Semiclassical quantization of an N-particle Bose-Hubbard model

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We derive a semiclassical approximation for an N-particle, two-mode Bose-Hubbard system modeling a Bose-Einstein condensate in double-well potential. This semiclassical description is based on the ‘classical’ dynamics of the mean-field Gross-Pitaevskii equation and is expected to be valid for large N. We demonstrate the possibility to reconstruct the quantum properties of the N-particle system from the mean-field dynamics. For example, the resulting WKB-type eigenvalues and eigenstates are found to be in very good agreement with the exact ones, even for small values of N, both in the subcritical and supercritical regime.

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Even for weakly interacting particles, a full many-particle treatment of Bose-Einstein condensates (BEC) is only possible for a small number N of particles. Most often a mean-field approximation is used, which describes the system quite well for large N at low temperature. In this mean-field approach, the bosonic field operators are replaced by c-numbers, the condensate wavefunctions. This constitutes a classicalization and therefore the result of the mean-field approximation, the Gross-Pitaevskii equation (GPE), is often denoted as ‘classical’, despite of the fact that the GPE is manifestly quantum, i.e. it reduces to the usual linear Schrödinger equation for vanishing interparticle interaction. In a two-mode approximation, a (possibly asymmetric) double well BEC can be described by a Bose-Hubbard model related to a classical non-rigid pendulum in the mean-field approximation (see, e.g., [1] and references therein).

In a number of recent papers, consequences of the classical nature of the mean-field approximation are discussed and semiclassical aspects are introduced. For a two-mode Bose-Hubbard model, Anglin and Vardi [2] consider equations of motion which go beyond the standard mean-field theory by including higher terms in the Heisenberg equations of motion. The classical-quantum correspondence has been studied in terms of phase space (Husimi) distributions [1] for such systems. Mossmann and Jung [3] demonstrate for a three-mode Bose-Hubbard model that the organization of the N-particle eigenstates follows the underlying classical, i.e. mean-field, dynamics. A generalized Landau-Zener formula for the mean-field description of interacting BEC in a two-mode system has been derived by studying the many particle system [4]. In [5] the commutability between the classical and the adiabatic limit for the same system is studied and first steps towards a semiclassical treatment of the problem are reported.

The purpose of the present paper is to show that the mean-field model is not only capable to approximate the interacting N-particle system in the limit of large N and to allow for an interpretation of the organization of the N-particle eigenvalues and eigenstates, but can also be used to reconstruct approximately the individual eigenstates in a semiclassical WKB-type manner with astounding accuracy even for a small number of particles. This will be demonstrated for N bosonic particles in a two-mode system, a many-particle Bose-Hubbard Hamiltonian, describing for example the low-energy dynamics in a double-well potential:

\[ \hat{H} = \varepsilon (\hat{n}_1 - \hat{n}_2) + v (\hat{a}_1^\dagger \hat{a}_2 + \hat{a}_2^\dagger \hat{a}_1) + g (\hat{n}_1^2 + \hat{n}_2^2) . \] (1)

Here \( \hat{a}_j, \hat{a}_j^\dagger \) are bosonic particle annihilation and creation operators for modes \( j \) and \( \hat{n}_j = \hat{a}_j^\dagger \hat{a}_j \) are the mode number operators. The mode energies are \( \pm \varepsilon \), \( v \) is the coupling constant and \( g \) is the strength of the onsite interaction. In order to simplify the discussion, we assume here that \( v \) is positive and \( g \) is negative. The Hamiltonian (1) commutes with the total number operator \( \hat{N} = \hat{n}_1 + \hat{n}_2 \) and the number \( N \) of particles, the eigenvalue of \( \hat{N} \), is conserved. For a given \( N \), we then have \( N+1 \) eigenvalues of the Hamiltonian (1).

The celebrated mean-field description can be most easily formulated as a replacement of operators by c-numbers \( \hat{a}_j \to \psi_j, \hat{a}_j^\dagger \to \psi_j^\ast \). Since the fact that the c-numbers commute in contrast to the quantum mechanical operators introduces ambiguities in the transition quantum \( \to \) classical and vice versa, one has to replace symmetrized products of the operators by the corresponding products of c-numbers. Therefore in the following we will start on the \( N \)-particle side with a symmetrized Bose-Hubbard Hamiltonian, where the \( \hat{n}_j \) are replaced by \( \hat{n}_j^\ast = (\hat{a}_j^\dagger \hat{a}_j + \hat{a}_j \hat{a}_j^\dagger)/2 \) (see also [3]). This symmetrization effects only the nonlinear term in (1) and the symmetrized \( \hat{H} \) is related to (1) by an additive constant term depending only on \( \hat{N} \). Note that thus the number operator \( \hat{N} = \hat{n}_1 + \hat{n}_2 = \hat{n}_1^\ast + \hat{n}_2^\ast - 1 \) is replaced by \( |\psi_1|^2 + |\psi_2|^2 - 1 \) and therefore the mean-field wavefunction is normalized as \( |\psi_1|^2 + |\psi_2|^2 = N + 1 \).

The mean-field time evolution is given by the two level
nonlinear Schrödinger equation, resp. GPE,

$$i\hbar \frac{d}{dt} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} \varepsilon + 2g|\psi_1|^2 & v \\ v & -\varepsilon - 2g|\psi_2|^2 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}, \quad (2)$$

where $\psi_1$ and $\psi_2$ are the amplitudes of the two condensate modes.

Like every Schrödinger equation, linear or nonlinear, the mean-field dynamics has a canonical structure of classical dynamics: The time dependence of the complex valued amplitudes can be written as canonical equations of motion with a Hamiltonian function $H$. The conservation of the particle number introduces an additional symmetry to the system which allows a reduction of the dynamics to an effectively one-dimensional Hamiltonian evolution by an amplitude-phase decomposition $\psi_j = \sqrt{n_j} + 1/2 e^{i\phi}$ in terms of the canonical coordinate $q_j = (q_1 - q_2)/2$, an angle, and the (angular) momentum $p = (n_1 - n_2)\hbar$, with Hamiltonian

$$H(p, q) = \frac{p^2}{2} + v \sqrt{N_s^2 - \frac{p^2}{h^2} \cos(2q)} + \frac{g}{2} \left( N_s^2 + \frac{p^2}{h^2} \right), \quad (3)$$

where $N_s = N + 1$ is the number of states. This describes the classical dynamics of a non-rigid pendulum where the phase space is a finite, $-N_s \hbar \leq p \leq N_s \hbar$, $0 \leq q \leq \pi$, if the lines $q = 0$ and $q = \pi$ are identified.

One of the prominent features of the two-mode system is the self-trapping effect [6]. A careful discussion of this effect, the relation between mean-field and $N$-particle behavior as well as its control by external driving fields can be found in [7].

The self-trapping transition is connected to a bifurcation of the stationary states, the fixed points of the Hamiltonian (3), in the mean-field approximation: In the subcritical regime one has a maximum, $E^+$, at $g = 0$ and a minimum, $E^-$, at $g = \pi/2$. In the supercritical regime the minimum bifurcates into two minima, $E_{\pm}$, and a saddle point, $E_{\text{saddle}} > E_{\pm}$. In phase space, the regions with oscillations around one of the two minima are separated by a separatrix passing through the saddle point. The period of the separatrix motion is infinite. Figure 1 shows phase space portraits of $H(p, q)$ for sub- and supercritical particle interaction. The stationary mean-field energies $H = E_{\pm}$ are related to the nonlinear eigenvalues, the chemical potentials $\mu$, by $\mu N_s = H + \frac{g}{2} (N_s^2 + p^2/h^2)$.

The multi-particle eigenvalues $E_n$ shown in Fig. 2 as a function of $\varepsilon$ form a net of avoided crossings clearly organized by a skeleton provided by the stationary mean-field energies, as reported before by several authors [8]. The $E_n$ are bounded by the maximum and minimum mean-field energies, and we observe a transition to a swallowtail structure in the supercritical regime. Here the mean-field energy $E_{\text{saddle}}^{-}$ forms a caustic of the multi-particle eigenvalue curves in the limit $N \rightarrow \infty$. To illustrate this issue, one can calculate the level density $\rho(E)$ (normalized to unity) as a function of the energy [9]. First we note that $\rho(E)$ approaches a smooth curve in the limit $N = 1500$ particles and different values of $\varepsilon$. The mean-field swallowtail curve between the cusps manifests itself as a peak in the density of the many particle energies. In

![Figure 1](image1.png) FIG. 1: (Color online) Phase space portrait of the mean-field Hamiltonian $H(p, q)$ in (3) for $v = 1$ and $\varepsilon = -0.5$ in the subcritical ($g = -1/N_s$) and supercritical ($g = -3/N_s$) regime for $N=10$.

![Figure 2](image2.png) FIG. 2: (Color online) Many particle energies $E_n$ and mean-field eigenvalues $H_n$ (red) as a function of the onsite energy $\varepsilon$ in the subcritical ($g = -0.5/N_s$, left) and supercritical regime ($g = -3/N_s$, right) for $v = 1$ and $N = 10$ particles.
the limit $N \to \infty$, this peak develops into a singularity. At the positions of the other mean-field eigenvalues one observes finite steps.

In the following, we will focus on the question to which extent the many particle information can be extracted from the mean-field system by an inversion of this ‘classical’ approximation in a WKB-type manner.

The most important ingredient of a semiclassical quantization is the action $S(E)$, i.e. the phase space area enclosed by the directed curve $\mathcal{H}(p, q) = E$. The action $S(E)$ increases with $E$ from zero at the minimum energy of $\mathcal{H}(p, q)$ to $2\pi\hbar$, the total available phase space area, at the maximum energy of $\mathcal{H}(p, q)$.

For the generalized pendulum Hamiltonian (3), one can express the position variable $q$ uniquely as a function of $p$ and $E$ and write down the action in momentum space in the form $S(E) = \int q(p, E) \, dp$. It is convenient [10, 11] to introduce the two ‘potentials’ $U_-(p) = \mathcal{H}(p, 0)$ and $U_+(p) = \mathcal{H}(p, \pi/2)$, which join smoothly at $p = \pm \hbar N_e$ and act as a classical potential for the variable $p$. The classically allowed energy region is given by $U_-(p) \leq E \leq U_+(p)$ as illustrated in Fig. 4 in the sub- and supercritical regimes. For a given energy $E$ the classical turning points $p_{\pm}$ (with $p_- \leq p_+$) are determined by $U_+(p_{\pm}) = E$ or $U_-(p_{\pm}) = E$. One has to distinguish three basic types of motion and, with $S = \int_{p_-}^{p_+} q(p, E) \, dp$, we find

(a) Orbits encircling a minimum of $\mathcal{H}(p, q)$. The classical turning points both lie on $U_-$ and we have $S(E) = 2S$. (b) Orbits encircling a maximum of $\mathcal{H}(p, q)$. The classical turning points both lie on $U_+$ and we have $S(E) = 2S + \pi(2N + 1h + p_- - p_+)$. (c) Rotor orbits extending over all angles $q$. We can find $p_-$ on $U_-$ and $p_+$ on $U_-$ with $S(E) = 2S + \pi(N + 1h - p_-)$ or $p_-$ on $U_-$ and $p_+$ on $U_+$ with $S(E) = 2S + \pi(N + 1h - p_+)$. In the case of a single classically accessible region, the semiclassical quantization condition is given by

$$S(E) = h(n + \frac{1}{2}), \quad n = 0, 1, \ldots, N. \quad (4)$$

A numerical solution of (4) determines the semiclassical energies $E_n$, $n = 0, \ldots, N$, where the total available phase space area, $0 \leq S(E) \leq hN_e$, restricts the number of semiclassical eigenvalues to $N_e$, exactly as the quantum ones.

In the linear case, $g = 0$, the action $S(E)$ is a linear function of the energy $E$, and the the semiclassical eigenvalues agree with the exact ones. This can be easily understood by recognizing that in this case the Hamiltonian (1) describes nothing but a system of two coupled harmonic oscillators, which can be transformed to two uncoupled ones by introducing normal-coordinates.

In the supercritical regime, the energy surface has two minima, hence the potential function $U_-(p)$ has two minima as well, separated by a potential barrier. In this case one has to distinguish different regions of the energy. For energies below the upper minimum (region I in Fig. 4) the quantization can be carried out like in the subcritical case by equation (4). For energies between the upper minimum and the barrier $E_{\text{barr}}$ (regions II in Fig. 4), there are four real turning points $p_-^{(1)} < p_+^{(1)} < p_-^{(r)} < p_+^{(r)}$. In this case one has to consider tunneling through the barrier. The semiclassical quantization condition can be achieved by a more elaborate expression [12] (see also [13]):

$$\sqrt{1 + \kappa^2} \cos(S_l + S_r - S_0) = -\kappa \cos(S_r - S_l + S_0) \quad (5)$$

where $S_l$ and $S_r$ are half the actions in the left resp. right region in Fig. 4 (note that also here one has to distinguish
the different cases (a) and (c)). The term
\[
\kappa = e^{-\pi S_\epsilon}, \quad S_\epsilon = -\frac{1}{\pi} \int_{p_+^{(r)}}^{p_+^{(i)}} |q(p, E)| \, dp
\]
accounts for tunneling through the barrier,
\[
S_\phi = \arg \Gamma(z + iS_\epsilon) - S_\epsilon \log |S_\epsilon| + S_\epsilon
\]
is a phase correction, and $S_\phi = 0$ below the barrier. Deep below the barrier, tunneling can be neglected and the semiclassical single well quantization is recovered (see also [5]).

Above the barrier, the inner turning points $p_+^{(i)}$, $p_-^{(i)}$ turn into a complex conjugate pair and different continuations of the semiclassical quantization have been suggested [12, 13]. Following [12] we replace these turning points by the momentum at the barrier $p_{\text{barr}}$ in the formulas for $S_{l,r}$, modify the tunneling integral $S_\epsilon$ as
\[
S_\epsilon = \frac{1}{4\pi} \int_{p_+^{(r)}}^{p_+^{(i)}} q(p, E) \, dp
\]
and introduce a non-vanishing action integral
\[
S_\theta = \int_{p_+^{(i)}}^{p_{\text{barr}}} q(p, E) \, dp + \int_{p_-^{(r)}}^{p_{\text{barr}}} q(p, E) \, dp.
\]
The combined semiclassical approximation is continuous if the energy varies across the barrier (from region II to III in Fig. 4) and continuously approaches the simple version with only two turning points $p_+^{(i)}$ and $p_-^{(i)}$ in region III high above the barrier.

Figure 5 shows the semiclassical many particle energy eigenvalues in dependence on the parameter $\epsilon$ in the supercritical regime for $N = 10$ particles. One observes an almost precise agreement with the exact eigenvalues shown in Fig. 2, even for such a small number of particles. A similar agreement is found in the subcritical regime where the structure and the semiclassical quantization condition (4) is much simpler. In particular the level distances at the avoided crossings are reproduced and allow furthermore a direct semiclassical evaluation. With increasing particle number $N$ the semiclassical deviation from the quantum eigenvalues decreases. Note that even for $N = 1$ the error is only 1%. Now it should be obvious that the quantum level densities shown in Fig. 3 for a large value of $\epsilon$ is directly related to the classical period $T$ of motion by $dS/dE = T$. The height of the steps in the density plots are simply given by the period of harmonic oscillation in the vicinity of the extremum and the singularity corresponds to the separatrix motion.

For the two-mode Bose-Hubbard system considered here, the classical description provided by the mean-field model has one degree of freedom and it is therefore integrable. For three and more modes, the classical dynamics is chaotic (see, e.g., the studies of the three-mode system [3, 14] or tilted optical lattices [15]). Chaoticity also appears in periodically driven two-mode systems [7] or the related kicked tops [11]. A semiclassical description of the quasienergy spectrum in these cases is a challenge for future studies.