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INTEGRABLE CHAIN OF ELECTRONS COUPLED WITH SQUEEZED PHONONS

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The exact wave function for a one-dimensional chain of electrons coupled with squeezed phonons is obtained. The ground state energy and the gap in the electron spectrum are calculated. It is shown that there exists an optimal phonon number $n^{ph} \neq 0$ for the ground state of the system. The results are generalized for a system of correlated electrons.

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The adiabatic approximation becomes less accurate in the presence of a strong anharmonic electron–phonon interaction, and the displaced-oscillator state does not properly represent the real phonon ground state[1]. For example, anharmonic coupling leads not only to a finite rigid displacement but also to a deformation of the phonon wave functions describing the squeezed phonons. For 3D systems this new ground state is known from the parametric photonic processes in quantum optics and is characterized by a super-Gaussian distribution with enhanced fluctuations of the particle number in comparison with the more familiar equilibrium Bose–Einstein distribution[2]. It has been shown [3] that phonon correlations together with electron–squeezed-phonon coupling have a substantial effect on the superconducting properties of a system.

It is of interest to consider the influence of the electron–squeezed-phonon coupling on the ground state properties of a system. In [4] an integrable chain of electrons coupled with harmonic phonons was considered. Here we construct an exactly solvable (via the Bethe ansatz) one-dimensional model of electrons interacting with squeezed phonons[5]. The modified electron hopping provides for decoupling of the electron and squeezed-phonon (rather than the initial harmonic-phonon) variables. We construct the exact wave function and calculate the ground state energy and the gap in the Fermi spectrum on the basis of the Bethe ansatz for the attractive Hubbard model [6].

We start with the Hamiltonian of tight-binding electrons interacting with local squeezed phonons at each site. The electron hopping is modulated by a term that

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depends on the phonon variables:

$$H = H_{hopp} + H_{on-site},$$

$$H_{on-site} = \Omega \sum_i b_i^+ b_i - g \sum_i (n_{i\uparrow} + n_{i\downarrow})((b_i^+)^2 + b_i^2) - \mu \sum_i n_{i\sigma},$$

$$H_{hopp} = -t \sum_{\langle ij \rangle \sigma} e^{-\gamma_{i\sigma}} c_{i\sigma}^+ c_{j\sigma} e^{\gamma_{j\sigma}}, \tag{1}$$

where

$$\gamma_{j\sigma} = -\frac{1}{4}\{\tanh^{-1}[\frac{2g}{\Omega} n_{j\bar{\sigma}}] - \tanh^{-1}[\frac{2g}{\Omega}(n_{j\uparrow} + n_{j\downarrow})]\}(b_j^2 - (b_j^+)^2) =$$

$$= [\tanh^{-1} \frac{2g\Omega n_{j\sigma}}{\Omega^2 - 4g^2(n_{j\sigma} + 1)n_{j\bar{\sigma}}}](b_j^2 - (b_j^+)^2). \tag{2}$$

Here $c_{i\sigma}^+(c_{i\sigma})$ are the electron creation (annihilation) operators and $b^+(b)$ are the phonon creation and annihilation operators, $[b, b^+] = 1$. For small g/Ω the electron hopping can be written approximately as

$$H_{hopp} \approx -t \sum_{\langle ij \rangle} c_{i\sigma}^+ c_{j\sigma} \{1 + \frac{2g}{\Omega}(n_{j\sigma}(b_j^2 - (b_j^+)^2) - n_{i\sigma}(b_i^2 - (b_i^+)^2))\}.$$

We see that it can be treated as correlated hopping that is dependent on the phonon numbers. We note that in the simplest mean field approximation (when the phonon operators b_i^+ and b_i are replaced by $\sqrt{n_i^{ph}}$) the correlation terms in the hopping term are zero.

The wave function of this Hamiltonian can be obtained exactly. The unitary "squeezed-phonon" transformation [7] of the phonon operators

$$b_i^+ = e^{\chi_i(a_i^2 - (a_i^+)^2)} a_i^+ e^{-\chi_i(a_i^2 - (a_i^+)^2)} = a_i^+ \cosh 2\chi_i + a_i \sinh 2\chi_i,$$

$$b_i = e^{\chi_i(a_i^2 - (a_i^+)^2)} a_i e^{-\chi_i(a_i^2 - (a_i^+)^2)} = a_i^+ \sinh 2\chi_i + a_i \cosh 2\chi_i, \tag{3}$$

$$4\chi_i = \tanh^{-1} \frac{2g}{\Omega}(n_{i\uparrow} + n_{i\downarrow}),$$

transforms the on-site term of the Hamiltonian in the following way:

$$H_{on-site} = \sum_i \eta_i a_i^+ a_i, \tag{4}$$

where

$$\eta_i = \Omega[\cosh 4\chi_i]^{-1} =$$

$$= \Omega[1 + (2 + \cosh(A + 2B) - \cosh A - 2\cosh B) n_{i\uparrow} n_{i\downarrow} +$$

$$+ (\cosh B - 1)(n_{i\uparrow} + n_{i\downarrow}),$$

$$A = \tanh^{-1} \frac{4g}{\Omega} - 2\tanh^{-1} \frac{2g}{\Omega}, \quad B = \tanh^{-1} \frac{2g}{\Omega}. \tag{5}$$

In the case under consideration, $g < \Omega/2$, the eigenfunctions of the on-site squeezed-phonon Hamiltonian are square-integrable. By virtue of the idempotent property of the $n_{i\sigma}$ operators, η_i has the following structure:

$$\eta_i = \Omega(1 + x n_{i\uparrow} n_{i\downarrow} + y(n_{i\uparrow} + n_{i\downarrow})). \tag{6}$$

For small g/Ω, the coefficients x and y can be calculated as perturbations of first order in this ratio, and the on-site Hamiltonian takes the form:

$$H_{on-site} = \Omega \sum_i (1 - \frac{4g^2}{\Omega^2} n_{i\uparrow} n_{i\downarrow} - \frac{2g^2}{\Omega^2}(n_{i\uparrow} + n_{i\downarrow})) - \mu \sum_{i\sigma} n_{i\sigma}). \tag{7}$$

Although the transformed on-site Hamiltonian has the functional form (4), (6) for all $g, \Omega/2$, the coefficients of $n_{i\uparrow} n_{i\downarrow}$ and $n_{i\uparrow} + n_{i\downarrow}$ should be calculated more precisely as g increases. Let us calculate the exact wave function for a chain of electrons with on-site part (7).

The operators a_i^+ and a_i depend on the electron number at site i. They obey the Bose commutation rule $[a_i, a_j^+] = \delta_{ij}$, but the vacuum for these transformed phonon operators is defined as

$$|\tilde{0}\rangle = e^{-\frac{1}{4}\tanh^{-1}\frac{2(n_\uparrow + n_\downarrow)g}{\Omega}(b^2 - (b^+)^2)}|0\rangle \tag{8}$$

where $n_{\uparrow,\downarrow}$ is the electron number, and $|0\rangle$ is the vacuum for the initial operators b^+, b. It is easy to calculate the eigenfunctions and eigenenergies of Hamiltonian (7) for a single site.

$$H_{on-site} = \Omega(1 - \frac{4g^2}{\Omega^2} n_\uparrow n_\downarrow - \frac{2g^2}{\Omega^2}(n_\uparrow + n_\downarrow)) a^+ a. \tag{9}$$

In the absence of electrons

$$F_0^{(n)} = (a^+)^n |0\rangle^{el} |0\rangle^{ph}, \qquad E_0^{(n)} = n\Omega. \tag{10}$$

Here and below n without indices denotes the phonon number. For one electron with spin σ we get

$$F_\sigma^{(n)} = c_\sigma^+ (a^+)^n |0\rangle^{el} |\tilde{0}\rangle^{ph}, \qquad E_\sigma^{(n)} = (1 - \frac{2g^2}{\Omega^2}) n\Omega \tag{11}$$

where n is the phonon number and the phonon vacuum is defined in accordance with (8). For two electrons

$$F_2^{(n)} = c_\uparrow^+ c_\downarrow^+ (a^+)^n |0\rangle^{el} |\tilde{0}\rangle^{ph}, \qquad E_2^{(n)} = (1 - \frac{8g^2}{\Omega^2}) n\Omega. \tag{12}$$

The energy $n\Omega$ (10) can be regarded as the phonon contribution to the energy. Thus the "electron" contribution to the energy due to the electron–phonon interaction can be considered as a sum of two parts: the one-particle energy $-2ng^2/\Omega$ and the energy of attraction of the electrons $-4ng^2/\Omega$. These are just the energy levels for noninteracting phonons ($n\Omega$) and electrons with one-particle energy $-2ng^2/\Omega$ and one-site attraction $-4ng^2/\Omega$.

For a chain we seek an exact wave function of the system in the following form:

$$\Psi = \sum_{x_1,\ldots,x_{N_e},\sigma} f(x_1,\ldots,x_{N_e};\sigma) \prod_{k=1}^{N_e} c^+_{x_k\sigma_k} \Phi(a_1^+,\ldots,a_N^+;x_1,\ldots x_{N_e})|0\rangle^{el}|0\rangle^{ph}. \qquad (13)$$

Here

$$|0\rangle^{ph} = \prod_{m=1}^{N} |0\rangle_m^{ph}, \quad |0\rangle^{el} = \prod_{m=1}^{N} |0\rangle_m^{el},$$

N is the number of sites and N_e is the number of electrons. The index σ specifies the spin projection variables of the electron amplitude f. We shall see that f obeys the equation of the Bethe ansatz for the Hubbard model with negative Hubbard energy $U = -4g^2n/\Omega$, and thereafter we shall drop the spin variables. We note that the phonon amplitude Φ depends on the electron coordinates. We can now show that if the phonon part of the wave function is chosen as a product of one-site wave functions in accordance with the electron number at this site (i.e., in accordance with the diagonalization of the Hamiltonian (9)):

$$\tilde{\Phi}(a_1^+,\ldots a_N^+;x_1,\ldots x_{N_e}) \prod_{m=1}^{N} (a_m^+)^n |0\rangle_m^{ph} \qquad (14)$$

then the electron part f obeys the equation for the wave function in the one-dimensional attractive Hubbard model.

The phonon amplitude Φ depends on the electron coordinates through the operators a_i^+ (Eq. (3)) and the vacuum $|0\rangle_i^{ph}$ (Eq. (8)). This dependence appears explicitly if the phonon amplitude is written in terms of the original b operators:

$$\Phi(b_1^+,\ldots b_N^+;x_1,\ldots x_{N_e}) \prod_{m=1}^{N} |0\rangle_m^{ph} =$$

$$= \prod_{m=1}^{N} \exp\left\{-\frac{1}{4}\tanh^{-1}\left(\frac{2g}{\Omega}\sum_{j=1}^{N_e}\delta_{x_j m}\right)(b_m^2 - (b_m^+)^2)\right\} (b_m^+)^n |0\rangle_m^{ph}. \qquad (15)$$

Here n is the number of squeezed phonons. Let us show that n is a good quantum number: $[N_j, H] = 0$, where $N = a^+a$ is the squeezed-phonon number operator. For the on-site part of the Hamiltonian this relation is obvious if $H_{on-site}$ is written in terms of the transformed phonon operators a (Eq. (7)), because the squeezed phonon operators a_i^+, a_i were defined in terms of the electron number operators $n_{i\sigma}$ rather than odd powers of the Fermi operators. The corresponding relation for H_{hopp} can be derived using the original b operators. The squeezed phonon number operator $N = a^+a$ depends on the number of electrons at the site and can be written as

$$N_j = \exp\left\{-\frac{1}{4}\tanh^{-1}\left[\frac{2g}{\Omega}(n_{j\uparrow} + n_{j\downarrow})\right](b_j^2 - (b_j^+)^2)\right\} \times$$

$$\times b_j^+ b_j \exp\left\{\frac{1}{4}\tanh^{-1}\left[\frac{2g}{\Omega}(n_{j\uparrow} + n_{j\downarrow})\right](b_j^2 - (b_j^+)^2)\right\}.$$

We have to check that $[N_j, e^{-\gamma_{i\sigma}} c^+_{i\sigma} c_{j\sigma} e^{\gamma_{j\sigma}}] = [N_i, e^{-\gamma_{i\sigma}} c^+_{i\sigma} c_{j\sigma} e^{\gamma_{j\sigma}}] = 0$.

Since the operator N_j commutes with the factor $e^{-\gamma_{i\sigma} c^+_{i\sigma}}$, it is sufficient to check the commutator $[N_j, c_{j\sigma} e^{\gamma_{j\sigma}}] = 0$. We can verify this last commutator by a direct calculation with simple algebra as

$$c_{j\sigma} e^{\gamma_{j\sigma}} N_j = c_{j\sigma} \exp\left\{-\frac{1}{4}\tanh^{-1}[\frac{2g}{\Omega} n_{j\bar{\sigma}}](b_j^2 - (b_j^+)^2)\right\} b_j^+ b_j \exp\left\{\frac{1}{4}\tanh^{-1}[\frac{2g}{\Omega} n_{j\bar{\sigma}}](b_j^2 -\right.$$

$$\left. -(b_j^+)^2)\right\} \exp\left\{-\frac{1}{4}\tanh^{-1}[\frac{2g}{\Omega} n_{j\bar{\sigma}}](b_j^2 - (b_j^+)^2)\right\} \exp\left\{\frac{1}{4}\tanh^{-1}[\frac{2g}{\Omega}(n_{j\sigma} + n_{j\bar{\sigma}})](b_j^2 -\right.$$

$$\left. -(b_j^+)^2)\right\} = c_{j\sigma} \exp\left\{-\frac{1}{4}\tanh^{-1}[\frac{2g}{\Omega} n_{j\bar{\sigma}}](b_j^2 - (b_j^+)^2)\right\} \times$$

$$\times b_j^+ b_j \exp\left\{\frac{1}{4}\tanh^{-1}[\frac{2g}{\Omega} n_{j\bar{\sigma}}](b_j^2 - (b_j^+)^2)\right\} e^{\gamma_{j\sigma}}.$$

It is easy to see that $N_j c_{j\sigma} e^{\gamma_{j\sigma}}$ has exactly the same form if we permute the operator $c_{j\sigma}$ on the left-hand side with the operator N_j, using the following relation for $N_j c_{j\sigma} e^{\gamma_{j\sigma}}$: $f(n_{j\sigma}, n_{j\bar{\sigma}}) c_{j\sigma} = f(0, n_{j\bar{\sigma}}) c_{j\sigma} = c_{j\sigma} f(0, n_{j\bar{\sigma}})$, which is valid for any function f that can be expanded in a Fourier series. We can check the indentity $[N_i, e^{-\gamma_{i\sigma}} c_{i\sigma}] = 0$ in the similar way.

The action of the one-site Hamiltonian (7) on the wave function (13) results in:

$$H_{on-site} F^{(n)} = \sum_{x_1 \ldots x_{N_e}} (n\Omega - \frac{2nN_e g^2}{\Omega} - \frac{4ng^2}{\Omega} \sum_{i<j} \delta_{x_i x_j}) f(x_1, \ldots x_{N_e}) \times$$

$$\times \prod_{i=1}^{N_e} c^+_{x_i \sigma_i} \tilde{\Phi}(a_1^+, \ldots a_N^+, x_1, \ldots x_{N_e}) \prod_{k=1}^{N} |\tilde{0}\rangle_k^{ph}.$$

The action of the hopping Hamiltonian results in:

$$-t \sum_{x_1 \ldots x_{N_e}} \sum_{i_1}^{N_e} \{f(x_1, \ldots x_{i-1}, x_i - 1, x_{i+1}, \ldots x_{N_e}) +$$

$$+ f(x_1, \ldots x_{i-1}, x_i + 1, x_{i+1}, \ldots x_{N_e})\} \prod_{i=1}^{N_e} c^+_{x_i \sigma_i} |0\rangle_i^{el} \Phi(a_1^+, \ldots, a_N^+, x_1 \ldots x_{N_e}) \prod_{k=1}^{N} |\tilde{0}\rangle_k^{ph}.$$

Because of the modulated factors in the hopping part, the electron arguments are unchanged. Therefore the phonon part of the wave function can be separated. The electron amplitude f obeys the equation for Hubbard model with negative $U = -4g^2 n/\Omega$. Let us apply the results of [6] to our model. We will not write out the Bethe ansatz equations, which have been thoroughly described many times, including in [6], where expressions were derived for the ground state energy for low and high electron densities $\varrho = N_e/N$. For low electron densities $\varrho t\Omega/4ng^2 \ll 1$ we obtain

$$\frac{E^{(n)}}{N} = n\Omega - 2t\varrho - \frac{\varrho n^2 g^4}{t\Omega^2} - \frac{2g^2 n\varrho}{\Omega} \qquad \left(\varrho \ll \frac{4ng^2}{\Omega t}\right). \tag{16}$$

For high electron densities $\varrho t\Omega/4ng^2 \gg 1$ we get

$$\frac{E^{(n)}}{N} = n\Omega - 2t\varrho - \frac{\pi^2 t\varrho^3}{12} - \frac{g^2 n\varrho^2}{\Omega} - \frac{2g^2 n\varrho}{\Omega} - \frac{g^4 n^2 \varrho \log^2(\varrho t\Omega/2ng^2)}{\pi^2 \Omega^2 t}$$

$$\left(\varrho \gg \frac{4ng^2}{\Omega t}\right) \tag{17}$$

The one-particle excitation spectrum has a gap which comes from the on-site attraction, and for low electron densities (or for small hopping) this gap is the binding energy of a pair. So, for small $\varrho t\Omega/4ng^2 \ll 1$:

$$\Delta E = \frac{2n^2g^4}{t\Omega^2}\left(1 + O\left((\varrho t\Omega/4ng^2)^3\right)\right) \tag{18}$$

while for $\varrho t\Omega/4ng^2 \gg 1$ the gap has the following form:

$$\Delta E = 4g\sqrt{2ne^{-1}/\Omega}\left(\frac{N_e}{N}\right)^{3/2}\exp(\pi^2\alpha_0)\exp(-\pi^2 N_e\Omega t/4g^2Nn) \tag{19}$$

where $\alpha_0 \approx 0.11$ [6].

We know from [6] that the ground state energy has a nonmonotonic dependence on the number of squeezed phonons. Therefore, unlike the case of a chain of electrons coupled with harmonic phonons[4], here the optimal number of squeezed phonons that minimizes the ground state energy can be nonzero, $n \neq 0$. The value depends on the parameters Ω, t, g.

The effective negative Hubbard energy depends on the number of phonons. The coupling parameter in the exponent in (19) is similar to the BCS one. We can see also from (18) and (19) that the energy gap tends to narrow as the ratio $N_e\Omega t/g^2Nn$ increases. We note that a system of correlated electrons with Hubbard energy I could be described in the same manner. In this case we should replace our effective Hubbard interaction $U = -4g^2n/\Omega$ by an effective on-site interaction $U = I - 4g^2n/\Omega$. The formula for the ground state energy and gap should change in accordance with this replacement, and for $U > 0$ the results of [8,9] should be applied. The sign of Hubbard interaction in this case depends on the relationship of I, g, Ω, and n. The effective interaction becomes attractive for large enough n.

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1. H.Zheng and K.Nasu, Phys. Rev. **B 45**, 2148 (1992).
2. S.Nakajima, Y.Toyozawa, and R.Abe, *The Physics of Elementary Excitations*, Springer Ser. In Solid State Sci. **12**, 1980.
3. T.Hakioglu, V.A.Ivanov, A.S.Shumovsky, and B.Tanatar, Phys. Rev. **B 21**, 15363 (1995).
4. M.Ye.Zhuravlev, V.A.Ivanov, and V.V.Achkasov, Pis'ma v JETP **63**, 83 (1996).
5. H.Zheng, Phys. Rev. **B 36**, 8736 (1987).
6. V.Ya.Krivnov and A.A.Ovchinnikov, JETP **67**, 1568 (1974).
7. H.Chen, Y.-M.Zhang, and X.Wu, Phys. Rev. **B39**, 546 (1989).
8. E.Lieb and F.Wu, Phys. Rev. Lett. **20**, 1445 (1968).
9. A.A.Ovchinnikov, JETP **57**, 2137 (1969).

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