langle\hat{B}\rangle\langle\hat{C}\rangle\langle\hat{D}\rangle, \end{aligned} \quad (7)$$

to obtain the HFB equations

$$i\frac{d}{d\tau}\hat{a}_j = (a_{j-1} + a_{j+1}) + La_j^*a_ja_j + L(2a_j\Delta_{jj}^n + a_j^*\Delta_{jj}^a), \quad (8)$$

$$\begin{aligned} i\frac{d}{d\tau}\Delta_{jk}^a = & (\Delta_{j-1,k}^a + \Delta_{j+1,k}^a + \Delta_{j,k-1}^a + \Delta_{j,k+1}^a) \\ & + 2L(|a_j|^2 + |a_k|^2 + \Delta_{jj}^n + \Delta_{kk}^n)\Delta_{jk}^a \\ & + \frac{L}{2}(a_k^2 + \Delta_{kk}^a)(2\Delta_{jk}^{n*} + \delta_{jk}) \\ & + \frac{L}{2}(a_j^2 + \Delta_{jj}^a)(2\Delta_{jk}^n + \delta_{jk}), \end{aligned} \quad (9)$$

$$\begin{aligned} i\frac{d}{d\tau}\Delta_{jk}^n = & (\Delta_{j,k-1}^n + \Delta_{j,k+1}^n - \Delta_{j-1,k}^n - \Delta_{j+1,k}^n) \\ & + 2L[(|a_k|^2 + \Delta_{kk}^n) - (|a_j|^2 + \Delta_{jj}^n)]\Delta_{jk}^n \\ & + L[(a_k^2 + \Delta_{kk}^a)\Delta_{jk}^{n*} - (a_j^2 + \Delta_{jj}^a)^*\Delta_{jk}^a], \end{aligned} \quad (10)$$

for the mean field $a_j \equiv \langle\hat{a}_j\rangle/\sqrt{N}$ and the two-point correlation functions $\Delta_{jk}^n \equiv [\langle\hat{a}_j^\dagger\hat{a}_k\rangle - a_j^*a_k]/N$, $\Delta_{jk}^a \equiv [\langle\hat{a}_j\hat{a}_k\rangle - a_ja_k]/N$, constituting the reduced single particle density matrix.

We note that the discrete HFB equations (8)–(10) are not UV divergent due to the natural momentum cutoff imposed by the lattice. However, due to the existence of a noncondensate anomalous density, U(1) symmetry is broken, in contrast to the gauge-invariant original field equations (2). U(1) symmetry may be restored for example, by omitting all anomalous quantities, to obtain the Hartree-Fock equations

$$i\frac{d}{d\tau}a_j = (a_{j-1} + a_{j+1}) + L(|a_j|^2 + 2\Delta_{jj}^n)a_j, \quad (11)$$

$$\begin{aligned} i\frac{d}{d\tau}\Delta_{jk}^n = & (\Delta_{j,k-1}^n + \Delta_{j,k+1}^n - \Delta_{j-1,k}^n - \Delta_{j+1,k}^n) \\ & + 2L[(|a_k|^2 + \Delta_{kk}^n) - (|a_j|^2 + \Delta_{jj}^n)]\Delta_{jk}^n. \end{aligned} \quad (12)$$

Equations (11) and (12), conserve separately the condensate population $\sum_j|a_j|^2$ and the noncondensed fraction $\sum_j\Delta_{jj}^n$. Thus, the HF approximation can not be used to account for condensate depletion during the evolution. If only the non-

condensate anomalous terms are neglected, one obtains the HFB-Popov [27] approximation, which allows for growth of fluctuations, but conserves the condensate population, so that the total number is not a constant of motion. In the following section we construct a U(1) invariant mean-field theory which conserves the total number of particles, yet includes dynamical depletion.

III. THE BOGOLIUBOV BACK-REACTION EQUATIONS

Instead of the conventional mean-field approaches, based on the site field operators \hat{a}_j , we construct a mean field formalism using the reduced single-particle density operator $\hat{a}_j^\dagger\hat{a}_k$, treating it as the fundamental quantity. We have previously applied this approach to the case of a two-site model [29,30]. Here we extend it to the general M site case. It is convenient to rewrite the Hamiltonian (1) in terms of the M^2-1 traceless operators which generate SU(M):

$$\begin{aligned} \hat{u}_{j,k} &= \hat{a}_j^\dagger\hat{a}_k + \hat{a}_k^\dagger\hat{a}_j, \quad 1 \leq k < j \leq M, \\ \hat{v}_{j,k} &= -i(\hat{a}_j^\dagger\hat{a}_k - \hat{a}_k^\dagger\hat{a}_j), \quad 1 \leq k < j \leq M, \\ \hat{w}_l &= -\sqrt{\frac{2}{l(l+1)}}\left(\sum_{j=1}^l \hat{n}_j - l\hat{n}_{l+1}\right), \quad 1 \leq l \leq M-1. \end{aligned} \quad (13)$$

Since it is easily verified that

$$\frac{1}{2}\sum_{j=1}^{M-1} \hat{w}_j^2 + \frac{1}{M}\hat{n}^2 = \sum_{j=1}^M \hat{n}_j^2, \quad (14)$$

where $\hat{n} = \sum_{j=1}^M \hat{n}_j$ is the total particle number, Eq. (1) can be rewritten, eliminating c -number terms, as

$$\hat{H} = J\sum_{j=1}^{M-1} \hat{u}_{j+1,j} + \frac{U}{4}\sum_{j=1}^{M-1} \hat{w}_j^2. \quad (15)$$

Using the SU(M) generators we construct a pseudospin vector operator

$$\hat{\mathbf{S}} = (\hat{u}_{21}, \hat{u}_{32}, \dots, \hat{u}_{31}, \hat{u}_{42}, \dots, \hat{v}_{21}, \hat{v}_{32}, \dots, \hat{v}_{31}, \hat{v}_{42}, \dots, \hat{w}_1, \hat{w}_2, \dots, \hat{w}_{M-1}), \quad (16)$$

so that the Hamiltonian (15) takes the form

$$\hat{H} = J\sum_{j=1}^{M-1} \hat{S}_j + \frac{U}{4}\sum_{j=M^2-M}^{M^2-1} \hat{S}_j^2. \quad (17)$$

The Heisenberg equations of motion for the operators \hat{S}_i and their products $\hat{S}_i\hat{S}_l$ then read

$$\begin{aligned} i\frac{d}{dt}\hat{S}_i = & J\sum_{j=1}^{M-1} \sum_{k=1}^{M^2-1} c_{ij}^k \hat{S}_k + \frac{U}{4}\sum_{j=M^2-M+1}^{M^2-1} \sum_{k=1}^{M^2-1} c_{ij}^k (\hat{S}_k\hat{S}_j + \hat{S}_j\hat{S}_k), \end{aligned} \quad (18)$$

$$\begin{aligned} i\frac{d}{dt}\hat{S}_i\hat{S}_l &= J \sum_{j=1}^{M-1} \sum_{k=1}^{M^2-1} (c_{ij}^k \hat{S}_k \hat{S}_l + c_{lj}^k \hat{S}_i \hat{S}_k) \\ &+ \frac{U}{4} \sum_{j=M^2-M+1}^{M^2-1} \sum_{k=1}^{M^2-1} c_{ij}^k (\hat{S}_k \hat{S}_j + \hat{S}_j \hat{S}_k) \hat{S}_l \\ &+ \frac{U}{4} \sum_{j=M^2-M+1}^{M^2-1} \sum_{k=1}^{M^2-1} c_{lj}^k (\hat{S}_k \hat{S}_j + \hat{S}_j \hat{S}_k), \end{aligned} \quad (19)$$

where the coefficients c_{ij}^k are the structure constants of the $SU(M)$ group. We note that for $M=2$ the Hamiltonian (15) and the dynamical equations (18) and (19) reduce to the familiar Bloch forms used in Refs. [29,30]. The M -site system is a direct extension of the two-mode case, in that hopping terms induce linear Rabi-like oscillations in the $\mathbf{v}\mathbf{v}$ subspace, whereas on-site interactions lead to nonlinear phase precession in the $\mathbf{u}\mathbf{v}$ subspace.

The reduced single-particle density matrix is obtained from the expectation value of $\hat{\mathbf{S}}$, according to

$$\rho = \frac{N}{2}\mathcal{I} + \frac{1}{2} \sum_{j=1}^{M^2-1} \langle \hat{S}_j \rangle \sigma_j, \quad (20)$$

where \mathcal{I} is a unit matrix of order M and σ_j are the $M \times M$ irreducible representations of the $SU(M)$ generators (e.g., Pauli matrices for $M=2$, Schwinger matrices for $M=3$ etc.). We will therefore focus on the dynamics of the “hyper-Bloch-vector” $\mathbf{S} \equiv \langle \hat{\mathbf{S}} \rangle / 2N$. The lowest-order mean-field approximation replaces the vector of operators $\hat{\mathbf{S}}$ by the vector of their expectation values \mathbf{S} , thus truncating $\langle \hat{S}_i \hat{S}_j \rangle \approx \langle \hat{S}_i \rangle \langle \hat{S}_j \rangle$. This results in the nonlinear pseudospin-precession form of the GP equations

$$\frac{d}{d\tau} \mathbf{S} = \mathbf{B}(\mathbf{S}) \otimes \mathbf{S}, \quad (21)$$

where

$$\mathbf{B}(\mathbf{S}) = (B_1, B_2, \dots, B_{M^2-1}), \quad (22)$$

with

$$B_j = \begin{cases} 1, & j = 1, \dots, M(M-1)/2, \\ 0, & j = M(M-1)/2 + 1, \dots, M(M-1), \\ LS_j, & j = M(M-1) + 1, \dots, M^2 - 1. \end{cases}$$

It is readily verified that Eq. (21) is exactly equivalent to the discrete GP equation (3). In addition to the conservation of the total number $\text{Tr}(\rho)$ there exist, within GP theory, $M-1$ independent constants of the motion $\text{Tr}(\rho^m)$ with $m=2, \dots, M-1$. For example, for $M=2$ the GP mean-field theory also conserves the single-particle purity $\text{Tr}(\rho^2)$, which is just the length of the three-dimensional Bloch vector. Deviations from this classical field theory, due to interparticle entanglement and loss of single particle coherence, will show up as a reduction in these classically conserved quantities.

The BBR approximation is obtained by going one level deeper in the hierarchy of dynamical equations for expecta-

tion values. Taking the expectation values of Eqs. (18) and (19) and truncating

$$\langle \hat{S}_i \hat{S}_j \hat{S}_k \rangle \approx \langle \hat{S}_i \rangle \langle \hat{S}_j \hat{S}_k \rangle + \langle \hat{S}_j \rangle \langle \hat{S}_i \hat{S}_k \rangle + \langle \hat{S}_k \rangle \langle \hat{S}_i \hat{S}_j \rangle - 2\langle \hat{S}_i \rangle \langle \hat{S}_j \rangle \langle \hat{S}_k \rangle, \quad (23)$$

we obtain the BBR equations of motion

$$i\frac{d}{d\tau} S_i = \sum_{j=1}^{M-1} \sum_{k=1}^{M^2-1} c_{ij}^k S_k + L \sum_{j=M^2-M+1}^{M^2-1} \sum_{k=1}^{M^2-1} c_{ij}^k \left(S_j S_k + \frac{\Delta_{jk}}{2} \right), \quad (24)$$

$$\begin{aligned} i\frac{d}{d\tau} \Delta_{il} &= \sum_{j=1}^{M-1} \sum_{k=1}^{M^2-1} (c_{ij}^k \Delta_{lk} + c_{lj}^k \Delta_{ik}) \\ &+ L \sum_{j=M^2-M+1}^{M^2-1} \sum_{k=1}^{M^2-1} c_{ij}^k (\Delta_{lj} S_k + \Delta_{lk} S_j) \\ &+ L \sum_{j=M^2-M+1}^{M^2-1} \sum_{k=1}^{M^2-1} c_{lj}^k (\Delta_{ij} S_k + \Delta_{ik} S_j), \end{aligned} \quad (25)$$

where $S_j = \frac{\langle \hat{S}_j \rangle}{2N}$ and $\Delta_{jk} = \frac{\langle \hat{S}_j \hat{S}_k + \hat{S}_k \hat{S}_j \rangle}{4N^2} - 2S_j S_k$. In the following section we compare the accuracy of the BBR approximation with respect to GP, HFB, and 2PI effective action.

IV. NUMERICAL RESULTS

In order to test the accuracy of the BBR approximation compared to other methods, we carried out exact numerical calculations for limited numbers of particles and sites (up to $N=100$ particles and $M=5$ lattice sites). The Hamiltonian (1)

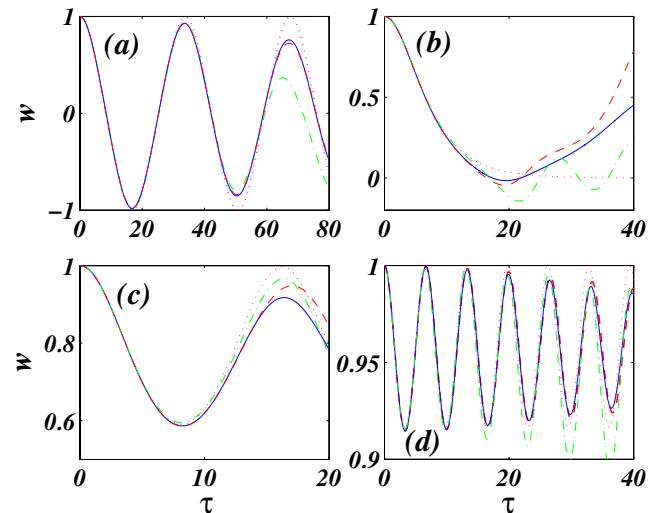
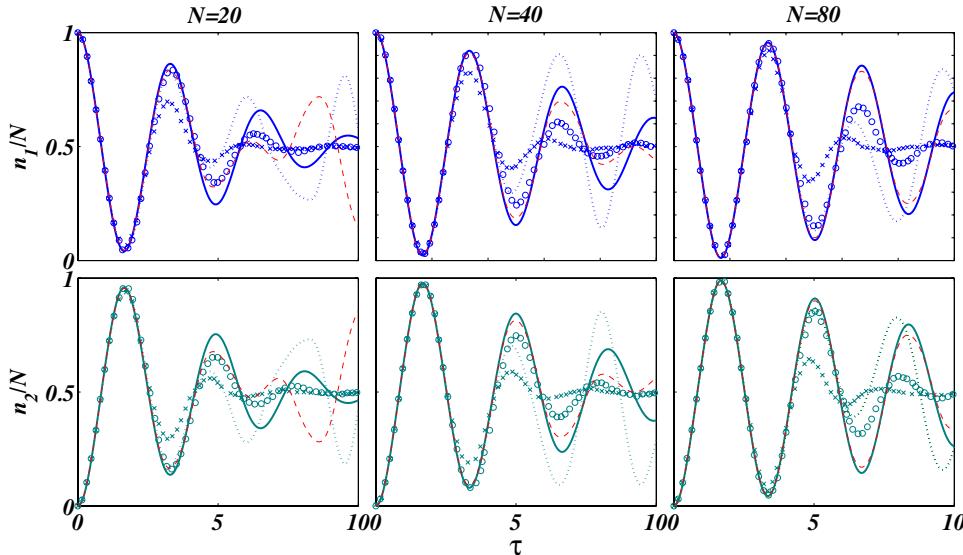


FIG. 1. (Color online) Population imbalance w in a two-site system as a function of rescaled time τ for $L=2$ (a), $L=4$ (b), $L=5$ (c), and $L=10$ (d). The total number of particles is set to $N=100$. Solid blue lines, corresponding to exact many-body numerical results, are compared to the GP (dotted lines), HFB (dash-dotted lines), and BBR (dashed lines) approximations.



was represented in terms of site-number states and the N -body Schrödinger equation was solved numerically, as in Refs. [24,29,30]. These many-body results were then compared with BBR mean-field calculations, as well as with GP, HFB, and variants of the 2PI effective action method.

In Fig. 1 the evolution of fractional population difference for a hundred particles in two-sites, is plotted for various values of the coupling parameter L . Within the GP mean-field theory, full-amplitude Rabi-like oscillations are predicted in the linear regime with $L < 2$ [Fig. 1(a)]. As the transition is made to the strong-coupling regime, the oscillation becomes increasingly more nonlinear, until when $L \geq 4$ macroscopic self-trapping is attained [Figs. 1(b)–1(d)]. The value of $L=4$ is particularly interesting because for this coupling a trajectory starting from a single-populated site becomes dynamically unstable when site-populations equilibrate. In previous work we have shown that this dynamical instability serves as a quantum-noise amplifier [29,30], so that the growth of the deviation of a quantum trajectory from the corresponding GP prediction is initially exponential, leading to a $\ln(1/N)$ slow convergence of the many-body quantum-field results to the classical GP prediction. Thus, while the naive expectation would be that quantum fluctuations would simply grow with the coupling parameter L , their role is in fact maximized for $L=4$, as evident in Fig. 1(b). It is clear from Fig. 1 that the BBR approximation gives a better description of the ensuing quantum dynamics, for longer time scales, than HFB does.

Convergence of various approximations with increasing number of particles is demonstrated in Fig. 2, where the two-sites population dynamics is plotted for increasing particle numbers, keeping a fixed coupling value of $L=2$. In addition to the exact, BBR, and HFB results, we also plot two calculations based on the 2PI effective action approach, taken from Fig. 5 of Ref. [24] (our exact and HFB results exactly coincide with the corresponding lines in that figure). Here too, the BBR approximation (red dashed lines) gives a more accurate description of the dynamics than any of the other methods, attaining a nearly perfect convergence in the given time-frame for $N=80$ particles. In comparison, standard HFB

FIG. 2. (Color online) Evolution of atomic site populations in a two-site system, starting with all population in one site, for $N=20, 40, 80$ and fixed $L=2$. Exact numerical results (solid) are compared with the HFB (dotted) and BBR (red dashed lines) approximations, as well as to the two approximations based on the 2PI effective action formalism: Second order (crosses) and $1/N$ (circles), taken from Fig. 5 in Ref. [24].

fails to depict the damping of coherent oscillations, whereas the 2PI effective action methods tend to overdamp. We note, that in terms of formalistic complexity alone, the BBR approximation is far simpler than the noninstantaneous integrodifferential equations used in the 2PI effective action methods [24]. In fact, it is even simpler than HFB, in that only normal quantities are involved, giving a total of nine equations for two sites, as opposed to fifteen in HFB.

Dynamical condensate depletion is also well-depicted by the BBR approximation. In Fig. 3 we plot the evolution of the leading eigenvalue of the reduced single-particle density matrix ρ and the single-particle von-Neumann entropy $-\text{Tr}(\rho \ln \rho)$, corresponding to the population dynamics of Fig. 2. While HFB calculations seem to give an abrupt deviation of the predicted condensate fraction from its exact

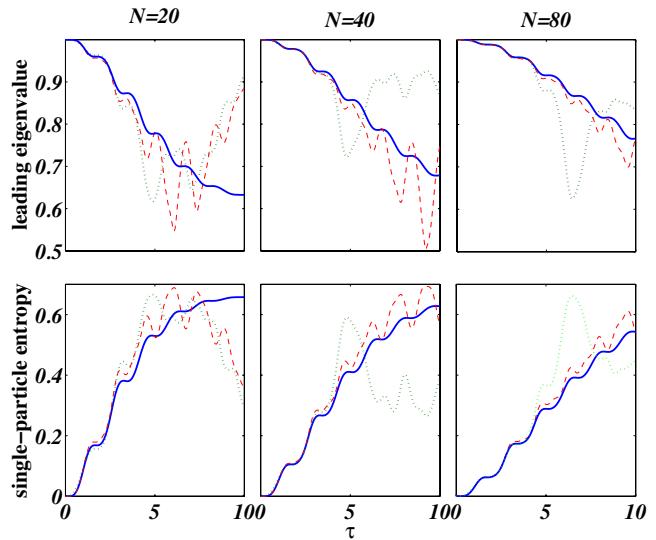


FIG. 3. (Color online) Evolution of the leading eigenvalue (above) and single-particle entropy (below) for a two-site system with $N=20, 40, 80$ and $L=2$. Exact many-body numerics (solid blue line) is compared with the HFB approximation (green dotted line) and the BBR approximation (red dashed line).

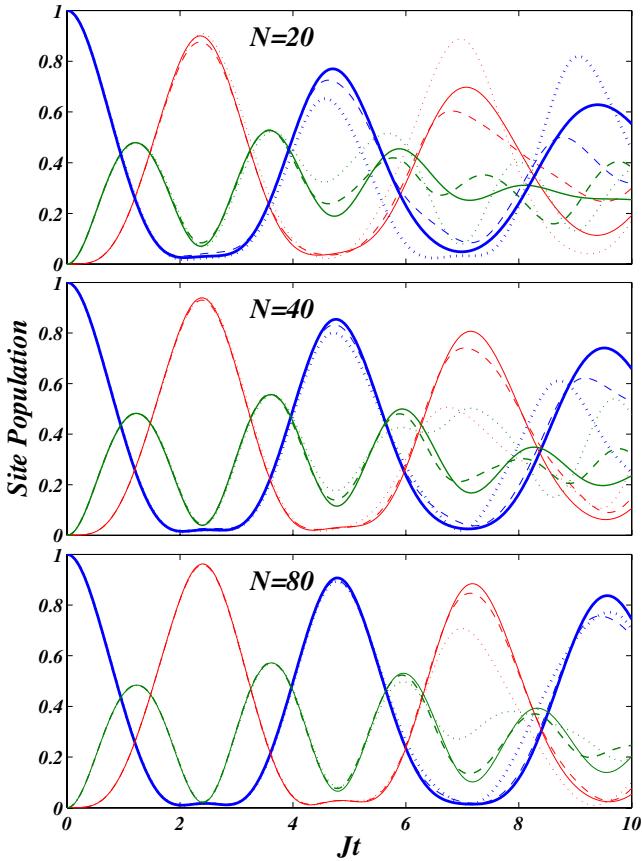


FIG. 4. (Color online) Site populations in a three-site system as a function of rescaled time τ for $N=20, 40, 80$ and fixed $L=2$. Blue (thick), green (medium), and red (thin) lines correspond to first, second, and third site populations, respectively. Solid lines depict the full many-body dynamics, whereas dotted and dashed lines correspond to the HFB approximation and the BBR approximation, respectively.

value, the BBR results converge well, giving a reasonably accurate description of BEC depletion.

The same qualitative behavior carries over to systems with more than two sites. In Figs. 4 and 5, population dynamics and condensate depletion are shown for a three-sites system with $N=20, 40, 80$ particles. Similarly to the two-sites case, the BBR approximation constitutes a significant improvement over the HFB approach, giving a better description of populations as well as coherences. The same is also true for the four-sites case shown in Fig. 6.

The faster convergence of BBR as compared with the HFB approximation is illustrated in Fig. 7, where characteristic breaktimes of the two approximations in a two-sites calculation, are plotted as a function of the total number of particles N . As anticipated, breaktimes grow as \sqrt{N} when the classical dynamics is regular [Figs. 7(a), 7(c), and 7(d)] and as $\ln N$ when the classical trajectory hits the dynamical instability [Fig. 7(b)]. The BBR calculations give consistently longer breaktimes, with a more regular convergence pattern.

V. DISCUSSION

The rich regime of strongly correlated many body physics, which ultracold atom experiments are now beginning to

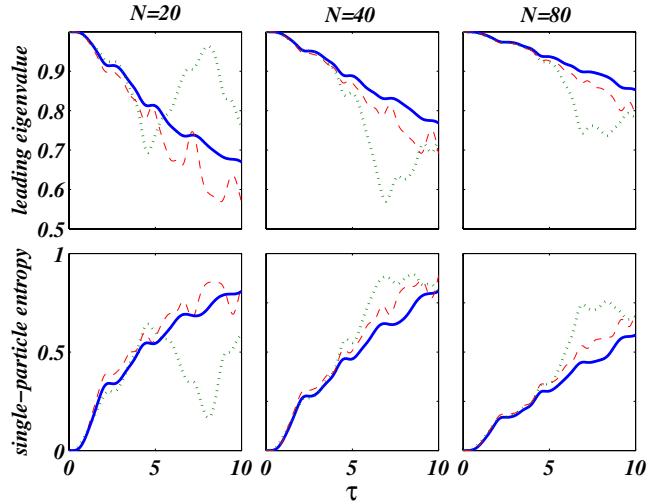


FIG. 5. (Color online) Leading eigenvalue of the reduced single-particle density matrix ρ and single-particle entropy $-\text{Tr}(\rho \ln \rho)$, as a function of rescaled time τ in a three-site system with $N=20, 40, 80$ and $L=2$. Exact results (solid blue lines) are compared to HFB calculations (dotted green lines) and BBR calculations (dashed red lines).

probe, will surely not be fully conquered by any simple hierarchy truncation scheme such as BBR. Nor does BBR offer anything similar to an exact solution even to the problems to which we have applied it in this paper; its improvements over its rivals are incremental rather than revolutionary. On the other hand it should be born in mind that incremental improvements in theory are more significant in the context of ultracold gases than in traditional condensed matter, because in the new atomic systems samples are precisely characterized, controlled, and measured, and relevant microphysics is clearly known. It is perfectly plausible in these systems that we may come to learn important qualitative principles from experimental discrepancies on the few percent level.

It is useful to contrast BBR with other previously proposed U(1) preserving schemes. Gardiner [25] has proposed a number-conserving variation of the Bogoliubov theory of linearized excitations around the Gross-Pitaevskii mean field, which does not account for back-reaction. In a closely related work, Castin and Dum [26] suggested an equivalent Bogoliubov reformulation, adding to it another step in their $N^{-1/2}$ perturbative expansion. This order consists of back-reactive corrections to the Gross-Pitaevskii wave function, from the Bogoliubov excitations, and is thus similar in spirit to our work here. There are, however, significant differences between BBR and the scheme of Ref. [26]. First, the two theories perturb different objects. Whereas [26] uses the standard perturbation of the condensate wave function, BBR perturbs the reduced single-particle density matrix and is thus of essentially higher order.

Another and perhaps more significant difference is the contrast between the perturbative rigor of [26] and the self-consistency of BBR. The formulation in Ref. [26] is a form of standard time-dependent perturbation theory. A small parameter is identified in the Heisenberg equations of motion for the bosonic field operator, in the presence of a Bose-

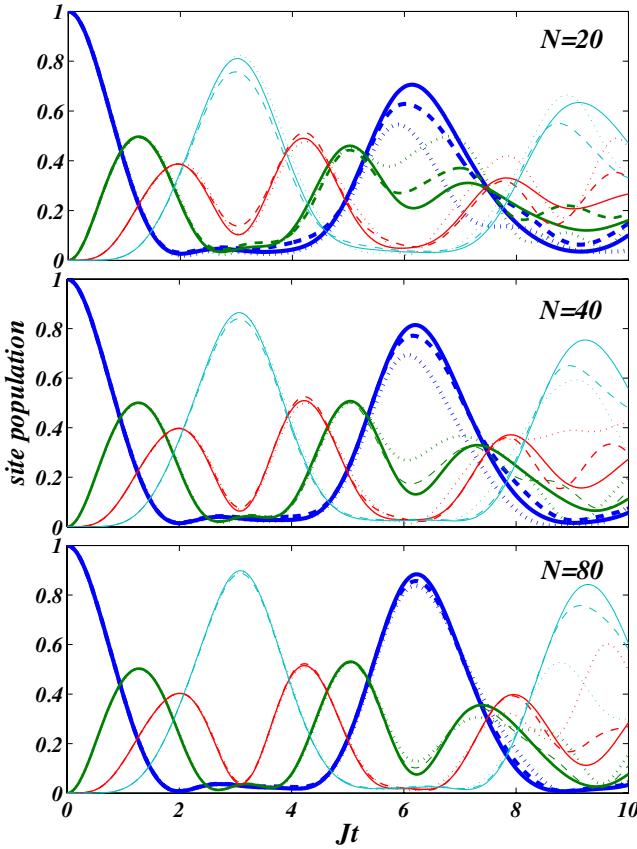


FIG. 6. (Color online) Site populations in a four-site system as a function of rescaled time τ for $N=20, 40, 80$ and fixed $L=2$. Blue, green, red, and cyan lines (in decreasing order of thickness) correspond to first, second, third, and fourth site populations, respectively. Solid lines depict the full many-body dynamics, whereas dotted and dashed lines correspond to the HFB approximation and the BBR approximation, respectively.

Einstein condensate as defined by Onsager and Penrose. The field operator is expanded systematically in this small parameter, and equations of motion are derived for each term, order by order, so that the small parameter itself never appears in any of their series of equations of motion.

Short time corrections to Gross-Pitaevskii can indeed be considered solved by the Castin-Dum approach. However, as with any simple time-dependent perturbation series, this method has some finite radius of convergence in time. It is not suitable for describing long-term, secular behavior, such as equilibration, dephasing, or damping. The quantum description of such phenomena, which has recently attracted much attention, requires other approaches.

The several different approaches that have been proposed to date are all still similar to Castin-Dum in that they construct equations of motion to various orders, the lowest order being Gross-Pitaevskii, the next being Bogoliubov, and so on. The key difference is that one seeks exact (“self-consistent”) solutions to these perturbatively derived equations. This apparently simple-minded procedure amounts to a partial resummation of the Castin-Dum perturbation theory, to all orders. Like most partial resummations, its accuracy is difficult to assess analytically with any rigor. But unlike the

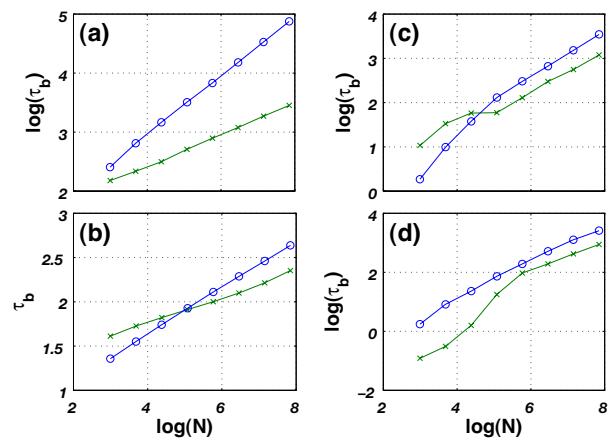


FIG. 7. (Color online) Characteristic times at which the Cartesian distance between the exact Bloch vector and its HFB (green, crosses) and BBR (blue, circles) approximants, reaches a predetermined threshold, as a function of N for $L=1$ (a), $L=4$ (b), $L=6$ (c), and $L=10$ (d). The break threshold is set to 0.2 in (a)–(c), and to 0.05 in (d).

Castin-Dum approach, it is in principle able to capture secular behavior.

A simple illustration of the difference between the two approaches would be an effective equation of motion for a damped particle. If to first order in γ one obtains the equation of motion $\ddot{x}+2\gamma\dot{x}=0$, then the Castin-Dum approach would produce the approximate solution $x(t)=A+Bt-\gamma Bt^2$. The self-consistent approach yields $x(t)=A+Be^{-2\gamma t}$. For an oscillator which really is damped in some way, the second approach is qualitatively better at late times; and with some tuning, it might well be made quantitatively accurate. Checking whether this long-time accuracy is really obtained, however, can be quite nontrivial, because the higher powers of γ that are included in the exponential are in the strictest sense inconsistent, given the perturbative derivation of the equation itself. It is a similar kind of nontrivial assessment that our paper has provided, for simple systems of equations that model interacting quantum gases instead of single damped particles.

The merits of BBR that we would like to emphasize, along with its very reasonable level of accuracy, are its simplicity and its direct relation to experimental reality. It involves only quantities which are directly observed in single- and two-particle number-conserving measurements, and it respects the fact that in current quantum gas laboratories atoms are neither created nor destroyed. And it is conceptually and computationally straightforward.

In one sense it is of course conceptually all too straightforward: as with all hierarchy truncation schemes since Boltzmann's, it is an uncontrolled approximation, whose accuracy is therefore arguably as much a puzzle as it is a solution. Insofar as truncating a hierarchy at a deeper level is grounds for expecting higher accuracy, however, the advantage of BBR is clear: it is a truncation at fourth order in field operators, compared to only second order for HFB. Deeper level truncation often involves proliferation of terms, to the point

of sharply diminishing returns in accuracy versus effort; but BBR avoids this, and manages to use fewer equations than HFB, because it eliminates all anomalous terms.

This leads us to conclude by indicating some of the potential future applications of the results of this paper. Why do hierarchy truncations often work as well as they do? What determines the best way of truncating a hierarchy? These are questions that have been raised ever since Boltzmann's *stosszahlansatz* produced the arrow of time, but they have yet to be fully answered. With current experimental capabilities for precise and controlled measurements on ultracold gases, introducing a physically motivated alternative truncation scheme, as this paper has done, may contribute to new progress on these questions.

Finally, another conceptual merit of BBR is that because it is based on the single particle density matrix, rather than

just the macroscopic wave function, it makes such a conceptually important quantity as the single particle entropy—the entropy of Boltzmann—a basic ingredient in the theory, rather than a perturbative afterthought. Rethinking entropy, heretofore mainly in the context of quantum information and computation theory, is another major thrust of current physics; the alternative viewpoint offered by BBR may potentially be of some value in a broader conception of this project.

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