объединенный
институт
ядерных
исследований
дубна

E17 - 12836

V.K.Fedyanin

PARTICLE-LIKE EXCITATIONS IN THE SYSTEMS DESCRIBED BY THE HUBBARD MODEL WITHOUT CHIRALITY CONDITION

1979

E17 - 12836

V.K.Fedyanin

PARTICLE-LIKE EXCITATIONS IN THE SYSTEMS DESCRIBED BY THE HUBBARD MODEL WITHOUT CHIRALITY CONDITION

Submitted to ТМФ

Федянин В.К. **E17 - 12836**

Частицеподобные возбуждения в системах, описываемых моделью Хаббарда при отказе от условия киральности

Показано, что в длинноволновом пределе при отказе от условия киральности /нормировки плотности на константу/ уравнения для шредингеровских амплитуд в модели Хаббарда имеют пару частицеподобных решений. Это существенно при обсуждении свойств квазиодномерных магнитных структур, где подобные возбуждения могут определять статическое и динамическое поведение системы.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1979

Fedyanin V.K. **E17 - 12836**

Particle-Like Excitations in the Systems Described by the Hubbard Model without Chirality Condition

This note is devoted to consequencies of the refusal from the chirality condition and assumptions on the character of dynamics in the Hubbard model used in paper[1]. A self-consistent pair of soliton solutions is obtained for the switched off electron-phonon interaction ($I=0$), and possible modifications are discussed for them for $I\neq 0$.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Preprint of the Joint Institute for Nuclear Research. Dubna 1979

1. Paper [1] has dealt with the study of the one-dimensional Hubbard model [2,3] in the continuum approximation, where alongside with the electron system also the effects of electron-phonon interaction have been taken into account. If one uses the Schrödinger wave function of the system proposed in [4,5] for the models, the dynamics of which is essentially determined by the ground state, then the Schrödinger wave function $\Phi_{\sigma}(\xi,t)$ obeys the following system of equations

$$i\dot{\Phi}_{\sigma} = T\Phi''_{-\sigma} + (2T-\hat{I}\sum_{\sigma'} \Phi^{*}_{\sigma'}\Phi_{-\sigma'})\Phi_{-\sigma} + v\,|\Phi_{-\sigma}|^{2}\Phi_{\sigma} - \mu\Phi_{\sigma} \qquad (1)$$

(in [1] we have considered, following [3], that the ground state in the Hubbard model is of the antiferromagnetic nature). Here $T=\bar{t}+\hat{I}\cdot a\cdot(1-k)$ is the kinetic energy of electron, renormalized by the effects of electron-phonon interaction $\hat{I}\cdot a\cdot(1-k)$, μ is the chemical potential; v, the Coulomb repulsion of electrons with opposite spins, $\hat{I}=4I^{2}M^{-1}(\omega^{2}-\omega_{0}^{2})^{-1}$, $\omega_{0}^{2}=\alpha/M$; deviations from the equilibrium states are assumed to be small $(\omega^{2}\neq\omega_{0}^{2})$. Specific expressions for the parameters in (1) in terms of the potential matrix elements and its derivatives with respect to the Wannier-states and also the notation accepted can be found in [1]. The system (1) is a system of four equations for $\Phi_{\uparrow}$, $\Phi_{\downarrow}$, $\Phi^{*}_{\uparrow}$, $\Phi^{*}_{\downarrow}$ ($\sigma=1/2$ corresponds to $\uparrow$ and $\sigma=-\frac{1}{2}$ to $\downarrow$). In deriving the system (1) we have used in [1] (in passing from the equations of motion for the Heisenberg operators to the equations for the Schrödinger amplitudes $\Phi_{\sigma}(\xi, t)$) splitting [4,5] of the three-particle matrix elements via one-particle elements and a particular choice of the dependence of the total shift $x(\xi, t)$ at point (ξ,t): $x=(\xi-\omega t)$. (The latter is however not necessary, but simplifies the derivation of the equation (see, e.g., ref. [4])).

Next, in paper [6] a possibility was analyzed for the existence of soliton solutions for the system (1). It was shown that in case 1) the chirality condition $|\Phi_\uparrow|^2+|\Phi_\downarrow|^2=\mathrm{const}$ is fulfilled; 2) the change in dynamics with time of Φ_σ is determined by the change in amplitude $|\Phi_{-\sigma}|^2$ and Φ_σ (neglecting in the equation for Φ_σ in the sum over σ' the term with $\sigma'=\sigma$), then (1) can be transformed to the mutually independent equations for $C_+(\xi,t)$, $C_-(\xi,t)$, where

$$C_+(\xi,t)=\Phi_\uparrow(\xi,t)+\Phi_\downarrow(\xi,t),\ C_-(\xi,t)=\Phi_\uparrow(\xi,t)-\Phi_\downarrow(\xi,t), \qquad (2)$$

solutions of which describing the particle-line excitations are given by the expressions

$$C_+(\xi,t)=\sqrt{2\bar{n}}\ \mathrm{sech}\,[\sqrt{\frac{v-\hat{I}}{T}\bar{n}}(\xi-\hat{u}t)]e^{-i\frac{\hat{u}}{2T}\xi-iV_+t},$$
$$C_-(\xi,t)=\sqrt{2\bar{n}}\tanh[\sqrt{\frac{v-\hat{I}}{T}n}(\xi-\hat{u}t)]e^{i\frac{\hat{u}}{2T}\xi-iV_-t}, \qquad (3)$$

and the frequencies V_+ and V_- are expressed via the signal velocity $\hat{u}$ and model parameters

$$V_+=2T-\mu-\frac{\hat{u}^2}{4T},\quad V_-=-2T-\mu+(v-\hat{I})\bar{n}+\frac{\hat{u}^2}{4T}. \qquad (4)$$

Physically $C_-(\xi,t)$ corresponds to the transition between two domains ("domain wall"); and $C_+(\xi,t)$, to the full probability of the spin in this interval (see (2)).

In this note we shall analyze consequences of the refusal from the conditions 1) and 2) and obtain soliton solutions for the "pure" Hubbard model.

2. Denoting $\hat{I}$ in eq. (1), before omitted in [1,6] terms, via α we can rewrite (1) in the form

$$i\dot{\Phi}_\sigma-T\Phi''_{-\sigma}-2T\Phi_{-\sigma}-(v-\hat{I})|\Phi_{-\sigma}|^2\Phi_\sigma+\mu\Phi_\sigma=-\alpha\Phi^*_\sigma\Phi_{-\sigma}\Phi_{-\sigma}. \qquad (5)$$

Passing from Φ and Φ to $C_\pm$ by formulae (2)

$$\Phi(\xi,t)=\frac{C_++C_-}{2},\ \Phi=\frac{C_+-C_-}{2} \qquad (6)$$

by some algebraic computations we obtain for $C_\pm$ the following system of equations

$$iC_+-TC''_+-(2T-\mu-(v-\hat{I})\frac{|C_+|^2+|C_-|^2}{2})C_+-(v-\hat{I})|C_+|^2C_+=$$
$$=\alpha[-(|C_+|^2+|C_-|^2)\frac{C_+}{2}+\frac{3}{4}|C_+|^2C_++\frac{C_+^*}{4}C_-^2]; \qquad (7)$$

$$iC_- + TC_-'' - (-2T - \mu - (v - \hat{I})\frac{|C_+|^2 + |C_-|^2}{2})C_- - (v - \hat{I})|C_-|^2 C_- =$$
$$= \alpha[-(|C_+|^2 + |C_-|^2)\frac{C_-}{2} + \frac{3}{4}|C_-|^2 C_- + \frac{C_-^*}{4}C_+^2]. \qquad (7)$$

If in (7) one postulates (posits) that

$$|\Phi_\uparrow|^2 + |\Phi_\downarrow|^2 \equiv \frac{|C_+|^2 + |C_-|^2}{2} = \bar{n} = \text{const}$$

and puts $\alpha = 0$, then one naturally gets the equations for $C_\pm$ of ref.[1] which have the soliton solutions (3). Without these constraints one arrives at the system (7) for four complex functions $C_\pm$, $C^*_\pm$. Along this way, a) the terms $\sim \alpha|C_\pm|^2 C_\pm$ merely renormalize the effective potential $(v - \hat{I})|C_\pm|^2 C_\pm$; b) the terms $\sim\alpha|C_\mp|^2 C_\pm$, along with $(v - \hat{I})|C_\pm|^2 C_\pm$, represent the effects of modification of this effective potential at the expense of the change in amplitude, "another" solution, that results in the dependence of the amplitude and phase C_+ on the amplitude C_- and vice versa (for details see below); c) the terms $\sim \alpha C^*_\pm C^2_\mp$ result in a "perturbed" system of equations. Note that in this case the deviation from integrability (perturbation) is fully due to the effects of electron-phonon interaction (in[4] it was related to the existence of anomalous terms in the Hamiltonian $\sim (a^+_n a^+_{n+1} - a_n a_{n+1})$; and in[5], to a different contribution from the x- and y-components of spin). The term $\alpha C^*_\pm C^2_\mp$ changes qualitatively the behaviour of solutions in a certain range of parameters that can be studied by modifying the methods developed in[7,8] as applied to a more simple model[4]. For the "pure" Hubbard model and things become much simpler: the system of equations following from (7)

$$iC_\pm = \pm TC_\pm'' + (\pm 2T - \mu)C_\pm + \frac{v}{2}(|C_\pm|^2 - |C_\mp|^2)C_\pm, \qquad (8)$$

as will be shown below, admits soliton solutions which describe the particle-like excitations. If the terms $\alpha\frac{C^*_\pm}{4}C^2_\mp$ in (7) are dropped, i.e., the effects of electron-phonon interaction are taken into account only partially, then we arrive at the following system of equations

$$iC_\pm = \pm TC_\pm'' + (\pm 2T - \mu)C_\pm + \frac{v - \hat{I} + \alpha/2}{2}|C_\pm|^2 C_\pm - \frac{v - \hat{I} + \alpha}{2}|C_\mp|^2 C_\pm \qquad (9)$$

Soliton solutions can be obtained for (9) also. However, in this case the amplitude of the second solutions modifies the effective potential with the weight

$$\eta = \frac{v - \hat{I} + \alpha}{v - \hat{I} + \alpha/2} \cong \frac{1}{1 - \hat{I}/2v}$$

that may turn out to be important in the use of these solutions for physical applications. The derivation of the solutions themselves for (9) may be carried out in close analogy to their derivation for the system (8). For this reason we will analyze this question conformably to the system (8).

3. Introducing the new variables

$$\xi' = \left(\frac{v}{2T}\right)^{1/2}\xi, \quad t' = \frac{v}{2}t \tag{10}$$

we get for $C_\pm(\xi',t')$, instead of (8), the system

$$i\dot{C}_\pm = \pm C''_\pm + \lambda_\pm C_\pm + (|C_\pm|^2 - |C_\mp|^2)C_\pm . \tag{11}$$

Further on we shall omit the prime of ξ,t. Then, making the phase transformation

$$C_\pm \to \tilde{C}_\pm e^{-i\lambda_\pm t} , \tag{12}$$

we obtain for $\tilde{C}_\pm$ the simple system

$$i\dot{C}_\pm = \pm C''_\pm + (|C_\pm|^2 - |C_\mp|^2)C_\pm , \tag{13}$$

the tilde will be also omitted. We shall look for solutions of (13) in a particle-like form

$$C_+(\xi,t) = \phi(\xi - ut)e^{i\alpha(\xi - v_+ t)} , \quad C_-(\xi,t) = f(\xi - ut)e^{i\beta(\xi - v_- t)} , \tag{14}$$

where $\phi(\xi - ut)$, $f(\xi - ut)$ are real function of $(\xi - ut)$, α, β, u, v_+ , v_- are parameters; the relation between them and amplitudes ϕ_0, f_0 will be established later. The substitution of (14) into (13) gives

$$\begin{aligned} -i(u\phi' + i\alpha v_+\phi) &= \phi'' + 2i\alpha\phi' - \alpha^2\phi + (\phi^2 - f^2)\phi, \\ -i(uf' + i\beta v_- f) &= -f'' - 2i\beta f' + \beta^2 f + (f^2 - \phi^2)f, \end{aligned} \tag{15}$$

where the prime means the derivative with respect to $(\xi-ut)$. Requirung the relations (10) $2\alpha=-u$, $2\beta=u$ hold, we arrive at the following system of equations

$$\begin{aligned} &\alpha v_+\phi=\phi''-\alpha^2\phi+(\phi^2-f^2)\phi, \\ &\beta v\_f=-f''+\beta^2 f+(f^2-\phi^2)f. \end{aligned} \tag{16}$$

Let us try to fulfil the system (16) by the following choice of $\beta\phi(\xi-ut)$ and $f(\xi-ut)$

$$\phi=\phi_0\,\mathrm{sech}[\lambda(\xi-ut)],\quad f=f_0\tanh[\lambda(\xi-ut)]. \tag{17}$$

The substitution of (17) into (16) gives

$$\begin{aligned} \frac{u}{2}v_+ &= \lambda^2-2\lambda^2\tanh^2[\lambda(\xi-ut)]+\frac{u^2}{4}-\phi_0^2\,\mathrm{sech}^2[\lambda(\xi-ut)]+ \\ &\quad +f_0^2\tanh^2[\lambda(\xi-ut)]; \\ \frac{u}{2}v_- &= 2\lambda^2\,\mathrm{sech}\ [\lambda(\xi-ut)]+\frac{u^2}{4}+f_0^2\tanh^2[\lambda(\xi-ut)]- \\ &\quad -\phi_0^2\,\mathrm{sech}^2[\lambda(\xi-ut)]. \end{aligned} \tag{18}$$

Imposing on the requirement

$$2\lambda^2=\phi^2+f^2,\quad \lambda=\sqrt{\frac{\phi_0^2+f_0^2}{2}}\ , \tag{19}$$

we arrive at the following relation of $v_\pm$ with the signal velocity and amplitudes

$$v_+=\frac{u}{2}+\frac{f_0^2-\phi_0^2}{u},\quad v_-=\frac{u}{2}+\frac{2f_0^2}{u}. \tag{20}$$

Here the amplitude modulation of soliton phases $C_\pm(\xi,t)$ is clearly seen. The formulae (14), (16), (19), and (20) solve the problem of derivation of the soliton solutions to the system of equations (8); arbitrary parameters here are u, ϕ_0, f_0.

Applying to (10) and (12), we turn back to the initial variables. For $C_\pm(\xi,t)$ we have

$$C_+(\xi, t) = \phi_0 \operatorname{sech}[(\frac{v}{T})^{1/2} \frac{\sqrt{\phi_0^2 + f_0^2}}{2} (\xi - \hat{u}t) e^{-i\frac{\hat{u}}{2T}\xi - i\hat{V}_+ t},$$

$$C_-(\xi, t) = f_0 \tanh[(\frac{v}{T})^{1/2} \frac{\sqrt{\phi^2 + f^2}}{2} (\xi - \hat{u}t) e^{i\frac{\hat{u}}{2T}\xi - i\hat{V}_- t}, \quad (21)$$

where

$$\hat{V}_+ = 2T - \mu - \frac{\hat{u}^2}{4T} - \frac{v}{4}(f_0^2 - \phi_0^2),$$

$$\hat{V}_- = -2T - \mu + \frac{\hat{u}^2}{4T} + \frac{v}{2} f_0^2, \quad \hat{u} = u \cdot (\frac{vT}{2})^{1/2} \quad (22)$$

(the relations (20) have been used). The solutions (21) define a self-consistent pair of particle-like excitations in the (ξ, t)-space, the amplitudes of which change considerably at distances $L \sim (\frac{T}{v})^{1/2} \frac{2}{\sqrt{\phi_0^2 + f_0^2}}$ and phases are given by the formulae (22). Requiring $\phi_0^2 = f_0^2 = 2\bar{n}$ the formulae (21), (22) convert to (3), (4) for $C_\pm$, $V_\pm$ at $I = 0$.

REFERENCES

1. Lindner V., Fedyanin V.K. phys.stat.sol. (b), 1978, 6, 89, p.123.
2. Hubbard J. (I). Proc.Roy.Soc., 1963, A276, p.238.
3. Lieb E.H., Wu F.Y. Phys.Rev.Lett., 1969, 20, p.1445.
4. Fedyanin V.K., Makhankov V.G., Yakushevich L.V. Phys.Lett., 1977, A61, p.256. Федянин В.К., Якушевич Л.В. ТМФ,1978, 37, с.371.
5. Fedyanin V.K., Yushanchai V.I. Phys.Lett., 1969, A470, p.459.
6. Lindner V., Fedyanin V.K. phys. stat.sol. (b), 1979, 95, p.K83.
7. Маханьков В.Г., Федянин В.К. ДАН СССР, 1977, 236, с.838.
8. Маханьков В.Г., Федянин В.К. ТМФ, 1979, 39, с.381.

Received by Publishing Department
on December 1 1979.