Energy spectrum of fermionized bosonic atoms in optical lattices

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We investigate the energy spectrum of fermionized bosonic atoms, which behave very much like spinless noninteracting fermions, in optical lattices by means of the perturbation expansion and the retarded Green's function method. The results show that the energy spectrum splits into two energy bands with single-occupation; the fermionized bosonic atom occupies nonvanishing energy state and left hole has a vanishing energy at any given momentum, and the system is in Mott-insulating state with a energy gap. Using the characteristic of energy spectra we obtained a criterion with which one can judge whether the Tonks-Girardeau (TG) gas is achieved or not.

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In the recent years, the strongly interacting system in cold atomic gases has been attracted great attention due to the developments in low-dimensional trapping[1−4], loading of optical lattices with ultracold atoms[5−11], and external modification of the inter-particle interactions[12,13]. The observation of the superfluid to Mott-insulator transition of ultracold bosonic gases in optical lattices has demonstrated the large degree of tunability offered by these techniques. Compared with three-dimensional (3D) system, one-dimensional (1D) system has different significances. Especially, in 1D gas the more important the inter-particle interactions become, the more dilute the gas is. Particularly, at sufficiently low density or a large s-wave scattering length a, the bosonic gas resembles a gas of classical hard spheres or spinless non-interacting fermions, the system enters Tonks-Girardeau (TG) region[14,15]. In experiment, the collective excitation spectrum of 1D bosonic gas was measured[16] and 1D superfluid to Mott-insulator transition was observed by adding an additional 1D optical lattice along the axis[17]. These experiments spurred the realization of 1D TG gases last year[18,19]. Realizing TG gas in optical lattices is a novel way. Paredes *et al.*[10] first achieved the TG regime experimentally. They measured the momentum distribution and found that it agrees closely with the theoretical prediction. TG gas is one of the main focus areas of experimental and theoretical investigation recently. A hydrodynamic formalism was shown to reproduce the stationary properties of the TG gas[20], the hydrodynamic method has been extended to the case of finite interactions, by employing the Lieb and Liniger (LL) model[21] and local density approximation[22]. Pedri *et al.* analyzed the properties of TG gases in harmonic trap[23−25]. Very recently, 1D TG gases in optical lattices have been investigated with quantum Monte carlo (QMC), the model is described by Bose-Hubbard Hamiltonian[26].

Over the past year, the Hubbard model has become more important, because it plays a crucial role in some topics in condensed matter physics, including 1D bosonic gases in optical lattices[26−28]. Reference [26] has shown that Bose-Hubbard Hamiltonian can describe TG gas in Ref. [18]. The energy spectrum is important for understanding the physics properties of TG gas loading in lattices. To the best of our knowledge, there is no analytic results for the energy spectrum of 1D TG gas in optical lattices. In this paper we will concentrate on analytic results for the energy spectrum. We consider 1D TG gas in optical lattices, which is described by Bose-Hubbard model, find the effective Hamiltonian of fermionized boson using perturbation expansion and Jordan-Wigner transform, and achieve the energy spectrum by means of double time retarded Green's function (GF) method.

Let's consider ultracold hard core bosonic gas loaded in the optical lattices at zero temperature, which is described in the Bose Hubbard model. In one dimension, the Bose-Hubbard Hamiltonian takes the form[18]

$$H_{\mathrm{B}} = -\frac{J}{2}\sum_i[\hat{b}_i^\dagger \hat{b}_{i+1} + H.c.] + \frac{U}{2}\sum_i \hat{b}_i^\dagger \hat{b}_i^\dagger \hat{b}_i \hat{b}_i, \qquad (1)$$

where the first term describes the hopping energy of the bosonic atom in optical lattice, J is the hopping matrix elements between nearest neighbor sites i and j; the second term gives the interactions between atoms on-site, U gives interaction strength. The bosonic operators $\hat{b}_i^\dagger$ ($\hat{b}_i$) create (annihilate) one bosonic atom at the ith site with canonical commutation relations $[\hat{b}_i, \hat{b}_j^\dagger] = \delta_{ij}$.

Our interest is in the strongly interacting ($U \gg J$ or TG) regime, in which two bosonic atoms cannot occupy the same lattice site. We can consider the bosons as the free-spin fermions in the TG regime[14], i.e., the state with site occupancy equal to or less than 1 ($n_i \leq 1$) will be available, because on-site interaction vanishes. It is well known that for sufficiently large U the bare energy band splits into the sub-bands. To describe the motion of bosonic atom in the TG regime, H_{B} is split into two complementary subspaces: $H_{\mathrm{B}} = H_{\mathrm{P}} \oplus H_{\mathrm{Q}}$, where projection operator P projects H_{B} onto the subspace H_{P} of states with the constraint ($n_i \leq 1$ for all ith sites); $Q = 1 - P$ projects onto the complementary subspace H_{Q}. The projection operators P and Q satisfy the relations: $P = P^+$, $P^2 = P$, $Q = Q^+$, and $Q^2 = Q$. Because the subspaces H_P and H_Q are orthogonal, we also have $QP = PQ = 0$. Thus we can find the effective Hamiltonian within the subspace H_P using perturbation expansion[29]

$$H_{\mathrm{eff}} = PH_\mathrm{B}P - PH_\mathrm{B}Q\frac{1}{QH_\mathrm{B}Q}QH_\mathrm{B}P + \cdots . \quad (2)$$

Our treatment of the effective Hamiltonian nearly traces Cazalilla's calculations[28], we will skip all the details and merely discuss some salient points of the calculations. One can remove the projection operator P if the boson operators are represented in terms of Pauli matrices $\sigma_{ix} = (\hat{b}_i^\dagger + \hat{b}_i)$, $\sigma_{iy} = i(\hat{b}_i^\dagger - \hat{b}_i)$, and $\sigma_{iz} = 1 - 2\hat{b}_i^\dagger \hat{b}_i$. Then using Jordan-Wigner transform[30] $\hat{b}_i = \exp(i\pi\Sigma_{l<i}\hat{c}_l)$ and $n_i = \hat{b}_i^\dagger \hat{b}_i = \hat{c}_i^\dagger \hat{c}_i$, one can obtain the fermionized effective Hamiltonian

$$H_{\mathrm{eff}} = -\frac{J}{2}\sum_i\left(\hat{c}_{i+1}^\dagger\hat{c}_i - \frac{J}{U}\hat{c}_{i+1}^\dagger n_i\hat{c}_{i-1} + H.c.\right) - \frac{J}{2U}\sum_{<i,j>}(n_{i+1}+n_{i-1})n_i + O\left(\frac{J^3}{U}\right), \quad (3)$$

where $\hat{c}_i^\dagger(\hat{c}_i)$ are the fernionized boson creating (annihilating) operators. We have, as usual for Bose operators,

$$[\hat{c}_i, \hat{c}_j] = 0, \quad [\hat{c}_i, n_j] = \hat{c}_i\delta_{ij}, \quad (4)$$

but introduce the fermionized boson constraint by limiting the eigenvalues from n_i to 0 and 1, i.e., $\hat{c}_i^2 = 0$, and $n_i^2 = n_i$. Together with Eq. (4), the basic commutation relation is implied as[31]

$$[\hat{c}_i, \hat{c}_j^\dagger] = (1-2n_i)\delta_{ij}. \quad (5)$$

Actually, Eq. (3) effectively represents the free-spin fermionized boson Hamiltonian. As following, we will calculate the energy spectrum and momentum distribution of TG gas in optical lattices in terms of the retarded Green's function and effective Hamiltonian H_{eff}. The double-time retarded single particle Green's function at zero temperature is defined by

$$G_{ij}(t) = -i\theta(t)\langle\{\hat{c}_i(t), \hat{c}_j^\dagger(0)\}\rangle \equiv \langle\langle\hat{c}_i(t); \hat{c}_j^\dagger(0)\rangle\rangle, \quad (6)$$

where the function $\theta(t-t')$ is the usual step function; the curly brackets $\{\cdots\}$ denote the anti-commutation relation; $\langle\cdots\rangle$ denotes the ground-state expectation value; the operators are expressed in the Heisenberg representation. Using the Fourier transform, the equation of motion for the Green's function becomes

$$\omega G(\omega) = \langle\{\hat{c}_i, \hat{c}_j^\dagger\}\rangle + \langle\langle[\hat{c}_i, H_{\mathrm{eff}}], \hat{c}_j^\dagger\rangle\rangle_\omega. \quad (7)$$

The subscript ω also indicates the Fourier transform. This equation can be solved by applying a suitable decoupling procedure in order to simplify the higher-order Green's function which appears on the right side. Substituting the effective Hamiltonian H_{eff} (Eq. (3) into Eq. (7), one has

$$\left(\omega + \frac{J^2}{U}\bar{n}\right)G_{ij}(\omega) = 1 - \frac{J}{2}[G_{i+1,j}(\omega) + G_{i-1,j}(\omega)] + \frac{J^2}{2U}\bar{n}[G_{i+2,j}(\omega) + G_{i-2,j}(\omega)] + \frac{J^2}{2U}\Gamma(\omega), \quad (8)$$

where

$$\Gamma(\omega) = \langle\langle\hat{c}_{i+1}^\dagger\hat{c}_i\hat{c}_{i-1} + \hat{c}_{i-1}^\dagger\hat{c}_{i+1}\hat{c}_i, \hat{c}_j^\dagger\rangle\rangle_\omega, \quad (9)$$

where $\bar{n} = \langle n_i\rangle$. We have used random phase approach decoupling $\langle\langle\hat{c}_{i+1}^\dagger\hat{c}_{i+1}\hat{c}_i, \hat{c}_j^\dagger\rangle\rangle_\omega \to \bar{n}\langle\langle\hat{c}_i, \hat{c}_j^\dagger\rangle\rangle_\omega$ and $\langle\langle\hat{c}_{i-1}^\dagger\hat{c}_{i-1}\hat{c}_i, \hat{c}_j^\dagger\rangle\rangle_\omega \to \bar{n}\langle\langle\hat{c}_i, \hat{c}_j^\dagger\rangle\rangle_\omega$. Applying the equation of motion to $\Gamma(\omega)$, one has

$$\left(\omega + \frac{J^2}{U}\bar{n}\right)\Gamma(\omega) = \frac{J^2}{2U}\bar{n}(1-\bar{n})G_{ij}(\omega). \quad (10)$$

For Eq. (10) we also used the random phase approach decoupling approximation and translation invariance: $\langle\hat{c}_{i+1}^\dagger\hat{c}_{i-1}\rangle - \langle\hat{c}_{i-1}^\dagger\hat{c}_{i+1}\rangle = 0$, $\langle\hat{c}_i^\dagger\hat{c}_{i-1}\rangle - \langle\hat{c}_{i-1}^\dagger\hat{c}_i\rangle = 0$, and $\langle\hat{c}_{i+2}^\dagger\hat{c}_{i-1}\rangle - \langle\hat{c}_{i-1}^\dagger\hat{c}_{i+2}\rangle = 0$. Transforming Green's functions from coordinate to momentum space, we have

$$\left[\omega + \frac{J}{2}\varepsilon_1 + \frac{J^2}{2U}\bar{n}(2-\varepsilon_2)\right]G(k,\omega) = 1 + \frac{J^2}{2U}\Gamma(k,\omega), \quad (11)$$

$$\left(\omega + \frac{J^2}{U}\bar{n}\right)\Gamma(k,\omega) = \frac{J^2}{2U}\bar{n}(1-\bar{n})G(k,\omega), \quad (12)$$

where $\varepsilon_1 = 2\cos(ka)$, $\varepsilon_2 = 2\cos(2ka)$, a is optical lattice constant linking nearest neighbor sites. From Eqs. (11) and (12), we obtain

$$G(k,\omega) = \frac{(Jr\bar{n} + \omega)}{(\omega-\omega_+)(\omega-\omega_-)}, \quad (13)$$

where $r = J/U$. The energy spectra are

$$\omega_\pm = \frac{J}{4}[(-\varepsilon_1 - 4\bar{n}r + \bar{n}r\varepsilon_2) \pm B], \quad (14)$$

where $B = (4\bar{n}r^2 - 4\bar{n}^2r^2 + \varepsilon_1^2 - 2\bar{n}r\varepsilon_1\varepsilon_2 + \bar{n}^2r^2\varepsilon_2^2)^{1/2}$. According to Eq. (14), we obtain the energy gap is

$$\Delta\omega = \omega_+ - \omega_- = \frac{J}{2}B. \quad (15)$$

From Eq. (13), we have Green function's standard formula

$$G(k,\omega) = \frac{A_-}{\omega-\omega_+} + \frac{A_+}{\omega-\omega_-}, \quad (16)$$

where $A_\pm = \frac{1}{2}\left(1 \pm \frac{\varepsilon_1 - \bar{n}r\varepsilon_2}{B}\right)$. We notice that

$$\omega_+ + \omega_- = \frac{J}{2}(-\varepsilon_1 - 4r\bar{n} + r\bar{n}\varepsilon_2), \quad (17)$$

i.e., the two bands are specularly symmetric with respect to $\omega = \frac{J}{4}(-\varepsilon_1 - 4r\bar{n} + r\bar{n}\varepsilon_2)$ and $A_+ + A_- = 1$. From $\omega_\pm$ and $A_\pm$ one knows that both the Hubbard bands and

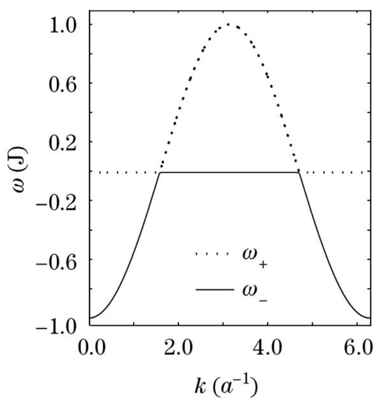

Fig. 1. The energy spectrum of fermionized Bose gas in optical lattices as a function of the momentum k, where $\bar{n} = 0.5$ (half-filling), $\gamma = 52.28$, and $U = 52.28$ J.

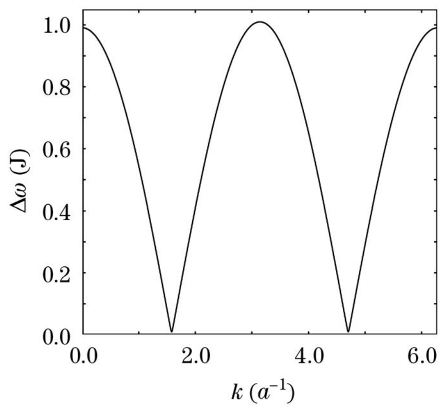

Fig. 2. The energy gap of fermionized Bose gas in optical lattices as a function of the momentum k, where the average occupancy factor is $\bar{n} = 0.5$.

their weights depend on $\bar{n}$, i.e., the average occupation of the fermionized bosons per site.

Figure 1 shows the energy spectrum of fermionized bosons in optical lattices, where $\bar{n} = 0.5$ (half-filling), $\gamma = 52.28$, the parameter is defined as $\gamma = U/J$. The energy spectrum is split into two bands, and there is gap $\Delta\omega$ between two spectral bands. The corresponding energy gap is given in Fig. 2. The existence of the energy gap indicates that the system is in Mott-insulating state when bosonic gas enters TG region. One knows that $\Delta\omega \to 0$ at $k = 1.07a^{-1}$, $4.71a^{-1}$ (see Fig. 2). It does not imply that the system enters the superfluid state, because the system enters TG region as the coherence length of the system, which is the de Broglie wavelength, approaches inter-particle spacing, the single-particle wave functions become spatially distinct[19]. In the asymptotic TG gas, the coherence length equals to inter-particle space, the single particle wave functions are completely distinct and separate. Therefore the superfluid state cannot occur in the TG region. One can obtain TG region by either increasing the interaction between bosons or decreasing 1D density of bosons (increasing inter-particle spacing).

From Fig. 1, we have the negative ground energy, because the effective Hamiltonian (Eq. (3)) has a negative nearest neighboring hopping energy $(-J)$ and the nearest neighboring attractive interaction due to perturbative expansion. Given any momentum k value, the energy approaches zero for one of two energy bands. This implies that single-occupation fermionized boson occupies lower nonvanishing energy band at smaller momentum state, and left empty-occupation hole has vanishing energy. For fermionized Bose gas in optical lattices, empty-occupation hole is static. These results are different from those of non-fermionized Bose gas in optical lattice. For single-component Bose gas, there are a constant lower energy band and an upper energy band[32]; for two component Bose gas, there are a constant lower energy band and two identical upper energy bands for each component[33]. Comparing fermionized bosons with soft-core bosons in optical lattices, the energy bands of the fermionized bosons are lower than those of the soft-core bosons. Lowering energy is the characteristic of the fermionization, which was demonstrated experimentally[19]. Comparing with the result calculated in terms of Bogoliubov approach[34], the ground state energy spectrum is in good agreement except the difference of a factor 2. This difference may be caused by the approximation itself. Therefore, one can predict whether a system enters the TG regime or not from the characteristic of the energy spectra in experiment.

In conclusion, using the fermionization technique of boson and double-time retarded Green's function method, we have found the analytic results of the energy spectrum in 1D fermionized Bose gas on presence of optical lattices. The energy spectrum splits two energy bands and the system is in Mott-insulator state. The characteristic of energy bands shows that the fermionized boson occupies the nonvanishing energy state, and left hole has vanishing energy at given momentum k. Our analytic results of fermionized bosonic energy spectra provides a criterion with which one can judge whether the system enters the TG region or not in experiment.

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