

## Semiclassical Quantization of the Bogoliubov Spectrum

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We analyze the Bogoliubov spectrum of the three-site Bose-Hubbard model with a finite number of Bose particles by using a semiclassical approach. The Bogoliubov spectrum is shown to be associated with the low-energy regular component of the classical Hubbard model. We identify the full set of the integrals of motion of this regular component and, quantizing them, obtain the energy levels of the quantum system. The critical values of the energy, above which the regular Bogoliubov spectrum evolves into a chaotic spectrum, is indicated as well.

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Recent experiments with cold bosonic atoms in optical lattices [1] has renewed the theoretical studies of the Bose-Hubbard model (BH model), which constitutes one of the fundamental Hamiltonians in the condensed matter theory. The number of phenomena, discussed in the frame of this model, is so diverse that sometimes it is difficult to see any link between them. In particular, this concerns the phenomena of superfluidity and quantum chaos. Indeed, the former phenomenon assumes the regular phononlike excitation spectrum, described by the Bogoliubov theory [2,3], while the latter phenomenon implies a highly irregular excitation spectrum, described by the random matrix theory [4–7]. This seeming contradiction is resolved by noting that these two spectra refer to different characteristic energies of the system. It is the aim of the present work to understand of how the regular Bogoliubov spectrum (BS) of the BH model evolves into an irregular one as the system energy is increased.

First, we recall the essentials of the BS. Having in mind Bose atoms in the 1D optical lattice, the Bose-Hubbard Hamiltonian reads

$$\hat{H} = -\frac{T}{2} \sum_{l=1}^L (\hat{a}_{l+1}^\dagger \hat{a}_l + \text{H.c.}) + \frac{U}{2} \sum_{l=1}^L \hat{n}_l (\hat{n}_l - 1), \quad (1)$$

where the first term in the right-hand side of (1), with  $T$  being the hopping matrix element, describes the tunneling of the atoms between different lattice sites, and the second term, with  $U$  being the microscopic interaction constant, takes into account the short-range interactions between the neutral atoms. The BS describes the low-energy excitations of the system (1), and there are at least two different methods to derive this spectrum: The first method is traced back to the original works by Landau and Bogoliubov and involves the famous Bogoliubov-de Gennes transformation [3]; the second approach uses the Leggett ansatz for wave functions, followed by analytic diagonalization of a 3-diagonal semi-infinite matrix [7]. Common features of the methods are that (i) the starting point of the analysis is the Hamiltonian of the BH model in the Bloch basis

$$\begin{aligned} \hat{H} = & -T \sum_k \cos\left(\frac{2\pi k}{L}\right) \hat{b}_k^\dagger \hat{b}_k \\ & + \frac{U}{2L} \sum_{k_1, k_2, k_3, k_4} \hat{b}_{k_1}^\dagger \hat{b}_{k_2}^\dagger \hat{b}_{k_3} \hat{b}_{k_4} \tilde{\delta}(k_1 + k_2 - k_3 - k_4) \end{aligned} \quad (2)$$

[which one obtains from (1) by using the canonical transformation  $\hat{b}_k = (1/\sqrt{L}) \sum_l \exp(i2\pi kl/L) \hat{a}_l$ ], and (ii) both methods assume the limit  $N \rightarrow \infty$ ,  $U \rightarrow 0$ ,  $g = UN/L = \text{const}$ , where  $g$  is the so-called microscopic interaction constant. After taking this limit, the spectrum of the system (2) is given by the direct sum of  $L$  linear spectra

$$E_m^{(k)} = E_0^{(k)} + \Omega^{(k)} m, \quad (3)$$

with  $\Omega^{(k)} = \sqrt{2g\delta_k + \delta_k^2}$  and  $\delta_k = T[1 - \cos(2\pi k/L)]$ . Let us also note that, since  $\Omega^{(-k)} = \Omega^{(k)}$ , it is convenient to restrict the index  $k$  in Eq. (3) to strictly positive values. Then the energy levels of every single spectrum (3) are  $(m+1)$ -fold degenerate. In what follows, we shall label the degenerate sublevels of the given Bogoliubov level by the index  $j$ .

We stress that the above result is valid only in the limit  $N = \infty$  and that for any finite  $N$  the BS (3) provides only an approximation to the low-energy spectrum of the BH model. Having in mind cold atoms in optical lattices, it is a problem of fundamental interest to find the finite- $N$  corrections to the BS. Indeed, in contemporary laboratory experiments with optical lattices, the number of atoms rarely exceeds  $N = 10^5$ , and it is not clear in advance how strong the finite- $N$  effects could be. In what follows, we analyze this problem by considering the simplest non-trivial case of the three-site BH model. For the three-site BH model, there is only one value for the single-particle excitation energy  $\delta = T[1 - \cos(2\pi/3)] = 3T/2$ , and, hence, the index  $k$  in Eq. (3) can be omitted. It is also worth noting that the three-site BH system has been intensively studied during the past decade with respect to the phenomenon of self-trapping in the system of coupled nonlinear equations [8,9], generalization of the dynamical

regimes of the celebrated two-site BH system [10,11], and as a model for multiparticle quantum chaos [4,6]. In the present work we use the three-site BH system as a model for studying the BS of the interacting Bose particles in a lattice.

To get answers to questions posed in the introductory part of the Letter, we employ the ‘‘semiclassical’’ method, where  $1/N$  plays the role of the effective Planck’s constant. This method explicitly refers to the classical dynamics of the BH system and provides in this way a deeper insight in the structure of its quantal spectrum. In particular, we show below that (i) the finite- $N$  BS is not linear, (ii) the Bogoliubov levels are split with respect to the second quantum number  $j$ , and (iii) that this splitting finally results in the transition from a regular to an irregular (chaotic) spectrum at higher energies. As an illustration to these statements and for the purpose of future references, Fig. 1 shows the energy spectrum of the three-site BH model for  $N = 40$  and  $0 \leq g \leq 4$ . All of the mentioned effects, which we shall quantify in the rest of the Letter, are clearly seen in the figure.

As an intermediate step, let us derive the BS (3) of the three-site BH model by using semiclassical arguments. The classical counterpart of the Hamiltonian (2) is obtained by

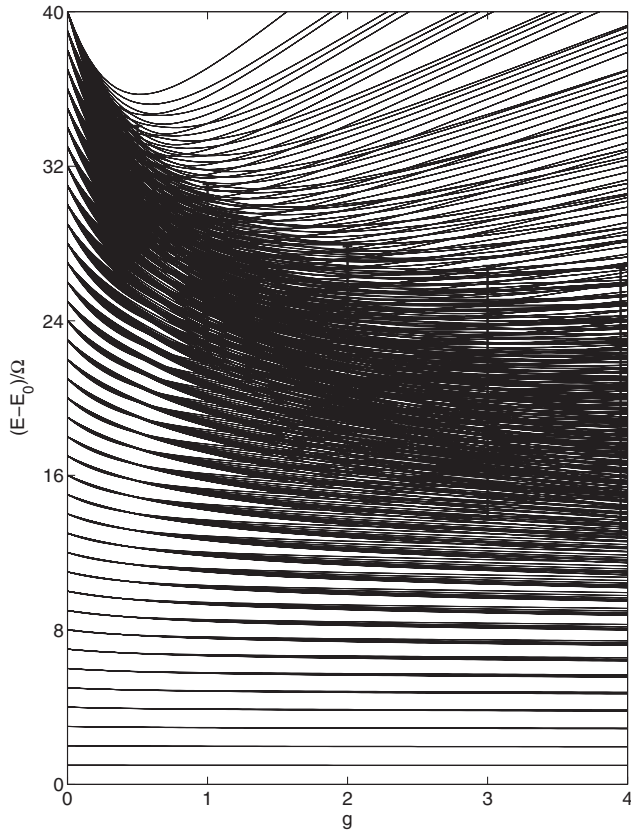


FIG. 1. Energy spectrum of the three-site BH model for  $N = 40$ . The energy is measured with respect to the ground energy  $E_0$  and scaled with respect to the Bogoliubov frequency  $\Omega = \Omega(g)$ . Error bars indicate the energy intervals, where the classical counterpart of the system shows chaotic dynamics.

scaling it with respect to the total number of particles  $\hat{H}/N \rightarrow H$ ,  $E/N = \tilde{E}$  and identifying the operators  $\hat{b}_k^\dagger/\sqrt{N}$  and  $\hat{b}_k/\sqrt{N}$  with pairs of canonically conjugated variables  $(b_k^*, b_k)$ , where  $k = -1, 0, 1$ . Next, we switch to the action-angle variable  $b_k = \sqrt{I_k} \exp(i\theta_k)$  and explicitly take into account that  $\sum_k I_k = 1$  is an integral of motion. This reduces our system of 3 degrees of freedom to a system of 2 degrees of freedom:

$$H = (\delta + g)(I_{-1} + I_{+1}) + 2gI_0\sqrt{I_{-1}I_{+1}} \cos(\theta_{-1} + \theta_{+1}) - g(I_{-1}I_{+1} + I_{-1}^2 + I_{+1}^2) + 2g\sum_{\pm} I_{\pm}\sqrt{I_0I_{\pm1}} \cos(2\theta_{\pm1} - \theta_{\pm1}), \quad (4)$$

where  $I_0 = 1 - I_{-1} - I_{+1}$  and the phases  $\theta_{\pm1}$  of variables  $b_{\pm1}(t)$  are measured with respect to the phase of  $b_0(t)$ . The low-energy dynamics of the system (4), which is associated with the low-energy spectrum of the system (1), implies  $I_{\pm1} \ll I_0$ . Keeping in the Hamiltonian (4) only the terms linear on  $I_{\pm1}$ , and using one more canonical transformation,

$$I = I_{+1} + I_{-1}, \quad \theta = (\theta_{+1} + \theta_{-1})/2, \\ J = (I_{+1} - I_{-1})/2, \quad \vartheta = \theta_{+1} - \theta_{-1}, \quad (5)$$

we have

$$H_{\text{eff}} = (\delta + g)I + g\sqrt{I^2 - 4J^2} \cos(2\theta). \quad (6)$$

Note that  $H_{\text{eff}}$  does not include phase  $\vartheta$ , and, hence, the action  $J$  is an integral of motion. Finally, we integrate the system (6) by introducing a new action  $\tilde{I} = (1/2\pi) \times \oint I(\theta, \tilde{E}) d\theta$  and resolving this equation with respect to the energy. This gives  $\tilde{E} = \Omega\tilde{I}$ , where, as before,  $\Omega = \sqrt{2g\delta + \delta^2}$  is the Bogoliubov frequency. Note that the energy is independent of the action  $J$ , which may be chosen arbitrary in the interval  $|J| \leq \tilde{I}/2$ . Referring to the original quantum problem, this action  $J$  obviously labels the degenerate sublevels of the excited Bogoliubov states. Indeed, the semiclassical quantization corresponds to  $\tilde{I} = m/N$ ,  $m = 0, 1, \dots$ , and  $J = j/N$ ,  $j = -m/2, -m/2 + 1, \dots, m/2$ . Thus, the energy spectrum is given by  $E_m = \Omega m$  with  $(m + 1)$ -fold degeneracy of every level.

Now we are prepared to discuss the finite- $N$  corrections to the BS. Let us analyze the dynamics of the classical system (4) in more detail, without assuming  $I_{\pm1} \ll I_0$ . First, we shall consider the symmetric solutions, where  $b_{-1}(t) = b_{+1}(t)$ . Expressing the Hamiltonian (4) in terms of the canonical variables (5) and setting there  $\vartheta = 0$  and  $J = 0$ , we have

$$H_{1D} = (\delta + g)I + g(1 - I)I \cos(2\theta) - 3gI^2/4 + gI\sqrt{2(1 - I)I} \cos(\theta). \quad (7)$$

The phase portrait of the 1D system (7) is depicted in Fig. 2(a). Our particular interest in this phase portrait is the trajectories near the origin  $I = 0$ , which can be asso-

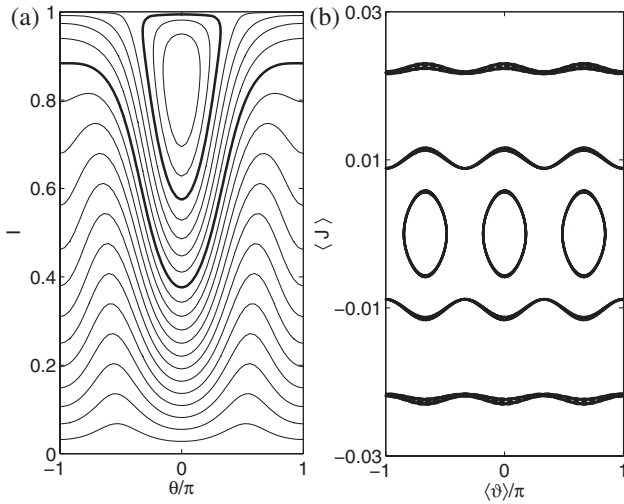


FIG. 2. (a) Phase portrait of the 1D system (7) for  $g = 1$ . The bold lines restrict the chaotic region, where the trajectories are unstable with respect to variation of  $(J, \vartheta)$ . (b) Slow dynamics of the variables  $\tilde{J} = \langle J \rangle$  and  $\tilde{\vartheta} = \langle \vartheta \rangle$  for  $g = 1$  and  $\tilde{I} = 0.133$ .

ciated with the Bogoliubov states. It is seen in the figure that these trajectories are strongly affected by the elliptic point in the upper part of the phase space. As a consequence, the eigenfrequency of the system depends on the action  $\tilde{I}$ . Namely,  $\tilde{\Omega} = \tilde{\Omega}(\tilde{I})$  vanishes for the separatrix action  $\tilde{I}^*$ , and for  $\tilde{I} \ll \tilde{I}^*$ , one has  $\tilde{\Omega}(\tilde{I}) = \Omega - \gamma\tilde{I}$ , where the nonlinearity  $\gamma$  is a unique function of  $g$ . (For instance, for  $g = 0.1, 1$ , and  $4$ , we have  $\gamma/\Omega = 0.1, 0.6$ , and  $1$ , respectively.) Referring to the original quantum problem, this result means that the energy difference between the  $(m + 1)$ th and  $m$ th Bogoliubov levels decreases as  $\gamma m/N$ .

Next, we address the “stability” of the symmetry plane trajectories depicted in Fig. 2(a) with respect to variation of  $J$ . Within the Bogoliubov approximation, the action  $J$  is an integral of motion and may be chosen arbitrary in the interval  $|J| \leq \tilde{I}/2$ . It should be understood, however, that in reality the action  $J$  does depend on time. An example of this dependence is given in Fig. 3. It is seen that the time evolution of the system is a superposition of fast dynamics, where  $J(t)$  and  $\vartheta(t)$  oscillate with the Bogoliubov frequency (more precisely, with the frequency  $\tilde{\Omega}$ ), and slow dynamics, with the characteristic frequency of the orders of magnitude smaller than the Bogoliubov frequency. Going ahead, we note that this new frequency defines the splitting of the Bogoliubov levels in Fig. 1, and for the moment we stress only that the system dynamics remains regular. This conclusion holds for any trajectory of the effective 1D system (7), providing the condition that a trajectory lies well below the separatrix. If we choose a trajectory closer to the separatrix, we observe a transition from regular to chaotic dynamics. We identify the border of the transition to chaos by calculating the Poincaré cross section of (4) for different values of the energy  $\tilde{E}$  and evaluating the volume of the chaotic component as the function of energy [12]. It is found that the chaotic region is restricted to a relatively

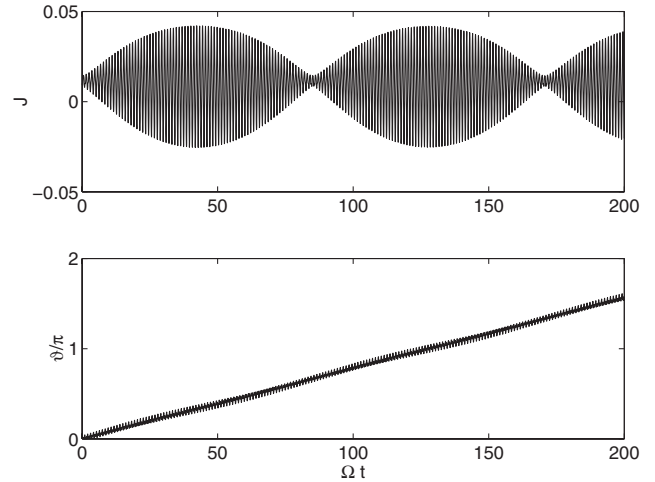


FIG. 3. An example of time evolution of the conjugated variables  $J(t)$  and  $\vartheta(t)$  in the regular regime. Parameters correspond to the second from top trajectory in Fig. 2(a).

narrow energy interval  $\tilde{E}_{\min}(g) \leq \tilde{E} \leq \tilde{E}_{\max}(g)$ . For  $g = 1$ , the phase trajectories of the system (7), corresponding to  $\tilde{E}_{\min}$  and  $\tilde{E}_{\max}$ , are marked by the bold lines in Fig. 2(a). Additionally, the error bars in Fig. 1 indicate the chaotic energy intervals for different values of  $g$ . The depicted borders are consistent with the visual analysis of the spectrum and suggest the following simple criteria of the transition to chaos: It takes place when the total splitting of the Bogoliubov levels with respect to the second quantum number  $j$  exceeds the mean distance  $\tilde{\Omega}$  between the levels.

To complete the visual analysis of the spectrum, we also mention its upper regular part, which is associated with the central stability island in Fig. 2(a). In principle, using as the starting point the classical counterpart of the Hamiltonian (1) [i.e., considering the three-site BH model as a system of three coupled nonlinear oscillators], one can estimate the upper border of chaos  $\tilde{E}_{\max}(g)$  analytically. In the present work, however, we are interested only in the lower border  $\tilde{E}_{\min}(g)$ .

The question on the sublevels splitting is in turn. As it was already mentioned, this splitting is defined by the slow dynamics of the system. To address this slow dynamics, we introduce the new variables  $\tilde{J} = (1/2\pi) \oint J d\tilde{\theta}$  and  $\tilde{\vartheta} = (1/2\pi) \oint \vartheta d\tilde{\theta}$ , where  $\tilde{\theta} = \tilde{\Omega}t$  is the phase conjugated to the action  $\tilde{I}$ . (Note that the action  $\tilde{I}$  is an adiabatic integral of motion and, hence, does not depend on time.) The Hamiltonian equations of the motion for the variables  $\tilde{J}$  and  $\tilde{\vartheta}$  read

$$\begin{aligned} \dot{\tilde{\vartheta}} &= \langle \partial H / \partial \vartheta \rangle \approx -2g\tilde{J}, \\ \dot{\tilde{J}} &= -\langle \partial H / \partial J \rangle \approx 6gV(g, \tilde{I}) \sin(3\tilde{\vartheta}/2), \end{aligned} \quad (8)$$

where  $V(g, \tilde{I}) \approx \langle (I/2)^{3/2} \cos \theta \rangle$  and  $\langle \cdots \rangle$  means time average over one period of the fast dynamics. Thus, the slow dynamics is defined by the pendulumlike Hamiltonian:

$$H_{\text{slow}} = -g\tilde{J}^2 + 4gV(g, \tilde{I}) \cos(3\tilde{\vartheta}/2). \quad (9)$$

It is worth noting that, to obtain (9), we have assumed the quantity  $V(g, \tilde{I})$  to be independent of  $\tilde{J}$ , which can be justified only for  $\tilde{J} \ll \tilde{I}/2$ . Nevertheless, the Hamiltonian (9) is found to capture well the main features of the low-energy regular dynamics for arbitrary  $\tilde{J}$ . In particular, it correctly predicts the existence of stable points at  $\tilde{\vartheta} = 0, \pm 4\pi/3$ , where the phases of  $b_{\pm 1}(t)$  are locked to 0 and 120 degrees with respect to each other [see Fig. 2(b)]. The size of the stability islands around these fixed points is obviously given by the separatrix trajectory of the pendulum, i.e., is proportional to  $|V(g, \tilde{I})|^{1/2}$ .

It is instructive to consider the limiting case  $g \rightarrow 0$ . As is easy to show, in this limit  $V(g, \tilde{I}) \rightarrow 0$  and, hence,  $H_{\text{slow}} \rightarrow -g\tilde{J}^2$ . Let us prove that these results correspond to the first-order quantum perturbation theory on  $U$ . Indeed, calculating the first-order corrections to the energies of the quasimomentum Fork states  $|\Psi_{m,j}\rangle = |m/2 - j, N - m, m/2 + j\rangle$ , we have  $\Delta E = (U/2L) \times \langle \Psi_{m,j} | \sum \hat{b}_{k_1}^\dagger \hat{b}_{k_2}^\dagger \hat{b}_{k_3} \hat{b}_{k_4} \tilde{\delta}(k_1 + k_2 - k_3 - k_4) | \Psi_{m,j} \rangle \sim -(U/L)j^2$ , or  $\Delta \tilde{E} = -g\tilde{J}^2$ . Thus, for small  $g$  the splitting between sublevels grows linearly with  $g$ . This linear regime changes to a nonlinear one as soon as the second term in the Hamiltonian (9) takes a non-negligible value. This second term also causes the rearrangement of the sublevels, clearly seen in Fig. 1. Needless to say, in this case the second quantum number is defined by the action  $\tilde{J} = (1/2\pi) \oint \tilde{J} d\tilde{\vartheta}$ , which amounts to the phase volume enclosed by the trajectories in Fig. 2(b).

We conclude the Letter by formulating quantitative criteria for the onset of quantum chaos. As mentioned earlier, the transition to an irregular spectrum occurs when the total splitting of the  $m$ th Bogoliubov level compares with the Bogoliubov frequency. Ignoring the nonlinear corrections, one has  $g(m+1)^2/4N \sim \Omega$ , or

$$m_{\text{cr}} \approx \left( \frac{4N\sqrt{\delta^2 + 2\delta g}}{g} \right)^{1/2}. \quad (10)$$

Through the relation  $E_{\text{cr}} \approx \Omega m_{\text{cr}}$ , this estimate defines the critical value of energy above which the regular spectrum transforms into a chaotic one. [For example, for  $N = 40$  the estimates (10) predict that  $m_{\text{cr}}$  drops to  $m_{\text{cr}} = 13$  at  $g = 4$ , which should be compared with  $m_{\text{cr}} = 16$  in Fig. 1.]

In conclusion, we have analyzed the BS of the finite- $N$  BH model. In the present work, we restricted ourselves by considering the three-site BH model, although many of the reported results hold for  $L > 3$  as well. An advantage of the three-site model is that, thanks to a relative low dimensionality of the system, its classical dynamics can be understood in every detail. In particular, the phase space of the system essentially consists of two regular and one chaotic component in between, where the low-energy regular component is shown to be associated with the BS. We identify the full set of the integrals of motion for this low-energy

regular component and, quantizing them, obtain the low-energy levels of the quantum BH model. These levels are labeled by two quantum numbers  $m$  and  $j$ . The first quantum number  $m$  corresponds to the usual Bogoliubov ladder, where the distance between neighboring levels is approximately given by the Bogoliubov frequency  $\Omega$  (i.e.,  $E_{m+1,j} - E_{m,j} \sim \Omega$ ). The second quantum number  $j$  labels  $(m+1)$  sublevels of the  $m$ th Bogoliubov level, where the splitting between the sublevels is proportional to the interaction constant  $g$  and inverse proportional to the system size  $N$  (i.e.,  $E_{m,j+1} - E_{m,j} \sim g/N$ ). If we go up the energy axis, the total splitting of the Bogoliubov levels compares the distances between them, and the energy spectrum shows a transition from a regular to an irregular (chaotic) one.

The described scenario of evolution of the BS into a regular, Bogoliubov-like spectrum and further into a chaotic spectrum also holds for the BH model with  $L > 3$  sites. However, to indicate the critical energies for these transitions remains an open problem. The qualitative difference between the three-site and, for example, five-site BH models is that the latter system has two different Bogoliubov frequencies, associated with two single-particle excitation energies. For some values of the macroscopic interaction constant  $g$ , these frequencies become commensurable, which strongly affects the onset of chaos. We reserve this problem of interacting Bogoliubov spectra for future studies.

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