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METHODS OF THEORETICAL PHYSICS

Excitation Spectrum in an Ensemble of Hubbard Bosons

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An approach that makes it possible to correctly derive equations describing the Bose–Einstein condensation and the spectrum of elementary excitations in the ensemble of Hubbard bosons in the strong correlation regime ($U \gg |t_{fm}|$) has been developed in the atomic representation using the Dyson method with the introduced indefinite metric. The kinematic Dyson interaction caused by the properties of the commutation relations of dynamic variables plays an important role in such a system. An effective Hamiltonian has been obtained using the operator form of perturbation theory at finite U values. It has been shown that the properties of the ensemble of Hubbard bosons have been determined by the kinematic interaction, correlated hopping, and the attraction between Hubbard bosons. Numerical calculations have demonstrated the effect of these interactions on the characteristics of the energy spectrum of excitations of the ensemble of Hubbard bosons and on the dependence of the density of condensate particles on the density of bosons in the system.

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1. INTRODUCTION

The static and kinetic properties of a single-component Bose system [1–3] and multicomponent mixtures of ultracold atoms [4–6] are determined to a great extent by the competition between Bose–Einstein condensation and interatomic interaction. Similar effects can also be observed in ultracold molecules [7]. Studies of the electromagnetically induced Bose–Einstein condensation of electron–hole pairs in strongly degenerate semiconductors are of current interest [8]. Since the magnitude of the interatomic interaction can be controlled by varying the Feshbach resonance conditions, an ultracold Bose ensemble of atoms, molecules, or electron–hole pairs is a promising platform to study multiparticle effects and to develop theoretical concepts [9].

Analytical methods for studying Bose–Einstein condensation are well developed in the case of a relatively weak interaction between bosons [10]. In this case, the use of the property of the macroscopic population of a state with zero quasimomentum and the mean-field approximation for the interaction operator provides satisfactory results.

If the interaction energy of bosons exceeds their kinetic energy, the Bogoliubov method [10] should be corrected. This correction can be made, e.g., in the atomic representation [11], which is actively used in the theory of strongly correlated electron systems [12–17]. In this representation, the boson interaction operator at a single site has a diagonal form, which allows one to correctly include the contribution from this operator to observables at any interaction parameter.

In this work, the atomic representation [11] and the Dyson method [18], which involves an indefinite metric, make it possible to study the Bose–Einstein condensation in the regime, where the interaction energy between bosons is much higher than their kinetic energy. In this case, the kinematic Dyson interaction [18], which is due to specific commutation relations between the Hubbard operators, affects the condensation of strongly correlated bosons.

2. BOSONS IN AN OPTICAL LATTICE

The authors of [19] showed that a system of ultracold atoms in the optical lattice is described by the Bose–Hubbard Hamiltonian

$$H = \sum_f \left[(\varepsilon - \mu)\hat{n}_f + \frac{U}{2}\hat{n}_f(\hat{n}_f - 1) \right] - \sum_{fm} t_{fm} c_f^+ c_m. \quad (1)$$

Here, the summation is performed over lattice sites specified by the subscripts f and m; c_f and c_m^+ are bosonic operators satisfying the conventional commutation relations $[c_f, c_m^+]_- = c_f c_m^+ - c_m^+ c_f = \delta_{fm}$, where δ_{fm} is the Kronecker delta; $\hat{n}_f = c_f^+ c_f$ is the boson number operator at the fth site; ε is the energy of the atom at the fth site; μ is the chemical potential of the system; t_{fm} is the atom hopping energy between the

nearest mth and fth sites; and U is the pair interaction energy between bosons at the same site.

Below, we consider the strong correlation regime $U \gg |t_{fm}|$. In this case, it is reasonable to use a formalism where the interaction operator is included in the zeroth-approximation Hamiltonian, whereas the perturbation operator contains hopping.

3. ATOMIC REPRESENTATION, HUBBARD BOSONS, AND KINEMATIC INTERACTION

As known, the formulated concept is implemented in the atomic representation. The eigenstates $|n\rangle$ of the operator c^+c are defined as

$$c^+c\,|n\rangle = n\,|n\rangle, \quad n = 0,1,2,\ldots. \tag{2}$$

Here, the site subscript f is temporarily omitted and can be easily reconstructed below, and n is the number of bosons in the state $|n\rangle$. Since

$$c|n\rangle = \sqrt{n}|n-1\rangle, \quad c^+|n\rangle = \sqrt{n+1}|n+1\rangle, \tag{3}$$

the operators c and c^+ in the atomic representation have the form

$$c^+ = \sum_{n=0}\sqrt{n+1}X^{n+1,n}, \quad c = \sum_{n=0}\sqrt{n+1}X^{n,n+1}. \tag{4}$$

Here,

$$X^{n+1,n} = |n+1\rangle\langle n|, \quad X^{n,n+1} = |n\rangle\langle n+1| \tag{5}$$

are the Hubbard operators, which transform states with n and $n+1$ bosons to states with $n+1$ and n bosons. Consequently, the operators $X^{n+1,n}$ and $X^{n,n+1}$ can be treated as the creation and annihilation operators of such a boson (it is called below the Hubbard boson by analogy with the Hubbard fermion introduced previously for strongly correlated electron systems), which is strictly related to a certain transition. For this reason, Hubbard bosons can be considered as colored.

This circumstance markedly distinguishes the initial boson described by the operators c and c^+ from colored Hubbard bosons. According to Eq. (4), the initial boson corresponds to a superposition of colored Hubbard bosons with weight factors.

A physical consequence of the color of Hubbard bosons is the kinematic interaction between them, which is mathematically due to the commutation relations between Hubbard operators

$$[X_f^{n,m}, X_g^{p,q}]_- = \delta_{fg}(\delta_{mp}X_f^{n,q} - \delta_{nq}X_f^{p,m}) \tag{6}$$

corresponding to the Lie algebra.

Dyson [18] was the first who focused on the existence of a specific interaction in systems whose dynamic variables are described by operators satisfying the Lie algebra and called this interaction kinematic. An important role of the kinematic interaction in strongly correlated electron systems was emphasized in [12–17].

Taking into account the above expressions, the Hamiltonian takes the necessary form

$$H = H_0 + \hat{T}. \tag{7}$$

Here,

$$H_0 = \sum_f\sum_{n=0}E_nX_f^{n,n}, \tag{8}$$

where

$$E_n = (\varepsilon - \mu)n + Un(n-1)/2 \tag{9}$$

is the diagonal operator exactly describing the single-site interaction between bosons, and

$$\hat{T} = -t\sum_{f\Delta}\sum_{n,m=1}\sqrt{nm}X_f^{n,n-1}X_{f+\Delta}^{m-1,m} \tag{10}$$

describes hopping processes of Hubbard bosons between the nearest sites.

We emphasize that, although the operator H_{int} is quadratic in X_l^{rt}, it indirectly reflects the above kinematic interaction between Hubbard bosons.

4. STRONG INTERACTION LIMIT

The effect of the kinematic interaction on the properties of the system of Hubbard bosons is first analyzed in the regime where the interaction is manifested in the pure form. To this end, the limiting case $U \to \infty, n < 1$, where the actual sector of the Hilbert space is based on the direct product of subspaces determined by the basis vectors $|0,f\rangle$ and $|1,f\rangle$, is considered.

The system of Hubbard bosons in this limit is described by the Hamiltonian

$$H_\infty = \sum_f(\varepsilon - \mu)X_f^{11} - t\sum_{f\Delta}X_f^{10}X_{f+\Delta}^{01}. \tag{11}$$

The Dyson method [18] is used to solve the problem of Bose–Einstein condensation and the excitation spectrum.

Let the pseudo-Hubbard operators be introduced in terms of new Bose operators a_f and a_f^+ as

$$\begin{aligned}\tilde{X}_f^{11} &= a_f^+a_f, \quad \tilde{X}_f^{00} = 1 - a_f^+a_f,\\ \tilde{X}_f^{10} &= a_f^+, \quad \tilde{X}_f^{01} = (1 - a_f^+a_f)a_f,\end{aligned} \tag{12}$$

which satisfy the same commutation relations as the Hubbard operators X_f^{nm}.

If $\tilde{X}_f^{nm} \equiv X_f^{nm}$ is formally set, Eqs. (12) correspond to the Dyson–Maleev transformations [18, 20] for $S = 1/2$ spin operators.

In reality, $\tilde{X}_f^{nm}$ and X_f^{nm} are different operators. First, they act in Hilbert spaces with different dimen-

sions. Second, according to Eqs. (12), the operators $\tilde{X}_f^{01}$ and $\tilde{X}_f^{10}$ are not mutually Hermitian.

Since Hermitian conjugation is directly related to the definition of the scalar product, Dyson [18] proposed a new metric (appearing indefinite) in which the mentioned operators are Hermitian conjugate.

The implementation of this program leads to the algorithm to obtain exact Bose analogs of $SU(2)$ and $SU(3)$ quantum Hamiltonians [21, 22]

$$H(a_f, a_f^+) = \hat{F}H(\tilde{X}), \tag{13}$$

where $\hat{F}$ is the metric operator. In our case, according to [21],

$$\hat{F} = \prod_f \hat{F}_f, \quad \hat{F}_f = 1 + \sum_{n=2} A_n (a_f^+)^n a_f^n, \tag{14}$$

$$A_2 = -1/2, \quad A_3 = 1/3, \quad A_4 = -1/8, \ldots, \tag{15}$$

and the operator $H(\tilde{X})$ is obtained from Eq. (11) by substituting pseudo-Hubbard operators (12) for Hubbard operators. The existence of the metric operator not only solves the problem of the Hermitian character of the boson Hamiltonian but also allows one to correctly remove contributions from so-called nonphysical states. The last circumstance is due to the fact that the single-site Hilbert space in the atomic representation is specified by two basis vectors, whereas the dimension of the single-site boson basis is infinite.

Using the above expressions and retaining terms up to the fourth order in secondary quantization operators in the Bose analog, we obtain the Hamiltonian of the system in the quasimomentum representation in the form

$$\begin{aligned} H &= \sum_k (\varepsilon - \mu - t_k) a_k^+ a_k \\ &- \frac{1}{N} \sum_{1-4} (\varepsilon - \mu - t_1 - t_4) a_1^+ a_2^+ a_3 a_4 \Delta(1 + 2 - 3 - 4), \end{aligned} \tag{16}$$

where t_k is the Fourier transform related to the parameters t_{fm} by the conventional relation $t_{fm} = (1/N)\sum_k \exp[ik(f-m)]t_k$ and $\Delta(1+2-3-4)$ is the Kronecker delta, which describes the conservation law of the quasimomentum in the interaction, where digits stand for quasimomenta.

The metric operator $\hat{F}$ in Eq. (13) leads to the renormalization of the matrix element of the interaction between bosons.

When calculating the spectrum of elementary excitations, it is necessary to take into account Bose–Einstein condensation at zero quasimomentum [10]. To this end, we perform the "shift" [23]

$$a_0 \to \sqrt{N_0} + \alpha_0, \quad a_0^+ \to \sqrt{N_0} + \alpha_0^+, \tag{17}$$

where N_0 is the average number of particles in the condensate and α_0 and α_0^+ are new operators related to fluctuations of the number of condensed particles.

The substitution of Eq. (17) into Eq. (16) gives

$$H = E_0 + H_{(2)} + H_{(4)}, \tag{18}$$

where

$$E_0 = (1 - n_0)(\varepsilon - \mu - t_0)N_0 + t_0 n_0 N_0 \tag{19}$$

is the energy of condensed particles obtained disregarding fluctuation renormalizations and $n_0 = N_0/N$ is the site density of the Bose–Einstein condensate. In Eq. (18), it is taken into account that the linear form of the operators α_0 and α_0^+ should be zero. This requirement provides the first equation for the determination of n_0 and μ:

$$(1 - 2n_0)(\varepsilon - \mu - t_0) = -2n_0 t_0. \tag{20}$$

The operator $H_{(2)}$ in Eq. (18) has the standard form

$$H_{(2)} = \sum_{k \neq 0} \left[A_k a_k^+ a_k + \frac{1}{2} B_k (a_k^+ a_{-k}^+ + a_{-k} a_k) \right], \tag{21}$$

where

$$\begin{gathered} A_k = (1 - 4n_0)\Gamma_k + t_0, \quad B_k = -2n_0 \Gamma_k, \\ \Gamma_k = \varepsilon - \mu - t_0 - t_k. \end{gathered} \tag{22}$$

The diagonalization of Eq. (21) using the Bogoliubov transformation

$$a_k = \cosh(\varphi_k) b_k + \sinh(\varphi_k) b_{-k}^+, \tag{23}$$

where $\cosh(2\varphi_k) = A_k/\omega_k$, $\sinh(2\varphi_k) = -B_k/\omega_k$, gives the excitation energy

$$\omega_k = \sqrt{(1 - 2n_0)(1 - 6n_0)\varepsilon_k^2 + 4n_0 t_0 \varepsilon_k}, \tag{24}$$

where $\varepsilon_k = t_0 - t_k$.

The second equation for the determination of n_0 and μ has the form

$$n = n_0 + \frac{1}{2N} \sum_k \frac{A_k - \omega_k}{\omega_k}. \tag{25}$$

The solution of Eqs. (20) and (25) using Eq. (24) yields the excitation spectrum as a function of the density of particles in the system.

Numerical calculations were carried out for a two-dimensional lattice including hopping only between the nearest sites with the hopping integral t. In this case,

$$t_0 = 4t, \quad t_k = 4t\gamma_k, \quad \gamma_k = (\cos(k_x) + \cos(k_y))/2.$$

Figure 1 shows the numerically calculated energy spectrum of elementary excitations in the ensemble of Hubbard bosons in the regime of extremely strong single-site correlation. The kinematic interaction between Hubbard bosons provides two effects. First, noncondensed particles appear because $n_0 < n$, and

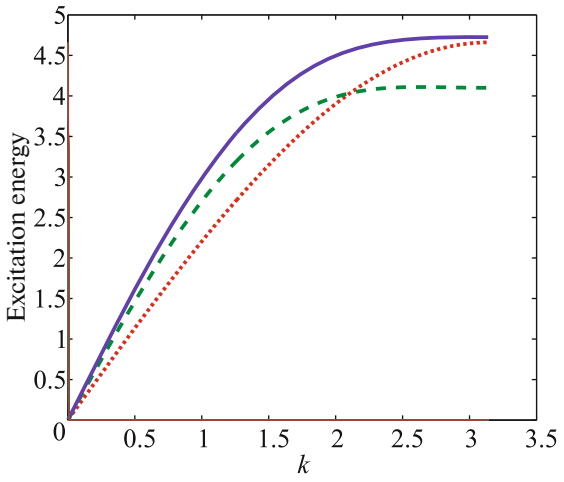

Fig. 1. (Color online) Quasimomentum dependences of excitation energies in the ensemble of Hubbard bosons at $U = \infty$ in the direction of the main diagonal of the Brillouin zone ($k_x = k_y = k$) at the parameters (red dotted line) $n = 0.25$ and $n_0 = 0.164$, (green dashed line) $n = 0.6$ and $n_0 = 0.282$, and (blue solid line) $n = 0.98$ and $n_0 = 0.341$.

the spectrum of elementary excitations at low quasimomenta becomes linear. The relative fraction of noncondensed particles increases with n, when the contribution from the kinematic interaction increases. Second, the rigidity of elementary excitations at low quasimomenta increases with n.

5. REGIME OF LARGE BUT FINITE U

If $|t_{fm}| \ll U < \infty$, hopping of Hubbard bosons even at $n < 1$ is accompanied by the appearance of doubly filled states. Since such states have a high energy, their generation is virtual and is manifested in the effective intersite interaction between Hubbard bosons.

This interaction can be determined using the operator form of perturbation theory [24, 25]. In the case under consideration, the actual sector of the Hilbert space is specified by the direct product of single-site subspaces constructed on the basis vectors $|f,0\rangle$ and $|f,1\rangle$.

Defining the projection operator on this sector in the form $\hat{P} = \prod_f (X_f^{00} + X_f^{11})$, we conclude that the effective Hamiltonian of the considered ensemble up to the second-order terms in the parameter $|t_{fm}|/U$ has the form

$$H_{\text{eff}} = \hat{P}H\hat{P} + \hat{P}\hat{T}\frac{1}{H_0 - E_0}(\hat{P}\hat{T}\hat{P} - \hat{T}\hat{P}), \qquad (26)$$

where E_0 is the energy in the zeroth approximation.

Simple algebra gives

$$H_{\text{eff}} = H_\infty - \hat{V},$$
$$\hat{V} = V\left(\sum_{f\Delta} X_{f+\Delta}^{11} X_f^{11} + \sum_{f\Delta\neq\Delta_1} X_{f+\Delta}^{10} X_f^{11} X_{f+\Delta_1}^{01}\right), \qquad (27)$$

where H_∞ is specified by Eq. (11), $V = 2t^2/U$, and summation over Δ and Δ_1 means summation over the nearest sites.

The same transition to the Bose representation for the Hamiltonian as in the preceding section indicates that A_q and B_q in the approximation under consideration are obtained with the substitution

$$A_q \to A_q - 2n_0\left(\frac{t_0^2}{U}\right)(1+\gamma_q)^2,$$
$$B_q \to B_q - 4n_0\left(\frac{t_0^2}{U}\right)\gamma_q. \qquad (28)$$

After that, the first equation for n_0 and μ takes the form

$$(1-2n_0)(\varepsilon - \mu) = [1 - 4n_0(1 - t_0/U)]t_0, \qquad (29)$$

and the second equation has the same form of Eq. (25).

Including the kinematic Dyson interaction, intersite attraction between Hubbard bosons, and correlated hoppings, the above formulas provide the following expression for the square of the frequency of elementary excitations in the ensemble of Hubbard bosons:

$$\omega_k^2 = [1 - 2n_0(1 - l_k)][1 - 2n_0(3 - r_k)]\varepsilon_k^2$$
$$+ 4n_0 t_0\left[1 - 2\frac{t_0}{U}\right]\left[1 + \frac{2n_0}{1-2n_0}l_k\right]\varepsilon_k, \qquad (30)$$

where

$$l_k = \frac{t_0 + t_k}{U}, \quad r_k = \frac{5t_0 + t_k}{U}. \qquad (31)$$

Figure 2 shows the numerically calculated spectrum of Bose excitations in the ensemble of Hubbard bosons at $U = 10t$ in the same nearest neighbor approximation. In this case, according to Eq. (27), attraction and correlated hoppings occur in addition to the kinematic interaction between Hubbard bosons.

It is seen that the contribution from attraction between bosons increases with the density of bosons in the system. As a result, a feature characterized by a decrease in the excitation energy with increasing quasimomentum appears in the quasimomentum dependence of ω_q. This picture qualitatively corresponds to the appearance of the roton section of the spectrum.

Figure 3 presents the dependences of the density of particles in the condensate on the total density of bosons in the system. It is seen that the difference

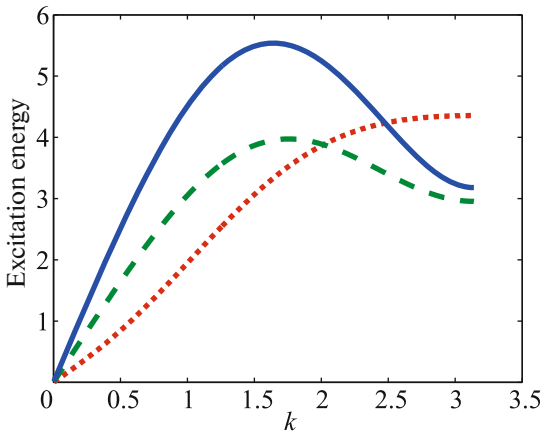

Fig. 2. (Color online) Quasimomentum dependences of excitation energies in the ensemble of Hubbard bosons at $U = 10t$ in the direction of the main diagonal of the Brillouin zone at the parameters (red dotted line) $n = 0.25$ and $n_0 = 0.2235$, (green dashed line) $n = 0.6$ and $n_0 = 0.40315$, and (blue solid line) $n = 0.98$ and $n_0 = 0.4558$.

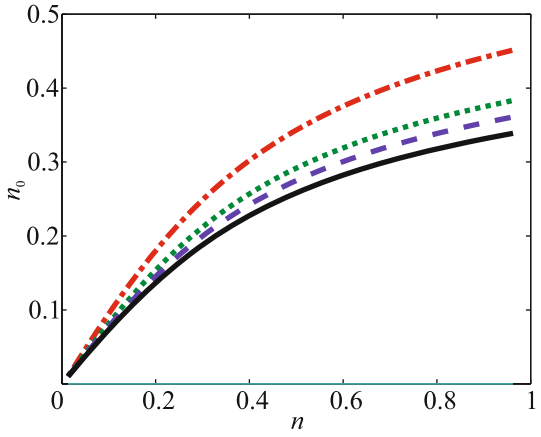

Fig. 3. (Color online) Density of particles in the condensate n_0 versus the total particle density n in the 2D lattice at U = (red dash-dotted) $10t$, (blue dotted line) $50t$, and (black solid line) ∞.

$n - n_0$ increases with n. This difference is maximal at $U = \infty$ because attraction between Hubbard bosons against the background of their kinematic interaction is $\sim t^2/U$, i.e., increases with decreasing U.

According to the presented dependences, the fraction of condensate bosons is no less than 30% even at $n \sim 1$, when the interaction is the most efficient. For comparison, this fraction in He-4 is no more than 10%. Such difference is due to the approximation used, where fluctuation contributions are ignored. They can be taken into account within the diagrammatic representation of perturbation theory. It is important that the proposed method allows one to determine bare Green's functions necessary to calculate loop renormalizations. The corresponding calculations will be reported elsewhere.

6. CONCLUSIONS

The method developed in this work to study the properties of a strongly correlated boson ensemble is based on concepts known in the theory of condensed matter.

The first concept is the atomic representation, which makes it possible to exactly take into account the strong boson interaction in the zeroth-approximation Hamiltonian and to consider the kinetic energy operator perturbatively.

In the atomic representation, dynamic variables are Hubbard operators describing intrasite transitions. Correspondingly, "colored" Hubbard bosons rather than initial bosons hop over sites of the lattice. Color appears because each intrasite transition unambiguously corresponds to its Hubbard boson. In this case, initial bosons are represented as weighted linear superpositions of colored Hubbard bosons.

Since commutation relations for Hubbard operators corresponds to a Lie algebra, the kinematic Dyson interaction occurs between Hubbard bosons.

The second concept is the Dyson method used to obtain an exact Bose analog of the Hamiltonian of the ensemble of Hubbard bosons by introducing pseudo-Hubbard operators and an indefinite metric. This metric allows one to recover the hermiticity of the resulting Bose Hamiltonian and to eliminate contributions from nonphysical states.

The effect of the kinematic interaction between Hubbard bosons on the characteristics of Bose–Einstein condensation and the spectrum of elementary excitations has been studied in the limit $U \to \infty$ and $n < 1$. The spectrum has been obtained in an analytical form and the dependence of the Bose–Einstein condensate density on the density of bosons has been calculated.

The third concept is the operator form of perturbation theory, which makes it possible to obtain the effective Hamiltonian at finite but large U values. In this case, in addition to the kinematic interaction between Hubbard bosons, correlated hoppings of such bosons and intersite attraction between them appear. The intensity of this attraction in the nearest neighbor approximation is given by the expression $V = 2t^2/U$, where t is the hopping parameter between the nearest sites. As a result, the competition between two interactions in the ensemble of Hubbard bosons at $t \ll U$ significantly affects the spectral and thermodynamic characteristics of the system. In particular, a feature corresponding to the roton section of the spectrum appears in the quasimomentum dependence of the energy of elementary excitations.

CONFLICT OF INTEREST

The author declares that he has no conflicts of interest.

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