The excitation spectrum of a one-dimensional Fermi gas

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The question of the exact calculation of the excited states of the one-dimensional Hubbard model with $\rho < 1$ (ρ is the number of electrons per unit cell) is considered in connection with the experimentally observed anomalies, indicating the existence of a lattice superstructure, in the x-ray scattering and neutron diffraction by TTF-TCNQ crystals. A new branch of excitations is found (two others were calculated earlier by Coll [Phys. Rev. B9, 2150 (1974)], the energy of which vanishes at $k = \pi\rho$ (k is the momentum of the excitation) irrespective of the value of the electron-electron interaction constant c. It is found that at $c \to 0$ these excitations are of the single-particle type. An analytic expression is obtained for their energy for small and large values of c. A generalization of the model considered to the case of an interaction potential of finite range a is proposed. Exact equations, valid for $\rho a \ll 1$ and determining the excitation spectrum in these model, are obtained. It is shown that in this case too the above-mentioned excitation branch possesses the property $\epsilon(\pi\rho) = 0$.

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As is well known, the one-dimensional Hubbard model is one of the few examples of a quantum-mechanical many-particle system for which it has been possible to obtain exact solutions. This model has been studied particularly fully in the case when $\rho = 1$ For this case, in particular, the different types of excitations have been classified and their energies calculated (see the review[1]).

The Hubbard model can be applied as the simplest model in the description of the electron states of quasi-one-dimensional donor-acceptor systems. However, since in the most interesting of these the charge transfer is not complete,[2] it is necessary to consider the Hubbard model with $\rho < 1$. In this connection it should be remarked that the properties of the model with $\rho = 1$ and that with $\rho < 1$ differ very sharply. Thus, e.g., unlike in the case $\rho = 1$, the single-particle excitation spectrum for $\rho < 1$ is gapless.[1]

Excited states in the Hubbard model with $\rho < 1$ have been studied in Ref. 3. Two branches $\Delta E_1(k)$ and $\Delta E_2(k)$ were found in the excitation spectrum, and, by analogy with the case $\rho = 1$, were classified as a spin-wave branch and a single-particle branch, respectively. As was shown in Ref. 3, irrespective of the strength c of the interaction these excitations possess the property $\Delta E_1(2k_F^0) = \Delta E_2(4k_F^0) = 0$, where k_F^0 is the Fermi momentum of a system of noninteracting electrons, connected with the density by the relation $k_F^0 = \pi\rho/2$.

This feature of the excitation spectra of the Hubbard model with $\rho < 1$ (the presence of the characteristic momenta $2k_F^0$ and $4k_F^0$) has been used to explain recent experiments on diffuse x-ray scattering[4,5] and inelastic neutron scattering[6,7] by TTF–TCNQ crystals, in which strong scattering at the wave-vector values $q = 0.295b^*$ and $0.59b^*$ was observed ($b^* = 2\pi/b$, where b is the lattice constant in the direction parallel to the stacks of molecules). According to Ref. 8, the values of q at which scattering occurs can be identified with the characteristic momenta $2k_F^0$ and $4k_F^0$ (in this case, the value of ρ for TTF–TCNQ is equal to 0.59), and the scattering at $q = 0.295b^*$ is associated with the direct excitation of spin waves. Although not all the features of the scattering observed in the above-mentioned experiments were explained in Ref. 8, there is no doubt that investigation of the excited states of the Hubbard model with $\rho < 1$ is of obvious interest from the point of view of the study of the properties of donor-acceptor complexes with incomplete charge transfer.

As already mentioned earlier, the energies of the excitations found by Coll[3] vanish at $k = 2k_F^0$ and $k = 4k_F^0$. The existence of these characteristic momenta in the Hubbard model with $\rho < 1$ is not surprising and is a consequence of the one-dimensionality of the problem. We shall explain this using the example of a one-dimensional Fermi gas without interaction, i.e., with $c = 0$. The spectrum of the single-particle excitations for this case is depicted in Fig. 1. The quantity $\Delta E(2k_F^0) = 0$, because the energy required to excite an electron from the state with $k = -k_F^0$ to the state with $k = k_F^0$ is equal to zero. At the same time, the single-particle branch found in Ref. 3 does not coincide in the limit $c = 0$ with the spectrum in Fig. 1. Moreover, as will be shown below, in this limit the above-mentioned branch corresponds to two-particle excitation. It also turns out that the very concept of an excitation of the single-particle type loses its meaning to a considerable extent for the model with $\rho < 1$, and can be introduced only in the limits of large and small values of c. We shall indicate a method by means of which such a classification could be made, and shall calculate the excitation branch (absent in Ref. 3) that possesses the correct single-particle behavior for $c \to 0$.

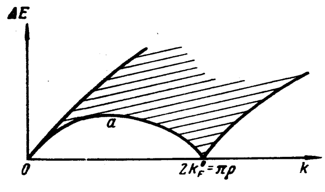

FIG. 1. Single-particle excitation spectrum of a noninteracting Fermi gas.

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Before proceeding to the calculation of the excitation spectrum we make the following remark. With no loss of generality we can assume that $\rho \ll 1$. In this case the Hubbard Hamiltonian reduces to the Hamiltonian of a one-dimensional Fermi gas with δ-function repulsion; this has the form

$$\hat{H}=-\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2}+2c\sum_{i<j}\delta(x_i-x_j). \qquad (1)$$

In (1) we have taken $\hbar=1$, $2m=1$. All the results obtained for the Hamiltonian (1) can be generalized without difficulty to the Hubbard model with $\rho<1$ (for more detail, see below).

According to Gaudin[9] and Yang,[10] the exact energy eigenvalues of (1) in states with momentum k are equal to

$$E=\sum_{j=1}^{N}p_j^2, \qquad (2)$$

$$k=\sum_{j=1}^{N}p_j, \qquad (3)$$

while the quasi-momenta p_j are determined by solving the transcendental system of equations

$$Lp_j=2\pi I_j-2\sum_{\alpha=1}^{M}\operatorname{arctg}\frac{2(p_j-\Lambda_\alpha)}{c},$$
$$2\sum_{j=1}^{N}\operatorname{arctg}\frac{2(\Lambda_\alpha-p_j)}{c}=2\pi J_\alpha+2\sum_{\beta\neq\alpha}\operatorname{arctg}\frac{\Lambda_\alpha-\Lambda_\beta}{c}. \qquad (4)$$

Here the Λ_α ($\alpha=1, 2, \ldots, M$) are a set of unequal numbers, the numbers I_j and J_α are integers or half-integers that label the eigenstates of the system, and L is the length of the one-dimensional chain. The total spin S of a state is equal to $S=\frac{1}{2}(N-2M)$. In the following we shall be interested only in states with $S=0$ (in particular, the ground state is always a singlet), and, therefore, $M=N/2$.

For the ground state it is necessary to choose I_j and J_α as follows[1]:

$$I_j^0=-{}^1/_2(N+1)+j, \quad j=1, 2, \ldots N,$$
$$J_\alpha^0=-{}^1/_2(M+1)+\alpha, \quad \alpha=1, 2, \ldots M. \qquad (5)$$

As shown in Ref. 1 for the Hubbard Hamiltonian with $\rho=1$ (for which the corresponding transcendental system of equations is analogous to (4)), the excited states of the spin-wave type correspond to the appearance of a hole in the distribution of the numbers J_α as compared with their distribution in the ground state, i.e.,

$$I_j=I_j^0,\ J_\alpha=J_\alpha^0+\theta(\alpha-t),\ 1\leqslant t\leqslant M,$$
$$\theta(x)=\begin{cases}1, & x\geqslant 0\\ 0, & x<0\end{cases}. \qquad (6)$$

The single-particle excitations for $\rho=1$ are characterized by the presence of a hole in the distribution of the numbers I_j, i.e.,

$$I_j=I_j^0+\theta(j-m),\ J_\alpha=J_\alpha^0,\ 1\leqslant m\leqslant N. \qquad (7)$$

This classification was used by Coll[3] in the calculation of the corresponding branches of the excitation spectrum. The following expressions were obtained for the lower bounds on the energies of the excitations of the spin-wave type ($\Delta E_1(k)$) and single-particle type ($\Delta E_2(k)$) (only in the limits $c\to 0$ and $c\to\infty$ is it possible to find them in analytic form):

$$\Delta E_1(k)=k(\pi\rho-k),\ c\to 0, \qquad (8)$$

$$\Delta E_1(k)=\frac{2}{3}\frac{(\pi\rho)^3}{c}\sin\frac{k}{\rho},\quad c\to\infty, \qquad (9)$$

$$\Delta E_2(k)=k(\pi\rho-k/2),\quad c\to 0, \qquad (10)$$

$$\Delta E_2(k)=k(2\pi\rho-k),\quad c\to\infty. \qquad (11)$$

As can be seen from (8)–(11), $\Delta E_1=0$ at $k=0$ and $k=\pi\rho=2k_F^0$, while $\Delta E_2=0$ at $k=0$ and $k=4k_F^0$. As shown by Coll,[3] these excitations will possess this property for arbitrary c.

We note, however, that (10) does not coincide with the expression for the energy of the single-particle excitations of a system of noninteracting electrons (curve a in Fig. 1). The reason for this disagreement is that the method of constructing the excited states (at any rate, the single-particle states), while correct for $\rho=1$, ceases to be correct for $\rho<1$.

A natural way of choosing the numbers I_j and J_α corresponding to such excitations can be found if we make use of the fact that the distribution of quasi-momenta for $c\to 0$ (for finite N) should correspond to the occupation of the momentum states for the ideal Fermi gas. We note here that, although Eqs. (4) are usually solved after taking the thermodynamic limit, for $c\to 0$ they can also be solved exactly for finite N.

First we shall consider the ground state. In this case the solution of (4), to within terms $\sim c$, has the form (see also Fig. 2)

$$p_{2a-1}=2\pi n_a/L-(c/L)^{1/2},$$
$$p_{2a}=2\pi n_a/L+(c/L)^{1/2}, \qquad (12)$$
$$\Lambda_a=2\pi n_a/L,$$

where $n_a=-(M+1)/2+a$, $a=1, 2, \ldots, M$. The expressions (12) are valid for $cL\ll 1$. We note also that (12) corresponds, in essence, to the concept, introduced by Gaudin,[9] of pairs of quasi-momenta.

The occupation of the states for $c=0$ in accordance with formula (2) is conveniently depicted schematically (see Fig. 3). We now consider Eqs. (4), with I_j and J_α corresponding to the choice (7). The solutions of (4) for $m=2t$ have the form ($cL\ll 1$)

$$p_{2a-1}=2\pi n_a/L-(c/L)^{1/2},\quad p_{2a}=2\pi n_a/L+(c/L)^{1/2}$$

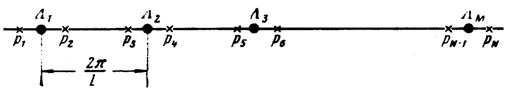

FIG. 2. Solutions (12) (schematic).

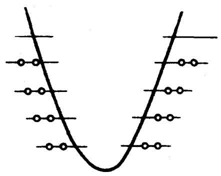

FIG. 3. Ground state for $c \to 0$ (schematic).

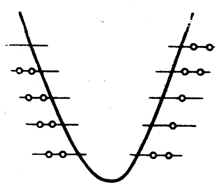

FIG. 4. Solutions (13) (schematic).

for $a < t$, and

$$p_{2a-1}=2\pi n_{a+1}/L-(c/L)^{1/2}, \quad p_{2a}=2\pi n_{a+1}/L+(c/L)^{1/2} \tag{13}$$

for $a > t$;

$$p_{2t-1}=2\pi n_t/L, \quad p_{2t}=2\pi n_{t+1}/L.$$

The solution (13) is shown schematically in Fig. 4. Comparison of (12) and (13) shows that for $c \to 0$ the states associated with the choice (7) of I_j and J_α correspond to two-particle excitations. The single-particle excitations for $c \to 0$ correspond to the scheme shown in Fig. 5. It is not difficult to convince oneself that the solutions of (4) that lead to this scheme correspond to choosing the numbers I_j and J_α in the form

$$I_j=I_j^0+\theta(j-2t), \quad J_\alpha=J_\alpha^0-\theta(\alpha-(t+1)). \tag{14}$$

The solution of (4) that corresponds to (14) for arbitrary c can be obtained by passing to a continuous distribution of the numbers p_j and Λ_α. We represent p_j and Λ_α in the form

$$p_j=p_j^0+\omega_j/L, \quad \Lambda_\alpha=\Lambda_\alpha^0+\xi_\alpha/L, \tag{15}$$

where p_j^0 and Λ_α^0 are the solutions of (4) for the ground state, and ω_j and ξ_α are functions of p and Λ, respectively. Introducing the functions $f(p)=g(p)\omega(p)$ and $\psi(\Lambda)=\sigma(\Lambda)\xi(\Lambda)$($g(p)$ and $\sigma(\Lambda)$ are the densities of the numbers p_j and Λ_α in the ground state), we obtain for them a system of integral equations:

$$2\pi f(p)=\int_{-\infty}^{\infty}\frac{4c\psi(\Lambda)\,d\Lambda}{c^2+4(p-\Lambda)^2},$$

$$2\pi\psi(\Lambda)-2\operatorname{arctg}\frac{2(\Lambda-q)}{c}+2\operatorname{arctg}\frac{2(\Lambda-Q)}{c}$$

$$=-2\pi\theta(\Lambda-\Lambda_0)+\int_{-Q}^{Q}\frac{4cf(p)\,dp}{c^2+4(\Lambda-p)^2}-\int_{-\infty}^{\infty}\frac{2c\psi(\Lambda')\,d\Lambda'}{c^2+(\Lambda-\Lambda')^2}, \tag{16}$$

where Q is determined from the condition

$$\int_{-Q}^{Q} g(p)\,dp=\frac{N}{L}=\rho, \tag{17}$$

and $q=p_{2t}^0$, $\Lambda_0=\Lambda_{t+1}^0$; Λ_0 can be expressed in terms of q by means of the relation

$$\int_{-Q}^{q} g(p)\,dp=2\int_{-\infty}^{\Lambda_0}\sigma(\Lambda)\,d\Lambda, \quad -Q\leqslant q\leqslant Q. \tag{18}$$

The energy ε and momentum k of an excitation have the form

$$\varepsilon=2\int_{-Q}^{Q} pf(p)\,dp+Q^2-q^2,$$

$$k=\int_{-Q}^{Q} f(p)\,dp+Q-q. \tag{19}$$

Introducing the new functions $f_1(p)=f(p)+\theta(p-q)$ and $\psi_1(\Lambda)=\psi(\Lambda)+\frac{1}{2}\theta(\Lambda-\Lambda_0)$ and taking the Fourier transform with respect to Λ in the second of Eqs. (16), we obtain for $f_1(p)$ the following integral equation:

$$2\pi f_1(p)=2\pi\theta(p-q)-2\operatorname{arctg}\exp\left(-\frac{(\Lambda_0-p)}{c}\pi\right)+\int_{-Q}^{Q} f_1(p')\,dp'\int_{-\infty}^{\infty}\frac{d\omega\, e^{i\omega(p'-p)}}{1+e^{|\omega|c}},$$

$$\varepsilon=2\int_{-Q}^{Q} pf_1(p)\,dp, \quad k=\int_{-Q}^{Q} f_1(p)\,dp. \tag{20}$$

We note the following property of $f_1(p)$. When $q=Q$ the quantity $\Lambda_0 \to \infty$, $f_1(p)=0$ and $\varepsilon(k=0)=0$. When $q=-Q$, on the other hand, $\Lambda_0 \to -\infty$, and, as is easily seen from (20), the function $f_1(p)\pi^{-1}$ coincides with the solution of the equation[11] for the density of the numbers p_j in the ground state, i.e., with the function $g(p)$. By virtue of (17), we have

$$\varepsilon(k=\pi\rho)=0. \tag{21}$$

Thus, the excitation energy $\varepsilon(k)$ vanishes at $k=2k_F^0$ for arbitrary values of c.

The equation (20) can be solved in analytic form for $c \to 0$ and $c \to \infty$. The quantity Λ_0 found from (18) for these cases is, respectively,

$$\Lambda_0=q \text{ and } \Lambda_0=-\frac{c}{\pi}\ln\operatorname{tg}\frac{\pi}{4}\left(1-\frac{q}{Q}\right).$$

In this case, for $\varepsilon(k)$ we have

$$\varepsilon(k)=k(\pi\rho-k), \quad c\to 0, \quad k>0, \tag{22}$$

$$\varepsilon(k)=4k\left(1-\frac{4\rho\ln 2}{c}\right)(\pi\rho-k)-\frac{2(\pi\rho)^3}{3c}\sin\frac{k}{\rho}, \quad c\to\infty. \tag{23}$$

The expression (22) attests that the excitation branch we have obtained is a single-particle branch for $c \to 0$, as we should expect from the way it was derived. At the same time, the Fermi velocity of these excitations for $c \to \infty$ is twice as large as we should expect starting

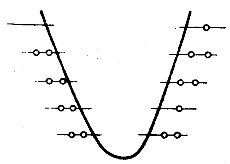

FIG. 5. Single-particle excitations for $c \to 0$.

from the idea that the Fermi gas becomes spinless as $c \to \infty$.[1] The reason for this is easily understood if we consider the solutions of (4) for finite N as $c \to \infty$. The expressions for p_j in this case have the following simple form:

$$p_j = \frac{2\pi I_j}{L} + \frac{2\pi}{NL} \sum_{\alpha} J_\alpha. \tag{24}$$

The solutions (24) for the ground state and the excitations corresponding to (6), (7) and (14) are shown schematically in Fig. 6. (The dashed lines in Figs. 6b and 6d show the positions of the levels for the ground state and the arrows indicate the corresponding shifts of the levels.) From the standpoint of these schemes the single-particle excitations found by Coll[3] are indeed single-particle for $c \to \infty$. In this limit, the excitation branch that we have found is, generally speaking, a combination of single-particle and collective (spin-wave) excitations (compare Figs. 6b and 6d, and also (9) and (23)). Thus, it turns out that the classification of the excited states depends in an essential way on the magnitude of c.

Up to this point our treatment has pertained to a one-dimensional Fermi gas with δ-function repulsion, i.e., to the Hubbard model with $\rho \ll 1$. However, everything expounded above can be generalized without difficulty to the case of a lattice Fermi gas with $\rho < 1$. Thus, e.g., Eq. (20) is replaced by the following equation:

$$2\pi f_1(p) = 2\pi\theta(p-q) - 2 \operatorname{arctg} \exp\left(-\frac{2(\Lambda_0 - \sin p)}{u}\pi\right)$$
$$+ \int_{-Q}^{Q} \cos p' f_1(p')\, dp' \int_{-\infty}^{\infty} \frac{\exp[i\omega(\sin p' - \sin p)]}{1+e^{|\omega|u/2}}\, d\omega, \quad u = 2c, \tag{25}$$
$$\varepsilon = 2\int_{-Q}^{Q} \sin p f_1(p)\, dp, \quad k = \int_{-Q}^{Q} f_1(p)\, dp.$$

It is not difficult to convince oneself, in a manner analogous to the way this was done above, that $\varepsilon(\pi\rho) = 0$ for any u. For $u \to 0$ the energy $\varepsilon(k)$ found from (25) coincides with the expression for the single-particle excitations of a noninteracting lattice Fermi gas, while for $u \to \infty$ it has the form

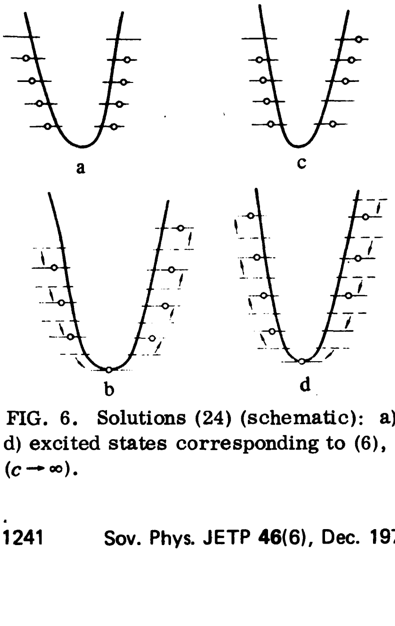

FIG. 6. Solutions (24) (schematic): a) the ground state; b, c, d) excited states corresponding to (6), (7), (14), respectively ($c \to \infty$).

$$\varepsilon(k) = 4\sin(\pi\rho - k)\sin k - \frac{16\rho\ln 2}{u}\Big[\sin\pi\rho\sin(\pi\rho - k)\cos k$$
$$-\sin(\pi\rho - 2k)\left(\frac{k}{\pi\rho}\sin\pi\rho + \sin(\pi\rho - 2k)\right)\Big]. \tag{26}$$

As we should expect, for $\rho \ll 1$ (26) goes over into (23).

Before proceeding to consider the other generalization of the model that we are investigating, we make the following remark. Our analysis of the excited states of the one-dimensional Fermi gas has been based on the exact solution of the Hubbard model with $\rho < 1$. Another approach to this problem, intensively developed in recent times in the papers of Luther, Emery and Peschel,[12-14] is associated with the investigation of a one-dimensional model with a linear spectrum (the linear model), which is a generalization of the well-known Luttinger model.[15] In particular, in Refs. 12–14 spin degrees of freedom were incorporated into the Luttinger model, and Umklapp processes and the interaction describing the backward scattering were taken into account. The most representative Hamiltonian, incorporating other types of interaction too, is given in the paper by Prigodin and Firsov.[16] On the other hand, linearizing the kinetic equation about k_F and introducing two kinds of particles with $k \simeq k_F$ and $k \simeq -k_F$ makes it possible to reduce the Hubbard Hamiltonian to a Hamiltonian $\hat{H}_{11n}$ coinciding with that given by Prigodin and Firsov.[16] True, all the possible types of interaction contained in $\hat{H}_{11n}$ appear here with the same constant c. According to Luther and Emery,[12] $\hat{H}_{11n}$ can be separated into commuting operators $\hat{H}_1$ and $\hat{H}_2$ describing the spin and single-particle excitations, respectively. Then, if $\rho < 1$, the Hamiltonian $\hat{H}_2$ can be diagonalized by the method of Lieb and Mattis.[15] It is easy to show that its excitation spectrum has the form $\varepsilon(k) = v_F'|k|$, where the renormalized Fermi velocity $v_F' = v_F(1 + 2c/\pi v_F)^{1/2}$ (in our notation, $v_F = \pi\rho$). It can be seen by comparing this expression with (22) and (23) (this comparison has meaning only for $|k| \ll \pi\rho$, since for large k the linearization of the Hubbard Hamiltonian is not legitimate) that the excitation spectra of a one-dimensional Fermi gas with the Hamiltonian (1) and the linear model coincide only for small values of $c (c/\rho \ll 1)$.

As regards the spin-excitation spectrum, here, unfortunately, it is not possible to carry out such a comparison, since the method proposed in Ref. 12 to diagonalize $\hat{H}_1$ is applicable only for a particular value of c, and this $c < 0$ (attraction).

We return now to the analysis of the one-dimensional Fermi gas with the Hamiltonian (1). Another generalization of this model is a Fermi gas with an interaction potential of finite range. For simplicity we shall consider the case when the interaction has the form of a potential step:

$$V(x) = \begin{cases} u_0, & |x| < a \\ 0, & |x| > a \end{cases}.$$

The boundary conditions relating the wavefunction and its derivative at $x_i - x_j = \pm a$ lead to a system of transcendental equations:

$$Lp_j=2\pi I_j-2\sum_{\alpha=1}^{M}\operatorname{arctg}\frac{2(p_j-\Lambda_\alpha)}{c_1}-\sum_{i=1}^{N}\operatorname{arctg}\frac{p_i-p_j}{c_1}+\sum_{i=1}^{N}\operatorname{arctg}\frac{p_i-p_j}{c_2},$$

$$2\sum_{j=1}^{N}\operatorname{arctg}\frac{2(\Lambda_\alpha-p_j)}{c_1}=2\pi J_\alpha+2\sum_{\beta\neq\alpha}\operatorname{arctg}\frac{\Lambda_\alpha-\Lambda_\beta}{c_1}; \qquad (27)$$

$$c_1=\gamma a^{-1}\operatorname{sh}2\gamma,\qquad c_2=\gamma a^{-1}\operatorname{th}2\gamma,\qquad \gamma=au_0^{1/2}.$$

We note that this generalization is valid if $\rho a \ll 1$ (otherwise, the Bethe hypothesis, on the basis of which Eqs. (27) were obtained, is certainly incorrect).

The system (27) can be reduced in the standard way to a system of integral equations, in terms of the solutions of which the energies of the ground and excited states are determined. In particular, the equation describing the excitation branch corresponding to the choice (14) of I_j and J_α has the form

$$2\pi f_1(p)=2\pi\theta(p-q)-2\operatorname{arctg}\exp\left(-\frac{(\Lambda_0-p)}{c_1}\pi\right)$$
$$+\int_{-Q}^{Q}f_1(p')\,dp'\int_{-\infty}^{\infty}\frac{d\omega\, e^{i\omega(p'-p)}}{1+\exp(|\omega|c_1)}+\int_{-Q}^{Q}\frac{c_2f_1(p')\,dp'}{c_2^2+(p-p')^2}-\int_{-Q}^{Q}\frac{c_1f_1(p')\,dp'}{c_1^2+(p-p')^2},$$
$$\varepsilon=2\int_{-Q}^{Q}pf_1(p)\,dp,\qquad k=\int_{-Q}^{Q}f_1(p)\,dp. \qquad (28)$$

It is possible to show, in a manner analagous to the way this was done in the derivation of (21), that $\varepsilon(\pi\rho)=0$ in this case too.

Thus, the excitations considered possess the property (21) irrespective of the strength of the interaction or of whether it is attractive. We note, however, that the excited states of the Fermi gas with an interaction potential of finite range have a number of features distinguishing them from those in the case of δ-function repulsion. We shall consider, e.g., the limit $\gamma\to\infty$ (a Fermi gas of hard rods). The presence of two "interaction constants" c_1 and c_2 in (27) and (28) leads to the result that, for $\gamma\to\infty$, the expression for $\varepsilon(k)$ is a series in powers of γ^{-1} and $\gamma^{-1}e^{-2\gamma}$:

$$\varepsilon(k)=4k(\pi\rho-k)\left(1-\frac{2\rho a}{\gamma}\right)\cdots$$
$$\cdots+\frac{16k(\pi\rho-k)}{\gamma}\rho a e^{-2\gamma}(1-2\ln 2)-\frac{4}{3}(\pi\rho)^3\frac{a}{\gamma}e^{-2\gamma}\sin\frac{k}{\rho}+\cdots \qquad (29)$$

As can be seen by comparing (29) and (23), the "collective" spin-wave contribution to $\varepsilon(k)$ is exponentially small. The energies of the spin-wave excitations corresponding to the choice (6) of I_j and J_α are just as exponentially small in the parameter γ. They have the form (9) with $c=\gamma a^{-1}e^{2\gamma}/2$.

This is a consequence of the fact that a potential step of infinite height is impenetrable, and the exchange integral that appears in the corresponding spin Hamiltonian is exponentially small for $\gamma\to\infty$.

In conclusion we note the following. The new branch of excitations of the Hubbard model with $\rho<1$, obtained in this work, possesses the property that its energy is equal to zero at $k=2k_F^0$. It is possible to assume that the excitations of this type are associated (together with the purely spin-wave excitations) with the scattering at $q=0.295b^*$ observed in the experiments of Refs. 4–7. A justification for this is provided by the fact that for $c\to\infty$ (and, evidently, $c\gg 1$ in TTF–TCNQ[8]), this branch is a combination of single-particle and collective excitations and is associated with both the neutron and the x-ray scattering. However, only by calculating the response of the system to a periodic perturbation is it possible to say this with certainty. Unfortunately, for the corresponding calculation in second order of perturbation theory in the external field it is necessary to know the wavefunctions of the unperturbed system, and these are too complicated to calculate, even for $c\to\infty$.

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