EXCITATION SPECTRUM IN THE ONE-DIMENSIONAL HUBBARD MODEL

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The spectrum of the lowest (quasi-homopolar) excitations in the one-dimensional Hubbard model are investigated within the framework of the exact method developed in articles[8-10]. The excitations are classified according to spin and momentum. The singlet states are states of the bound type. It is shown that both singlet and triplet excitations start from zero, i.e., they do not have a gap. The magnitude of the gap is determined for the spectrum of quasi-ionic states to which an optical transition is possible. Its dependence on the parameter characterizing the electron interaction is investigated.

1. INTRODUCTION

In order to describe the metal-dielectric transition associated with an increase of the repulsion between electrons, Hubbard[1] proposed a model of a Fermi lattice gas having an interaction of the electrons only at one center. In the case of a one-dimensional cyclic chain, the corresponding Hamiltonian has the following form:

$$H = \sum_{m,n}^{N} \sum_{\sigma} T_{m,n} a_{m\sigma}^{+} a_{n\sigma} + \frac{\gamma}{2} \sum_{n}^{N} \sum_{\sigma} a_{n-\sigma}^{+} a_{n-\sigma} a_{n\sigma}^{+} a_{n\sigma}, \qquad (1)$$

where $a_{n\sigma}^{+}$ and $a_{n\sigma}$ denote the creation and annihilation operators for an electron with spin σ in atom n; all $T_{m,n} = 0$ except $T_{n\pm1,n} = -\beta$ $(\beta > 0)$.

The Hamiltonian (1) was used in article[2] in order to explain the appearance of a gap in the optical spectrum of long polymers with conjugated bonds. In this connection it was shown, within the framework of the generalized Hartree-Fock method, that an excited state to which an optical transition is possible is separated from the ground state by a gap for arbitrary values of the parameter γ. For a suitable choice of γ it was possible to obtain agreement with the experimentally observed dependence of the magnitude of the first transition on the length of the chain. In addition to the excitations of the indicated type, the Hamiltonian (1) has below a gap a set of singlet and triplet quasi-homopolar excitations.[3,4] Here, as shown in the work by Kohn[5] and Bulaevskiĭ[3], an optical transition to these states is forbidden or very weak. Meanwhile these states play a major role in the determination of the physical and chemical properties of long systems with conjugated bonds. For example, the fact that the spectrum of the triplet excitations starts from zero leads, for infinitely long chains, to an appreciable paramagnetism of these molecules.[6]

The goal of the present article is a determination of the spectrum of the lowest quasi-homopolar excitations of the Hamiltonian (1) and their classification. We shall use the exact expression for the wave function of the Hamiltonian which was obtained in articles[7-9], where Bethe's idea[10] was extended.

Let us consider an eigenfunction of the Hamiltonian (1) with the number of electrons equal to the number of sites, i.e., N, and with the z-component of the total spin equal to zero (we shall assume N to be even). We shall seek it in the form

$$\Psi_Q(n_1, n_2, \ldots, n_N) = \sum_P [Q, P] \exp\left\{ i \sum_{j=1}^{N} k_{P_j} n_{Q_j} \right\},$$
$$1 \leqslant n_{Q_1} \leqslant n_{Q_2} \leqslant \ldots \leqslant n_{Q_N} \leqslant N. \qquad (2)$$

Here $k_1, k_2, \ldots, k_N$ denotes the set of quasimomenta for which the equation will be written down; $(Q_1, Q_2, \ldots, Q_N)$ and $(P_1, P_2, \ldots, P_N)$ denote permutations among the coordinates and momenta respectively. The summation in (2) is carried out over all permutations of the momenta k_i; the $[Q, P]$ are coefficients which simultaneously depend on Q and P and which are represented by a square matrix of order $N! \times N!$, which must be determined. The Schrödinger equation gives the following relation between these coefficients:

$$[Q, P] = Y_{nm}^{ab} [Q, P'], \qquad (3)$$

where the operator Y_{nm}^{ab} has the form[10]

$$Y_{nm}^{ab} = -\frac{i\gamma/2 + (\sin k_n - \sin k_m) P^{ab}}{\sin k_n - \sin k_m + i\gamma/2};$$
$$Q_i = a = Q_j', \quad Q_j = b = Q_i', \quad P_i = m = P_j', \quad P_j = n = P_i', \qquad (4)$$

$Q_k = Q_k'$, $P_k = P_k'$ for $k \neq i, j$ and the operator P^{ab} interchanges the sites Q_i and Q_j. In this connection the characteristic energy of the system is expressed in terms of the quasimomenta k_i in the following way:

$$E = -2\beta \sum_{j=1}^{N} \cos k_j. \qquad (5)$$

By successively applying the operator Y_{mn}^{ab}, one can express any arbitrary coefficient $[Q, P]$ in terms of (a vector of dimension N!) the coefficient $[Q, I]$, where I denotes the identity permutation among the momenta $k_1, k_2, \ldots, k_N$.

Utilization of the conditions for the cyclic nature and symmetry of the wave function leads to a system of equations for the coefficients $[Q, I]$. Omitting the subsequent calculations which are rather completely given in the article by Yang,[9] let us write down the transcendental equations for the quasimomenta k_i arising upon the solution of this system

$$Nk_j = 2\pi I_j + \sum_{\beta=1}^{N/2} \varphi(j\beta), \tag{6a}$$

$$\sum_{j=1}^{N} \varphi(j\alpha) = 2\pi J_\alpha + \sum_{\beta=1}^{N/2} \psi(\beta\alpha) + \pi, \tag{6b}$$

$$e^{i\varphi(j\beta)} = \frac{\sin k_j - \Lambda_\beta + ic/2}{\sin k_j - \Lambda_\beta - ic/2}, \tag{7a}$$

$$e^{i\psi(\beta\alpha)} = \frac{\Lambda_\beta - \Lambda_\alpha + ic}{\Lambda_\beta - \Lambda_\alpha - ic}, \quad c = \frac{\gamma}{2\beta}. \tag{7b}$$

Here Λ_α ($\alpha = 1, 2, \ldots, N/2$) denotes a set of numbers, all of which are different, and which in general may be complex. The phases $\psi(\alpha\beta)$ and $\varphi(j\beta)$ are determined so that

$$-\pi < \mathrm{Re}\,\psi(\alpha\beta),\ \mathrm{Re}\,\varphi(j\beta) < \pi,$$

I_j ($j = 1, 2, \ldots, N$) and J_α ($\alpha = 1, 2, \ldots, N/2$) are integers; they label the eigenstates of the system. For example, the total momentum Q of the system is expressed in terms of them in the following manner:

$$Q = \sum_{j=1}^{N} k_j = \frac{2\pi}{N}\left(\sum_{j=1}^{N} I_j + \sum_{\alpha=1}^{N/2} J_\alpha\right). \tag{8}$$

2. SPECTRUM OF THE TRIPLET EXCITATIONS

Let us consider the solution of the system of Eqs. (6) and (7) in the limit $\gamma \to \infty$. As is well-known, in this limit all eigenstates of the Hamiltonian (1) are divided into groups of almost degenerate states: homopolar, ionic, doubly ionic, etc. The first group consists of 2^N states with almost zero energy. The splitting of the energy levels among this group is described by the Heisenberg spin Hamiltonian. The second group consists of 2^N N states with energy $\sim\gamma$. A lowest excited state, to which an optical transition is possible, is found among this group. The third group contains $N(N-1)2^{N-1}$ states with energy $\sim 2\gamma$ and so forth. We will primarily be interested in the first group of states. Since the excited states of the spin Hamiltonian are well-known, then this makes it possible to classify the quasihomopolar states of the Hamiltonian (1) according to spin and momentum.

As $\gamma \to \infty$, Eqs. (6a), (6b) and (7a), (7b) go over into the following system of equations:

$$Nk_j = 2\pi I_j + \sum_{\beta=1}^{N/2} p_\beta, \quad \xi_\alpha = \mathrm{ctg}\frac{p_\alpha}{2} = -\frac{2\Lambda_\alpha}{c},$$

$$Np_\beta = 2\pi J_\beta + \sum_{\alpha(\neq\beta)} \psi(\alpha\beta), \quad 0 < p_\beta < 2\pi,$$

$$\mathrm{ctg}\frac{\psi(\beta\alpha)}{2} = \frac{1}{2}(\xi_\alpha - \xi_\beta). \tag{9}$$

This system agrees with the system of equations for the case of the spin Hamiltonian.[4] For the ground state of the system it is necessary to choose J_α and I_j in the following way:

$$J_\alpha = 1, 3, 5, \ldots, N-1, \tag{10}$$

$$I_j = -N/2, -N/2+1, \ldots, N/2-1. \tag{11}$$

For the quasi-homopolar levels all kj are real, and for convenience one can reduce them to the interval $(-\pi, \pi)$.

In order to determine the excited triplet states, following[11] let us choose J_α in the form

$$J_\alpha = 0, 2, 4, \ldots, 2n-2, 2n+1, \ldots, N-1, \tag{12}$$

where n is a certain number which determines the total quasimomentum of the system. The solution of Eqs. (6) and (7) is obtained by changing to a continuous distribution of the numbers k_j and Λ_α. In this connection one can use the formal equation $\rho(k) = dj/dk_j$ for the density of the numbers k_j in the interval $(-\pi, \pi)$ and $\sigma(\Lambda) = d\alpha/d\Lambda_\alpha$ for the density of the numbers Λ_α over the entire axis $(-\infty, \infty)$. Carrying out the required differentiation in Eqs. (6) and (7) under the conditions (11) and (12), we obtain the following system of equations for the triplet states:

$$\rho(k) = \frac{1}{2\pi} + \frac{\cos k}{2\pi}\int_{-\infty}^{\infty} \frac{4c\sigma(\Lambda)\,d\Lambda}{c^2 + 4(\Lambda - \sin k)^2}, \tag{13}$$

$$\int_{-\pi}^{\pi} \frac{4c\rho(k)\,dk}{c^2 + 4(\Lambda - \sin k)^2} = 2\pi\sigma(\Lambda) + \int_{-\infty}^{\infty} \frac{2c\sigma(\Lambda')\,d\Lambda'}{c^2 + (\Lambda - \Lambda')^2} + \frac{2\pi}{N}\delta(\Lambda - \Lambda_n),$$

$$E = -2N\beta\int_{-\pi}^{\pi} \rho(k)\cos k\,dk. \tag{14}$$

Here Λ_n is equal to its own unperturbed value, i.e., it is obtained from the solution of Eqs. (6) and (7) by utilization of the numbers J_α and I_j, just as for the ground state (10) and (11). Taking the Fourier transform of the function $\sigma(\Lambda)$, one can easily obtain an expression for $\rho(k)$ and $\sigma(\Lambda)$. Omitting this calculation, we cite the answer for the energy of the triplet states

$$E_t(q) = E_0 + 2\beta\int_0^{\infty} \frac{J_1(\omega)\cos\omega\Lambda_n\,d\omega}{\omega\,\mathrm{ch}(\omega c/2)}. \tag{15}$$

Here E_0, the energy of the ground state which was first determined by Lieb and Wu,[10] is given by

$$E_0 = -4N\beta\int_0^{\infty} \frac{J_1(\omega)J_0(\omega)\,d\omega}{\omega(1 + e^{\omega c})},$$

$J_0(\omega)$ and $J_1(\omega)$ are Bessel functions. The quantity Λ_n is expressed in terms of the quasimomentum of the system $q = 2\pi n/N$ in the following way:

$$q = \frac{\pi}{2} + \int_0^{\infty} \frac{J_0(\omega)}{\omega}\frac{\sin\omega\Lambda_n}{\mathrm{ch}\,(\omega c/2)}\,d\omega. \tag{16}$$

The system (15) and (16) parametrically determines the $E_t(q)$ dependence. The function $E_t(q)$ possesses a double periodicity and reaches a maximum at $q = \pi/2$. If $\gamma \to \infty$

$$\varepsilon_t(q) = E_t(q) - E_0 \cong (4\pi\beta^2/2\gamma)\,|\sin q|,$$

which agrees with the expression for the triplet excitations[11] in the Heisenberg model with an exchange integral equal to $4\beta^2/\gamma$.

3. SPECTRUM OF THE SINGLET EXCITATIONS

As was shown in[4] the lowest singlet states of an antiferromagnetic Heisenberg chain necessarily belong to the bound state type, i.e., they correspond to complex momenta in the spin system. Our calculation of the spectrum of the singlet quasi-homopolar excitations of the Hamiltonian (1) will be entirely based on an analogy with a similar calculation for the spin Hamiltonian.

Let us choose sets of numbers I_j and J_α in the

following way. Let us leave the set I_j unchanged, as given by Eq. (11), but

$$J_\alpha = 1, 3, \ldots, 2\beta_1 - 1, 2\beta_1 - 1, \ldots, 2\beta_2 - 3, 2\beta_2 + 1, \ldots, N - 1. \quad (17)$$

According to[4] two complex-conjugate numbers $\Lambda_a = \lambda + i\kappa$ and $\Lambda_b = \lambda - i\kappa$ will correspond to two identical numbers J_{β_1}. We note that the total quasi-momentum of such a system will be determined in the following way:

$$q = 2\pi (J_{\beta_1} - J_{\beta_2}) / N. \quad (18)$$

One can choose all remaining Λ_α to be real. From the imaginary part of Eq. (6c) for α = a we have $\kappa = c/2$. Changing to a continuous distribution of the numbers Λ_α and k_j and introducing the corresponding densities according to the formulas of the preceding Section, we obtain the following system of equations:

$$\rho(k) = \frac{1}{2\pi} + \frac{\cos k}{2\pi} \int_{-\infty}^{\infty} \frac{4c\sigma(\Lambda)\,d\Lambda}{c^2 + 4(\Lambda - \sin k)^2} - \frac{1}{2N\pi} T(k),$$

$$T(k) = \left[2\pi\delta(\sin k - \Lambda) - \frac{2c}{c^2 + (\sin k - \lambda)^2} \right] \cos k$$

$$+ \cos k \sum_{m=1,2} \left[\frac{4c}{c^2 + 4(\bar{\Lambda}_{\beta_m} - \sin k)^2} - 2\pi\delta(\sin k - \bar{\Lambda}_{\beta_m}) \right]; \quad (19)$$

$$\int_{-\pi}^{\pi} \frac{4c\rho(k)\,dk}{c^2 + 4(\sin k - \Lambda)^2} = 2\pi\sigma(\Lambda) + \int_{-\infty}^{\infty} \frac{2c\sigma(\Lambda')\,d\Lambda'}{c^2 + (\Lambda - \Lambda')^2} + \frac{D(\Lambda)}{N},$$

$$D(\Lambda) = -4\pi\delta(\Lambda - \lambda) + \frac{4c}{4(\Lambda - \lambda)^2 + c^2} + \frac{12c}{4(\lambda - \Lambda)^2 + 9c^2}$$

$$+ \sum_{m=1,2} \left[2\pi\delta(\Lambda - \bar{\Lambda}_{\beta_m}) - \frac{2c}{c^2 + (\Lambda - \bar{\Lambda}_{\beta_m})^2} \right]. \quad (20)$$

In connection with the derivation of these equations we added to the system of real numbers Λ_α two additional numbers $\bar{\Lambda}_{\beta_1}$ and $\bar{\Lambda}_{\beta_2}$ which satisfy the same equations as the number Λ_α for $J_{\beta_1} = 2\beta_1 - 1$, $J_{\beta_2} = 2\beta_2 - 1$. The function $\sigma(\Lambda)$ is represented out of the density of real numbers Λ_α together with the two additional numbers $\bar{\Lambda}_{\beta_1}$ and $\bar{\Lambda}_{\beta_2}$.

The solution of the system of equations is obtained by transition to the Fourier transform for the function $\sigma(\Lambda)$. Omitting the calculations, we write down an expression for the energy of the singlet quasi-homopolar excitations

$$E_s(q) = E_0 + 8\beta \int_0^{\infty} \frac{d\omega J_1(\omega)}{\omega \operatorname{ch}(\omega c/2)} (\cos \omega\bar{\Lambda}_{\beta_1} + \cos \omega\bar{\Lambda}_{\beta_2} - \cos \omega\lambda). \quad (21)$$

In this connection, just as in[4], the following restriction is imposed on $\bar{\Lambda}_{\beta_1}$, $\bar{\Lambda}_{\beta_2}$, and λ:

$$|\bar{\Lambda}_{\beta_1}| > 1, \; |\bar{\Lambda}_{\beta_2}| > 1, \; |\lambda| > 1. \quad (22)$$

The condition for solvability of the system of equations for the number Λ_α (here it is required that $\Lambda_\alpha \neq \Lambda_\beta$ for $\alpha \neq \beta$) at once gives the equation

$$\lambda = \bar{\Lambda}_{\beta_2}. \quad (23)$$

The real part of Eq. (6b) for α = a together with Eq. (23) leads to the relation

$$2\beta_1 = \beta_2. \quad (24)$$

Finally Eqs. (18) and (24) make it possible to relate the total momentum q of the system to Λ_{β_1}:

$$|q| = \pi - 2 \int_0^{\infty} \frac{d\omega J_0(\omega) \sin \omega\bar{\Lambda}_{\beta_1}}{\omega \operatorname{ch}(\omega c/2)}. \quad (25)$$

Equation (25) together with the equation which follows from (21) and (23),

$$\varepsilon_s(q) = 8\beta \int_0^{\infty} \frac{d\omega J_1(\omega) \cos \omega\bar{\Lambda}_{\beta_1}}{\omega \operatorname{ch}(\omega c/2)} \quad (26)$$

give the parametric dependence of the energy of the singlet excitations on the quasimomenta. Here one should keep in mind the limiting condition $|\bar{\Lambda}_{\beta_1}| > 1$. It leads to the result that the singlet excitation spectrum has a termination point at

$$q_0 = \pi - 2 \int_0^{\infty} d\omega \frac{J_0(\omega) \sin \omega}{\omega \operatorname{ch}(\omega c/2)}. \quad (27)$$

For $\gamma \to \infty$ the value $|q_0| = \pi/2$. If $\gamma = 0$ then $q_0 = 0$, which indicates the absence of bound states in this limit. For small q the spectra of singlet and triplet excitations have identical slopes:

$$\varepsilon_{t,s}(q) = |q| \frac{2\beta I_1(\pi/c)}{I_0(\pi/c)}, \quad (28)$$

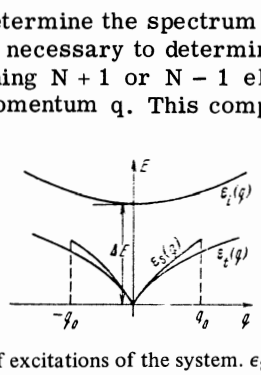
where I_1 and I_0 are Bessel functions of imaginary argument. For large values of q the singlet levels always lie above the triplet levels. For sufficiently large but not infinite values of N, the energy of the first triplet level tends to zero in the following way:

$$\varepsilon_t(N) = -\frac{4\pi\beta}{N} \frac{I_1(2\pi\beta/\gamma)}{I_0(2\pi\beta/\gamma)} \quad (29)$$

Let us make several remarks about the energy of the singlet quasi-ionic states. A strong optical transition takes place precisely to these states. The quasi-ionic states possess a nonvanishing current. The energy of the lowest current state and, consequently, the gap in the optical spectrum in the one-dimensional Hubbard model were calculated in the article by Lieb and Wu.[10] For its determination they obtained an energy $E_+ = E_0 + \mu_+$ for the ground state of the system containing N + 1 electrons and an energy $E_- = E_0 + \mu_-$ for the ground state of the system containing N − 1 electrons. The gap in the spectrum of the quasi-ionic states is then determined in the following way:

$$\Delta E = E_+ - E_- = \mu_+ - \mu_-. \quad (30)$$

In order to determine the spectrum of the quasi-ionic states it is necessary to determine the energy of a system containing N + 1 or N − 1 electrons and having a total momentum q. This computation is quite



Different types of excitations of the system. $\epsilon_s(q)$ is the spectrum of singlet homopolar excitations for small q, as given by Eqs. (25) and (26); q_0 given by Eq. (27) is the point of termination of the spectrum; $\epsilon_t(q)$ is the spectrum for the homopolar triplet excitations which are described by Eqs. (15) and (16); $\epsilon_i(q)$ is the spectrum for the ionic excitations, and ΔE given by Eq. (33) is the gap in the spectrum of the ionic states.

analogous to the one given in the text. Without giving it in detail, in the figure we show the general form of the spectra for the lowest excited states. Different types of excitations of the system. $\epsilon_s(q)$ is the spectrum of singlet homopolar excitations for small q, as given by Eqs. (25) and (26); q_0 given by Eq. (27) is the point of termination of the spectrum; $\epsilon_t(q)$ is the spectrum for the homopolar triplet excitations which are described by Eqs. (15) and (16); $\epsilon_i(q)$ is the spectrum for the ionic excitations, and ΔE given by Eq. (33) is the gap in the spectrum of the ionic states.

Lieb and Wu[10] arrived at the following expression for the gap ΔE:

$$\Delta E = \gamma - 4\beta + 8\beta \sum_{n=1}^{\infty} (-1)^n [(1 + c^2 n^2)^{1/2} - cn]. \quad (31)$$

It is possible to give a more convenient expression for ΔE. For this purpose let us represent the series in (31) in terms of an integral along a contour C_0 which encompasses the real axis from c to ∞:

$$\sum_{n=1}^{\infty} (-1)^n [(1 + c^2 n^2)^{1/2} - nc] = \frac{1}{2ic} \int_{C_0} \frac{dz}{\mathrm{sh}(\pi z/c)} (\sqrt{z^2 + 1} - z). \quad (32)$$

Deforming the contour C_0 until it coincides with the imaginary axis, we can represent ΔE in the form

$$\Delta E = \frac{16\beta^2}{\gamma} \int_1^{\infty} \frac{\sqrt{y^2 - 1}\, dy}{\mathrm{sh}(\pi y/c)}. \quad (33)$$

For $\gamma \to \infty$ the gap is given by $\Delta E \approx \gamma - 4\beta + (8\beta^2/\gamma) \ln 2 + \ldots$. If the strength of the electron interaction is decreased, i.e., if $\gamma \to 0$, then

$$\Delta E \approx 8\pi^{-1} \sqrt{\gamma\beta}\, e^{-2\pi\beta/\gamma}. \quad (34)$$

We note that to within the pre-exponential factor this expression agrees with the expression given in article[2] for the gap as $\gamma \to 0$.

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