Dynamical Mean Field Theory of the Bose-Hubbard Model

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Quantum dynamics of the Bose-Hubbard model is investigated through a semiclassical Hamiltonian picture provided by the time-dependent variational principle method. The system is studied within a factorized slow/fast dynamics. The semiclassical requantization procedure allows one to account for the strong quantum nature of the system when $t/U \ll 1$. The phase diagram is in good agreement with quantum Monte Carlo results and third order strong coupling perturbative expansion. [S0031-9007(98)05433-7]

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In recent years outgrowing interest has been devoted to many-body systems which can be modeled in terms of bosonic degrees of freedom. Examples are granular superconductors, short-length superconductors, and Josephson junction arrays [1]. The relevant physics of these systems is captured by the Bose-Hubbard model (BHM) which represents a boson gas of identical charges hopping through a D dimensional lattice. The boson dynamics is described by the second quantized Hamiltonian

$$H = \sum_i [U(n_i - 1) - \mu] n_i - \frac{t}{2} \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i), \tag{1}$$

where the operators $n_i \doteq a_i^\dagger a_i$ count the number of bosons at site i, while the annihilation and creation operators a_i, $a_i^\dagger$ obey the canonical commutation relations $[a_i, a_j^\dagger] = \delta_{ij}$. The parameters of Hamiltonian (1) $U > 0$, t, and μ correspond to the strength of the Coulomb on-site repulsion, the hopping amplitude, and the chemical potential, respectively. The rich structure of the BHM phase diagram has been investigated by a number of theoretical methods, from mean field [2], variational [3] and perturbative [4] approaches, to quantum Monte Carlo [5] technique.

At $T = 0$ and integer fillings, the system undergoes a quantum phase transition, between a Mott insulator (MI) and a superfluid (SF) phase. At $t = 0$ the filling is fixed to the integer n that minimizes the on-site contribution of the Hamiltonian (1). In this limit, the existence of a finite energy $\mu = 2U$, required to add one boson to the system, reflects the MI nature of this phase, characterized by a vanishing compressibility (gapped particle-hole excitations). The MI survives (except for the degeneration points with $\mu/U = 2n$) when $t/U > 0$, inside extended *lobes* in the t/U, μ/U plane attached to the intervals $I(n) = (2(n-1)U, 2nU)$ of the μ/U axis [2]. Elsewhere, in the phase plane, the system is superfluid and appears to be compressible since the addition of a particle free to hop through the lattice brings up a reduction of the Coulomb repulsion. A crucial property has to be mentioned, at this point, concerning the MI-SF phase lobe boundary. At the transition points the appearance of superfluidity is announced by the vanishing of the energy gap between the states corresponding to n $(n-1)$ and $n+1$ (n) particles (holes). Such a feature characterizes the whole frontier between the MI and the SF phase and will play a central role in the sequel.

In spite of the great amount of work devoted to studying the several aspects of the BHM, no investigation, to the best of our knowledge, has been made on the dynamics of boson degrees of freedoms. The attempt of relating the onset of the macroscopic order leading to the MI and SF phases with the microscopic behavior of the system motivates the dynamical approach to the BHM. This should be useful as well to study both the emergence of vortex dynamics and the transport properties. In particular, in the present paper we shall show the mean field phase diagram of the BHM results to be quite improved if the *dynamics* of the SF order parameter is accounted for.

Indeed, it is possible to develop such a program, although several features of Hamiltonian (1) (nonlinearity, the many-body character, and its quantum nature) make the investigation of its dynamical behavior a hard problem.

The time-dependent variational principle (TDVP) method [6] offers a quite general procedure for constructing an approximate macroscopic wave function for many-body systems. Such a method, recently employed for studying the fermionic Hubbard Model dynamics [7], is based on the idea of constraining the time evolution of the system's state $|\Phi\rangle$ via the weaker form of the Schrödinger equation $\langle\Phi|(i\hbar\partial_\tau - H)|\Phi\rangle = 0$. Upon setting $|\Phi\rangle = \exp(iS/\hbar)|Z\rangle$ one obtains

$$\dot{S} = i\hbar\langle Z|\partial_\tau|Z\rangle - \langle Z|H|Z\rangle, \tag{2}$$

where the *trial macroscopic state* $|Z\rangle$, the basic ingredient of the method, must be structured so as to contain as much information as possible on the microscopic dynamics. The label Z is thus identified with a vector of microscopic parameters that are required to account for the dominating physical processes at microscopic

level and represent the effective dynamical variables of the system. For this reason $\dot{S}$ and $\langle Z|H|Z\rangle$ can be properly seen as functions of Z and we denote them by $\mathcal{L}[Z]$ and $\mathcal{H}[Z]$, respectively. The TDVP theory identifies the effective Lagrangian of the system with $\mathcal{L}[Z]$ and its semiclassical model Hamiltonian with $\mathcal{H}[Z]$. The quantum dynamics is thus described through a set of semiclassical Hamiltonian equations obtained by implementing the stationarity condition $\delta S = 0$ on the action S of $\mathcal{L}[Z]$.

A thorough analysis of the semiclassical equations related to H is interesting in itself due to their complexity. Here, we intend instead to employ the TDVP method for finding the ground-state configurations of the model and examining their dependence from the microscopic parameters t/U and μ/U. In other words, we aim to work out the phase diagram of the BHM starting from the study of the semiclassical equations of motion. Let us apply the TDVP method to the BHM model (1). We write the state $|\Phi\rangle$ as $|\Phi\rangle \equiv \exp[iS/\hbar] \otimes_i |z_i\rangle$ once the trial macroscopic state $|Z\rangle$ is assumed to have the form $|Z\rangle \equiv \otimes_i |z_i\rangle$. Here the states $|z_i\rangle$ are the Glauber coherent states [6] associated with the boson lowering operators a_i, solutions of the equation $a_i|z_i\rangle = z_i|z_i\rangle$ for each i. The choice of $|Z\rangle$, of course, is suggested by the fact that H belongs to the enveloping algebra of the N_s-boson Weyl-Heisenberg algebra $\{\mathbf{I}, a_j, a_j^\dagger, n_j : j \in \Lambda\}$, N_s being the number of sites of the lattice Λ. In this case Eq. (2) becomes

$$\mathcal{L}[Z] = i\hbar \sum_i \frac{1}{2}(\bar{z}_i \dot{z}_i - \dot{\bar{z}}_i z_i) - \mathcal{H}(Z), \qquad (3)$$

where the semiclassical model Hamiltonian $\mathcal{H}(Z) = \langle Z|H|Z\rangle$ is easily shown to have the form

$$\mathcal{H} = \sum_i (U|z_i|^2 - \mu)|z_i|^2 - \frac{t}{2}\sum_{\langle i,j\rangle}(\bar{z}_i z_j + \bar{z}_j z_i). \quad (4)$$

Lagrangian (3) yields the equations of motion

$$i\hbar \dot{z}_i = -\mu z_i + 2U z_i |z_i|^2 - \frac{t}{2}\sum_{j\in(i)} z_j, \qquad (5)$$

where (i) indicates the set of the nearest neighbor sites around i and we have omitted the equation for $\bar{z}_i$ directly ensuing from Eqs. (5) via complex conjugation. Notice that Eqs. (5) can be obtained as well through the standard formulas $i\hbar \dot{z}_j = \{z_j, \mathcal{H}\}$, based on the canonical Poisson brackets $\{z_k, \bar{z}_j\} = \delta_{kj}/i\hbar$ replacing commutators $[a_i, a_j^\dagger] = \delta_{ij}$ in the TDVP semiclassical scenery. This checks their hamiltonian character. As expected, Eqs. (5) are not integrable (integrability occurs only when either $U = 0$ or when $t = 0$) since the only known constant of motion, a part from $\mathcal{H}$, is the semiclassical version $\mathcal{N} = \sum_i |z_i|^2$ of number operator $N = \sum_i n_i$.

We simplify the structure of Eqs. (5) by separation of slow and fast dynamics, a procedure which is in some way the analog, in a dynamical contest, of the mean field approximation (MFA) usually employed in statistical mechanics. To this end we set, at each site, $z_i = \psi_i + \eta_i$ and assume that ψ_i is a slow variable whereas η_i is a fast oscillating term describing the complex, high-frequency part of the dynamics taking place on the microscopic interactions time scale (the hopping interaction, in this case). Then $\psi_j = \langle z_j\rangle_\tau$ ($\langle\bullet\rangle_\tau$ denotes time average) when the time scale τ is larger than that of the η_j's. The onset of order in the system at the macroscopic scale should reflect the dominating role of the ψ_j's in the lattice dynamics. Imposing the standard condition $(z_i - \psi_i)(\bar{z}_j - \overline{\psi}_j) = \eta_i \overline{\eta}_j \approx 0$ of the MFA procedure involves the dynamical mean field decoupling $z_i \bar{z}_j \approx \psi_i \bar{z}_j + \overline{\psi}_j z_i - \psi_i \overline{\psi}_j$ which implies, in turn, the random phase approximation $\langle \bar{z}_j z_i\rangle_\tau \approx \langle \bar{z}_j\rangle_\tau \langle z_j\rangle_\tau$. The dynamical scenery just depicted together with an ergodic assumption leads thus naturally to defining

$$\Psi \equiv \frac{1}{N_s}\sum_j \langle z_j\rangle_\tau \qquad (6)$$

as the macroscopic order paramenter revealing when order issues from the lattice dynamics.

When our dynamical MFA is applied to Hamiltonian (4), and the further assumption $\psi_j \equiv \psi_i$ for $j \in (i)$ is made (smoothing condition), the kinetic term modifies as follows:

$$\frac{t}{2}\sum_{\langle i,j\rangle}(\bar{z}_i z_j + \bar{z}_j z_i) \to \frac{qt}{2}\sum_i (\bar{z}_i \psi_i + \overline{\psi}_i z_i - |\psi_i|^2), \qquad (7)$$

where q denotes the number of nearest neighbors per site. The resulting Hamiltonian reduces thus to a sum of on-site terms: $\mathcal{H}_{\rm mf} = \sum_j \mathcal{H}_j$, where

$$\mathcal{H}_j = U|z_j|^4 - \mu|z_j|^2 - \frac{qt}{2}(\bar{z}_j \psi_j + \overline{\psi}_j z_j - |\psi_j|^2). \qquad (8)$$

The Hamiltonian equations ensuing from Eq. (8),

$$i\hbar \dot{z}_i = -\mu z_i + 2U z_i |z_i|^2 - \frac{qt}{2}\psi_i, \qquad (9)$$

bear memory of the off-site dynamics only through the on-site term ψ_i. When compared with the exact ones (5), they imply the relation $q\psi_i \approx \sum_{j\in(i)} z_j$ consistently leading to an identity once time average is carried on and the smoothing conditions are used. It is important to notice that $\mathcal{N} = \sum_i |z_i|^2$ is no longer a constant of motion while the mean field Hamiltonian $\mathcal{H}_{\rm mf} = \sum_j \mathcal{H}_j$, that should approximate $\mathcal{H}$, might represent a time-dependent total energy (which $\mathcal{H}$ is not) since it depends on ψ_j's. In order to recover such features, it seems reasonable to introduce some restriction on the form of $\psi_j(\tau)$, whose time behavior, so far, has not been specified at all. We do this looking for solutions of Eqs. (9) where θ_j, χ_j, the phases of $z_j = |z_j|e^{i\theta_j}$, $\psi_j = |\psi_j|e^{i\chi_j}$, respectively, are locked one to the other in such a way that $\Delta\phi \doteq \theta_j - \chi_j = \text{const}$, the constant

being zero or π. In view of Eqs. (9), this entails that any $|z_j|^2$ has a zero time derivative, thereby restoring the particle total number $\mathcal{N}$ to its proper role of time-independent quantity. The same effect is obtained for any $\mathcal{H}_j$, and thus for $\mathcal{H}_{\rm mf}$, only adding the further condition $|\psi_j| = \text{const}$. Solutions of the form $z_j(\tau) = |z_j| e^{i\theta_j(\tau)}$ whose phase, due to Eq. (9), obeys the equation

$$-\hbar |z_j| \dot{\theta}_j = (2U|z_j|^2 - \mu)|z_j| - \frac{qt}{2}|\psi_j|, \qquad (10)$$

successfully fulfill the conditions just stated. Despite the elimination of any residual dynamical complexity, we are able to characterize the MI and some features of the SF phase via the phase dynamics of Eq. (10).

We examine first the dynamics related to the MI. In this case, ψ_i must have a zero time average along macroscopic time scales. Such a behavior occurs when the uniform filling conditions $n_i = n$, for all i (we identify here number operators n_i's with their integer spectral values) is inserted in (10) by setting $|z_i|^2 = n$. Such a substitution is the natural consequence of the requantization process [6] of the actionlike variables $|z_i|^2$ (notice that $\{|z_i|^2, \theta_j\} = \delta_{ij}/\hbar$) strongly requested from the pure quantum character of the MI. Equation (10) is thus solved by $\theta_j(\tau) = \lambda_\pm \tau/\hbar + \alpha_j$ (α_j is the initial condition), where

$$\lambda_\pm \doteq \frac{1}{\sqrt{n}}\left(U\delta\sqrt{n} \pm \frac{qt}{2}|\psi_i|\right), \qquad (11)$$

$\delta = \mu/U - 2n$, and λ_- (λ_+) is related to the choice $\Delta\phi = \pi$ ($\Delta\phi = 0$). Notice that the index j does not label $\lambda_\pm$ since the request $\langle z_j \rangle_\tau \equiv \psi_j(\tau)$ leads to $|\psi_j| = \sqrt{n}$ at each site. In the present theory, the frequencies $\lambda_\pm$ play the role of time correlation length governing the phase transition. Our theory gives $\lambda_\pm = U\sqrt{n}(\mu - \mu_c)$ for fixed t and $\lambda_\pm = q|\psi_i|/2(t - t_c)$ for fixed μ (μ_c and t_c are the critical values of μ and t). Defining the critical exponents z and ν as in the Ref. [2], we argue that [8]

$$z\nu = 1. \qquad (12)$$

By replacing in the reduced Hamiltonian (8) the value of $|\psi_i|$ provided by Eq. (11), the energy of the MI reads

$$E_n(\mu, t; \lambda_\pm) = n\left[U\delta - Un + \frac{2}{qt}(\lambda_\pm + U\delta)^2\right], \qquad (13)$$

where the subscript n reminds us that the filling n is accounted for. The oscillating behavior of $\Psi = (e^{i\lambda_\pm \tau}/N_s)\sum_j \psi_j e^{i\alpha_j}$, having a vanishing long time average, identifies the MI. This, in fact, implies that the gauge symmetry breaking expected in the SF phase cannot take place. Notice that the ordinary (time-independent) MFA cannot describe the MI for $t > 0$, since the hopping term of the reduced Hamiltonian is canceled by the vanishing of the order parameter $\psi = 0$. Within our scheme, instead, the condition $\langle \Psi \rangle_\tau = 0$ can be realized also for $\psi \neq 0$.

All dynamics disappears at the degeneration points $\mu/U = 2n$, $t/U = 0$, that represent the limiting points of the SF domain separating $I(n)$ from $I(n+1)$. Within our theory, the fixed points of the equations of motion ($\lambda_\pm = 0$) correspond to the SF system configurations. This is but the oversimplified version of the low frequency dynamics expected in the SF phase. Considering such configurations (the trivial case $\dot{z}_j = 0$ due to $z_j = \psi_j = 0$ is excluded) allows one to recast Eq. (9) in the form

$$\psi_j = \frac{2}{qt}(2U|z_j|^2 - \mu)z_j, \qquad (14)$$

making ψ_j a function of z_j. The energy associated to the Hamiltonian $\mathcal{H}_j$, in turn, reduces to

$$\epsilon(\mu, t, z_j) = |z_j|^2\left[\frac{2}{qt}(\mu - 2U|z_j|^2)^2 + (\mu - 3U|z_j|^2)\right],$$

once (14) is inserted in (8). $\epsilon(\mu, t, z_j)$ is the on-site energy accounting for the absence of dynamics. The limit $\lambda_\pm \to 0$, in fact, shows that $E_n(\mu, t; \lambda_\pm) \to \epsilon(\mu, t, z_j)$ provided $|z_j|^2 = n$. Its lowest value is found to be, via minimization, $\epsilon(\zeta) = -U|\zeta|^4$, where the value of $|z_j|^2$ corresponding to the minimum is $|\zeta|^2 = (\mu + 2t)/(2U)$. It is worth noticing that inserting $|\zeta|$ in (14) implies $\psi_j = z_j$ so that the minimum energy configuration naturally satisfies the consistency condition on which our dynamical MFA is based.

Let us consider, instead, how the MI characters reflect on the macroscopic phase—viable to experimental observations—S. Notice, first, that inserting Eqs. (5) in the Lagrangian (3) implies $\dot{S} = U\sum_j |z_j|^4$ and that the same result is found in the MFA scheme in that $\psi_j \approx z_j$. Then the exponential factor of $|\Phi\rangle$ has a frequency $\dot{S}$ which reduces to

$$\dot{S} = UN_s n^2, \qquad (15)$$

when the system is a MI with $|z_j|^2 = n$ for each j. A transition leading from the n lobe to the $(n+1)$-lobe thus involves a change of the phase frequency of $UN_s(2n+1)$, whereas in the case of a transition between any two superfluid states, where $\dot{S}_{\rm mf} = UN_s|\Psi|^4$, since $z_j = \Psi$ for each j, no quantization of the frequency variation appears, in that Ψ takes continuous values.

Now, we employ the expression (13) for the on-site energy to reconstruct the lobelike structure of the phase diagram. In the SF phase, the states with n and $n+1$ (adding a particle), as well as the states with $n-1$ and n (adding a hole) must be degenerate. The curves representing the n-lobe boundary are identified by implementing both gauge symmetry breaking through the limits $\lambda_\pm \to 0$ and vanishing of the energy gaps $E_n - E_{n\pm1}$. In other words, we require

$$\lim_{\lambda_+ \to 0}(E_n - E_{n+1}) = 0 \qquad (\delta < 0), \qquad (16)$$

$$\lim_{\lambda_- \to 0}(E_{n-1} - E_n) = 0 \qquad (\delta > 0). \qquad (17)$$

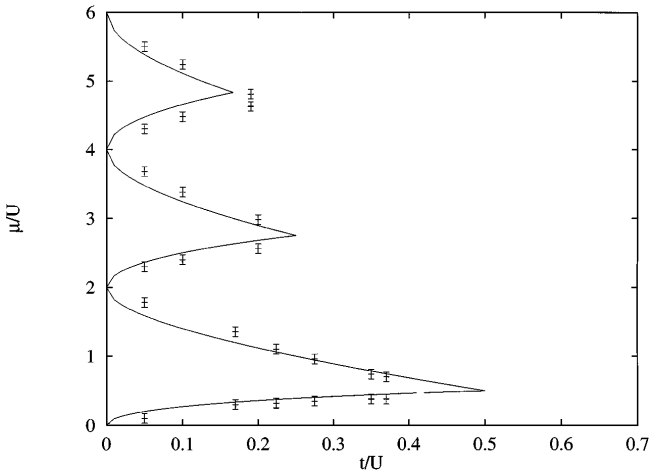

FIG. 1. The phase diagram of the BHM for $D = 1$. The error boxes are the QMC results of Batrouni *et al.* Relatively to the first lobe ($n_i = 1$), $(t_c/U) = 0.5$. QMC gives $(t_c/U) = 0.43 \pm 0.002$ and the SCPE $(t_c/U) = 0.43$. For ($n_i = 3$), QMC and SCPE give $(t_c/U) = 0.2$ and $(t_c/U) = 0.18$, respectively. Our theory gives $(t_c/U) = 0.16$.

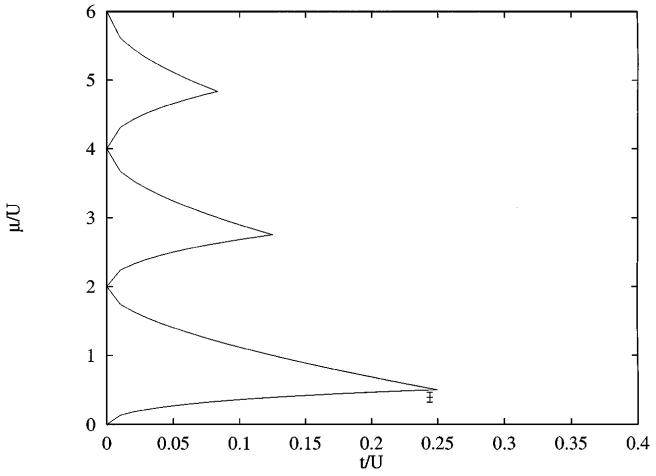

FIG. 2. The phase diagram of the BHM for $D = 2$. The error box indicates the QMC tricritical point obtained by Krauth and Trivedi [5]. For $n_i = 1$, $(t_c/U) = 0.25$ while QMC gives $(t_c/U) = 0.244 \pm 0.002$ and SCPE provides $(t_c/U) = 0.272$.

For solving Eqs. (16) and (17) we introduce the variables $\delta_\pm = \mu/U - 2n + (1 \pm 1)$. By inserting $\delta_+ \geq 0$ [$\delta_- \leq 0$] in Eq. (16) [(17)], and defining $r = qt/4U$, one gets the quadratic equations $\delta_\pm^2 + 2r\delta_\pm - 2r(2n \mp 1) = 0$ providing the curves

$$\frac{\mu_\pm}{U} = 2[n - (1 \pm 1)] - r \pm [r^2 + 2r(2n \mp 1)]^{1/2}. \tag{18}$$

The lower branch $\mu_+(t)$ and the upper $\mu_-(t)$ constitute the boundary encircling the nth lobe. We conclude by retrieving from Eq. (18) the position of the farthest point on the n-lobe boundary from the μ axis. By setting $\mu_-(t) = \mu_+(t)$ one finds the lobe tip coordinates

$$t_c = U/qn \tag{19}$$

and $\mu(t_c)/U = 2n - 1 - (1/2n)$. In the captions of Figs. 1 and 2 the values of t_c furnished by the present approach are compared for the $D = 1$ and $D = 2$ cases with QMC [5] and the strong coupling perturbative expansion (SCPE) [4].

The dynamical approach we have developed appears to succeed in describing the quantum MI-SF phase transition of BHM. The resulting phase diagram indeed exhibits an excellent agreement with QMC simulations and SCPE results. This suggests that Eqs. (5), here faced solely within the dynamical MFA, deserve a systematic investigation by the methods of dynamical system theory. The dynamics they account for, in fact, should describe not only zero temperature configurations but also excited states involving density waves as well as vortices. Moreover, a systematic analysis of Eqs. (5) should be interesting both in relation to the dynamical scaling theory [9] and for calculating the dynamical correlation functions in the MI. Work is in progress along these lines.

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