Electric current due to excitations in the Hubbard model

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A calculation is described of the electric current due to various excitations in the Hubbard model. The electric charge for one-particle excitation is found and its value is shown to depend in a continuous manner on the electron occupancy of the system and on the single-site repulsion potential.

INTRODUCTION

Quasi-one-dimensional highly conducting compounds have been the subject of major interest in the last decade. The most interesting effects in these compounds are associated with the electron-phonon and electron-electron interactions. The electron-phonon interaction creates charge density waves associated with the transition of a material from a metallic to an insulating state (Peierls effect). The excited states of a Peierls insulator are self-localized states such as solitons or polarons, which exhibit an anomalous coupling of the spin to the charge. A theory of the Peierls effect has been developed on the basis of discrete and continuum models in a semiclassical (in respect of the phonon degrees of freedom) approximation which can be solved exactly.[1-6] It has been found that the properties of a Peierls insulator depend strongly on the electron density ρ in a unit cell; if $\rho = 1$, then the steady-state excitations of the system are solitons (kinks) carrying a spin $s = 1/2$ or a charge $q = \pm e$ and polarons with $q = e$ and $s = 1/2$; if $\rho \neq 1$, then spin-carrying ($s = 1/2$) zero-charge solitons are the excited states.[2] The effects of the commensurability[4] and of the discrete nature of the lattice,[5,7] together with an allowance for the dispersion of the phonon spectrum,[8] are responsible for the fractional charge which depends continuously on the occupancy ρ. The charge of such excitations is localized in a finite region of size ξ which is of the order of dimensions of a soliton or a polaron.

In real systems the Coulomb interaction may modify considerably the structure and properties of the ground state and of excitations of a system that carry an electric current and spin. We shall consider a situation opposite to that found in a Peierls insulator: we shall deal with a one-dimensional system of electrons interacting with one another but not with the lattice deformation. We shall investigate a current due to excitations in the Hubbard model, which describes a system of N electrons on a discrete chain of N_a sites with repulsion between electrons at the same site. The Hubbard model is used because of its simplicity and because it provides an exactly solvable quantum model. In contrast to kinks in the Peierls model, excitations in the Hubbard model are delocalized. The Hubbard model can be used to interpret the properties of quasi-one-dimensional compounds in which the Coulomb interaction is much stronger than the electron-phonon interaction.

The content of the present paper is arranged as follows. A model to be used later is formulated in Sec. I and the properties ofthe ground state needed later are given; a description is also provided of the investigated types of excited states and an expression is obtained for an electric current carried by excitations. A consistent analysis is made of various excited states in Sec. II and this is followed by a calculation of the current j, the energy ε, the momentum p, and the velocity of excitations v; the electric charge is found for one-particle excitations. The electric charge of such excitations is found as the coefficient of proportionality between the current $j(p)$ carried by excitations and the velocity $v = d\varepsilon/dp$.[1)] It is shown that in general the charge of these excitations is fractional and its value is governed by the energy of the Hubbard repulsion U and by the occupancy ρ of the electron energy band. It follows from our results that the excitation of such a system, for example by introduction of an additional particle, results in a redistribution of the quasimomenta of all particles in the system. Therefore, the motion of an excited particle is accompanied by the motion of its background, so that the total electric charge consists of contributions made by a current due to a screened particle and a countercurrent of the homogeneous background. This is the reason for the fractional charge of the excitations.

I. PRINCIPAL DEFINITIONS

The Hubbard model describes a system of interacting electrons on a discrete chain represented by the Hamiltonian[10]

$$H=-t\sum_{i=1}^{N_a}\sum_{\sigma}(c_{i,\sigma}^{+}c_{i+1,\sigma}+c_{i+1,\sigma}^{+}c_{i,\sigma})+U\sum_{i=1}^{N_a}n_{i,\uparrow}n_{i,\downarrow}, \qquad (1)$$

where $c_{i,\sigma}^{+}$ and $c_{i,\sigma}$ are the operators representing creation and annihilation of electrons with spins $\sigma = \uparrow,\downarrow$ at the ith site; $n_{i,\sigma} = c_{i\sigma}^{+}c_{i,\sigma}$; U is the repulsion energy of electrons with opposite spins at the same site; t is the integral representing hopping between neighboring sites. The exact solution of the system was obtained by Lieb and Wu.[11] The excitations in this model were investigated in Refs. 12–14. The energy and momentum of the system for the ground and excited states were determined in Ref. 11 in terms of quasimomenta k_j, which can be found from the following equations[11]

$$N_a k_j=2\pi I_j+\sum_{\beta=1}^{M}\theta(2\sin k_j-2\lambda_\beta), \quad j=1,\ldots,N, \qquad (2)$$

$$\sum_{j=1}^{N}\theta(2\sin k_j-2\lambda_\alpha)=2\pi J_\alpha-\sum_{\beta=1}^{M}\theta(\lambda_\alpha-\lambda_\beta), \quad \beta=1,\ldots,M, \qquad (3)$$

where $\theta(x) = -2\tan^{-1}(2x/u)$; M is the number of electrons with a spin $\rho = \downarrow$; I_j and J_α are sets of integral (or half-integral) numbers; here and later we shall assume that $u = U/t$ and $t = 1$. In the case of the ground state, we have

$$J_{\alpha+1}-J_\alpha=1,\quad I_{j+1}-I_j=1,\quad \sum J_\alpha+\sum I_j=0.$$

The quasimomenta k_j for the ground state are distributed in an interval $-Q < k_j < Q$, where Q is expressed in terms of the electron density $\rho = N/N_a$ as follows[15]:

$$Q=\pi\rho-4\rho(\ln 2)\sin(\pi\rho)/u+O(1/u^2). \tag{4}$$

We shall consider excitations of the following type.

1. Triplet states of the spin wave type with a distribution I_j as in the ground state, and with a distribution J_α given by

$$J_{\alpha+1}-J_\alpha=1+\delta_{\alpha,\alpha_0} \tag{5}$$

(such a state is called by Lieb and Wu "a hole in the λ distribution").

2. One-particle excitations: a) "a hole in the k distribution"

$$I_{j+1}-I_j=1+\delta_{j,n},\quad J_{\alpha+1}-J_\alpha=1; \tag{6}$$

b) "a particle in the k distribution"

$$I_{j+1}-I_j=1+A\delta_{N-1,j},\quad J_{\alpha+1}-J_\alpha=1. \tag{7}$$

The spectra of excitations of types 1 and 2 were investigated in Refs. 12 and 13. One-particle excitations 2 associated with a redistribution of the charge and differing from the ground state only by the distribution of the momenta should occur obviously only in a chain for which the electron band is not half-filled ($N/N_a = \rho \neq 1$), since for $\rho = 1$ all the k_j states are occupied [k_j are defined by Eq. (3) apart from 2π].

3. Excitations with complex wave numbers. In contrast to excitations of types 1 and 2, these excitations describe states in which there are electron pairs occupying (at least in the limit of high values of u) one lattice site. In contrast to zero-gap excitations 1 and 2, these excitations have a gap (of the order of u in the limit of high u) and they can appear both for a $\rho = 1$ and for $\rho \neq 1$. As demonstrated by Woynarovich,[14] such excitations should be described by complex wave numbers $k_j = \varkappa \pm i\chi$. For simplicity, we shall consider the case of excitations with one pair of complex wave numbers.

4. Excitations formed on introduction of an additional $(N+1)$-th particle or a hole into the system. In this case we have excited states of two types: states of type 2, differing from the ground state by a redistribution of the quasimomenta in the case when $\rho \neq 1$ and states of type 3 with complex quasimomenta in the case of an arbitrary value of ρ.

We shall calculate the current carried by various excitations. The operator describing the electric current is readily obtained from Eq. (1):

$$j=i\sum_{n,\sigma}(c^+_{n+1,\sigma}c_{n,\sigma}-c^+_{n,\sigma}c_{n+1,\sigma}). \tag{8}$$

The expression for the current given by Eq. (8) is derived in a standard manner, as for any other physical system, from the law of conservation of the electric charge:

$$d\rho_n/dt+\operatorname{div} j=0,$$

where $d\rho/dt = i[H,\rho]$; $\rho_n = c^+_{n,\sigma}c_{n,\sigma}$; H is the Hamiltonian of Eq. (1). In the discrete case, we have $\operatorname{div} j = j_{n+1} - j_n$. The current operator of Eq. (8) commutes with the Hamiltonian (1). Using the explicit form of the wave functions, taken from Ref. 11, we can find from Eq. (8) the following expressions for the current in the system:

$$j=\sum_{j=1}^{N}\sin k_j.$$

We can readily see that the wave function of this sytem is in the form of a Bloch function analogous to the wave function of quasiparticles in the crystal lattice:

$$\psi(x_1,\ldots,x_N)=u(x_1,\ldots,x_N)\exp\left[ip\left(\sum x_i\right)\Big/N\right],$$
$$u(x_1+1,\ldots,x_N+1)=u(x_1,\ldots,x_N).$$

Therefore, we can determine similarly the quasimomentum p from the condition

$$\hat{T}\psi(x_1,\ldots,x_N)=\psi(x_1+1,\ldots,x_N+1)=e^{ip}\psi(x_1,\ldots,x_N).$$

The quasimomentum found in this way can be expressed in terms of a set of numbers k_j using the relationship $p = \Sigma k_j$ (Ref. 11). By analogy with a definition of the velocity of quasiparticles in a periodic crystal chain, we can adopt the momentum representation and readily show that the velocity $v(p)$ of excitations with the quasimomentum p is of the standard form $v(p) = d\varepsilon(p)/dp$. The electric charge of an excitation is found in the usual way as the ratio of the current transported by an excitation to the excitation velocity: $q(p) = j(p)/v(p)$.

II. DETERMINATION OF THE ELECTRIC CURRENT AND CHARGE DUE TO EXCITED STATES

1. Triplet states (spin wave)

Subtracting from Eqs. (2) and (3) the equations for the ground state, we find—allowing for Eq. (5)—that in the limit $N_a \to \infty$

$$2\pi\rho(k)=\int_{-\infty}^{\infty}\frac{8u\tilde\sigma(\lambda)\,d\lambda}{u^2+16(\sin k-\lambda)^2},$$

$$\int_{-Q}^{Q}\frac{8u\tilde\rho(k)\cos k\,dk}{u^2+16(\sin k-\lambda)^2}=2\pi\tilde\sigma(\lambda)+\int_{-\infty}^{\infty}\frac{4u\tilde\sigma(\lambda')\,d\lambda'}{u^2+4(\lambda-\lambda')^2}-2\pi\theta(\lambda-\lambda_0). \tag{9}$$

where

$$\tilde\rho(k_j)=N_a\rho_0(k_j)\delta k_j,\quad \tilde\sigma(\lambda_\alpha)=N_a\sigma_0(\lambda_\alpha)\delta\lambda_\alpha,$$

$\rho_0(k)$ and $\sigma_0(\lambda)$ are the functions of the ground state: δk_j and $\delta\lambda_\alpha$ are the shifts of the values of k_j and λ_α relative to the values for the ground state; $\delta k_j \propto \delta\lambda_\alpha \propto \sim O(1/N_a)$. An investigation of the excitation spectrum reported in Ref. 13 was based on equations for the function $\rho_1(k)$: $\rho(k) = \rho_0(k) + \rho_1(k)/N_a$; however, no allowance was made there for the asymmetry of the quasimomenta k_0 and k_N ($k_0 \neq -k_N$) or for the limits of integration in integrals of the $\int f(k)\rho(k)dk$ type. Hence, the momentum or current could not be calculated using expressions of the type

$$p=N_a\int k\rho(k)\,dk,\quad j=2N_a\tilde\rho(k)\sin k\,dk,$$

but the energy was found in Ref. 13 employing an expression $E=-2\int\rho(k)\cos k dk$ with symmetric integration limits. The calculated energy is correct at least in the leading order with respect to u and this is due to the even nature of the function $\cos k$ in the integrand, because the contributions due to asymmetric boundary conditions balance out.

The Fourier transformation given in Ref. 9 yields the following equation for $\tilde\rho(k)$:

$$\tilde\rho(k)=\frac{1}{\pi}\operatorname{arctg}\left\{\exp\left[-\frac{2\pi(\lambda_0-\sin k)}{u}\right]\right\}$$
$$+\int_{-Q}^{Q}dk'\cos k'\tilde\rho(k')\frac{4}{u}R\left(\frac{4}{u}[\sin k-\sin k']\right),\qquad(10)$$

where

$$R(x)=\frac{1}{4\pi}\int_{-\infty}^{\infty}\frac{e^{ixy/2}}{e^{|y|}+1}dy.$$

We shall now write down the expressions for the energy, momentum, and current in terms of $\tilde\rho(k)$:

$$\varepsilon=E-E_0=2\int_Q^Q\tilde\rho(k)\sin k\,dk,$$
$$p=\int_{-Q}^{Q}\tilde\rho(k)\,dk,\quad j=2\int_{-Q}^{Q}\tilde\rho(k)\sin k\,dk.\qquad(11)$$

It follows from Eq. (10) that $\tilde\rho(k)$ is a function of $\tilde\rho(\sin k)$; if $\rho=1$, $Q=\pi$, we find that

$$\tilde\rho(k)=\pi^{-1}\operatorname{arctg}\exp[-2\pi(\lambda_0-\sin k)/u],\quad j=0.\qquad(12)$$

We shall consider the case of high values of u when $\rho\ll1$; in the leading order with respect to $1/u$, we obtain

$$\tilde\rho(k)=\operatorname{arctg}\exp[-2\pi(\lambda_0-\sin k)/u]$$
$$+4\pi^{-2}u^{-1}\operatorname{arctg}[\exp(-2\pi\lambda_0/u)]\sin Q\ln 2,\qquad(13)$$
$$j=2p\sin(\pi\rho)/\pi\rho,\quad p=2\rho\operatorname{arctg}\exp(-2\pi\lambda_0/u).$$

It follows from Eq. (13) that if $\rho=1$ the current vanishes [it is clear from Eq. (10) that $j=0$ for any value of u]. This is to be expected because in the $\rho=1$ case the phase of a spin density wave is fixed so that there is no electric current.

The spectrum of a spin wave was found earlier,[13] and it was shown in Refs. 16 and 17 that in the states with spin waves there is an electric current proportional to the quasimomentum, in accordance with Ref. 16.

A compact expression cannot be obtained for the spin current. However, in the limit of high values of u the equations for spin excitations in the Hubbard model reduce for $\rho=1$ to equations for triplet excitations in a Heisenberg chain with an exchange integral $J=4t^2/u$. The current is calculated readily in the spin model and the value obtained should correspond to the spin current in the Hubbard model. Equations of the Bethe ansatz for a chain of spins can be written in the form[18]

$$NP_\alpha=2\pi J_\alpha+\sum_{\beta=1}^{N}\psi_{\alpha\beta},$$
$$2\operatorname{tg}(\psi_{\alpha\beta}/2)=\operatorname{tg}(P_\alpha/2)-\operatorname{tg}(P_\beta/2).\qquad(14)$$

The energy, momentum, and spin currents are described by

$$E=-\sum_j(1+\cos P_j),\quad p=\sum_j P_j,\quad j_{sp}=\sum_j\sin P_j.\quad(15)$$

In the case of high values of u, Eqs. (2) and (3) become identical with the expressions in the system (14), if they are written in the form

$$N_ak_j=2\pi I_j+\sum_\alpha P_\alpha,\quad P_\alpha=2\operatorname{arctg}(4\lambda_\alpha/u),$$
$$NP_\alpha=2\pi J_\alpha+\sum_\beta\psi_{\alpha\beta},\quad\psi_{\alpha\beta}=2\operatorname{arctg}[2(\lambda_\alpha-\lambda_\beta)/u].\qquad(16)$$

Following the procedure used to obtain Eq. (11), we can use Eq. (16) and write down the equations for $\tilde\sigma(\lambda)$ in the case of triplet excitations ($J_{\alpha+1}-J_\alpha=1+\delta_{\alpha,\alpha_0}$):

$$2\pi\tilde\sigma(\lambda)=2\pi\theta(\lambda-\lambda_0)-\int\frac{4u\sigma(\lambda')\,d\lambda'}{u^2+4(\lambda-\lambda')^2},$$

which is readily solved to give

$$\tilde\sigma(\lambda)=\frac{1}{\pi}\int_0^\infty\frac{\sin[\omega(\lambda-\lambda_0)]\,d\omega}{\omega[1+\exp(-\omega u/2)]}+\frac{1}{4}.\qquad(17)$$

The spin current is defined by analogy to the electric current employing a relationship $dS_{z,n}/dt+\operatorname{div}j_{sp}=0$, where $S_{z,n}$ is the spin density at the nth site in the chain. Using the variables λ and $\tilde\sigma(\lambda)$, we can write down the expressions for the spin current and momentum with the aid of Eqs. (16) and (17):

$$p=\int_{-\infty}^{\infty}\frac{8u\tilde\sigma(\lambda)\,d\lambda}{u^2+16\lambda^2}=2\operatorname{arctg}\exp\left(-\frac{2\pi\lambda_0}{u}\right),$$
$$j_{sp}=\int_{-\infty}^{\infty}\frac{8u(u^2-16\lambda^2)}{u^2+16\lambda^2}\tilde\sigma(\lambda)\,d\lambda=-\frac{\pi}{2}\operatorname{th}\frac{2\pi\lambda_0}{u}$$
$$-\frac{i}{2}\left[\psi\left(\frac{1}{4}+\frac{i\lambda_0}{u}\right)-\psi\left(\frac{1}{4}-\frac{i\lambda_0}{u}\right)\right]\qquad(18)$$

where $\psi(x)$ is the Euler function. In the limit of high values of λ_0 (low p), it follows from Eq. (18) that

$$j_{sp}\approx u/4\lambda=\pi/2\ln(2/p).\qquad(19)$$

In contrast to the electric current, which is zero for $\rho=1$, the spin current of Eq. (19) does not vanish.

For comparison we shall write down the expression for the current in an antiferromagnetic chain obtained for an approximation utilizing the Holstein–Primakoff transformation. The current carried by a magnon is $j=4J\sin^2(k/2)$ (J is the exchange integral for the nearest neighbors), and the dispersion law for magnons has the familiar form: $\varepsilon_0(k)=2J\sin k$.

2. Particle and hole states

a) Hole states differ from the ground state by a hole in the distribution of the quasimomenta k_j of the particles. Subtracting from Eq. (2) the equation for the ground state, we obtain subject to Eq. (6)

$$2\pi\tilde{\rho}(k)=2\pi\theta(k-k_0)+\int\frac{8u\tilde{\sigma}(\lambda)\,d\lambda}{u^2+16(\sin k-\lambda)^2},$$
$$\int_{-Q}^{Q}\frac{8u\tilde{\rho}(k)\cos k\,dk}{u^2+16(\sin k-\lambda)^2}=2\pi\tilde{\sigma}(\lambda)+\int\frac{4u\tilde{\sigma}(\lambda')\,d\lambda'}{u^2+4(\lambda-\lambda')^2}, \tag{20}$$

where $k_0=k_{j_0}$, whereas $\tilde{\rho}(k_j)$, $\tilde{\sigma}(\lambda_\alpha)$ are defined as in Eq. (9). The following equation for the function $\tilde{\rho}(k)$ follows readily from Eq. (20):

$$\tilde{\rho}(k)=\theta(k-k_0)+\int_{-Q}^{Q}dk'\cos k'\tilde{\rho}(k')\times\frac{4}{u}R\left(\frac{4}{u}[\sin k-\sin k']\right). \tag{21}$$

In the case of high values of u, we find from Eq. (21) that

$$\tilde{\rho}(k)=\theta(k-k_0)+2(\pi u)^{-1}(\sin Q-\sin k_0)\ln 2. \tag{22}$$

The expressions for the energy, momentum, and current are now

$$\varepsilon=E-E_0=-2\{\cos\pi\rho-\cos(\pi\rho-p)+\gamma[\sin^2\pi\rho-\sin^2(\pi\rho-p)]\},\quad p=\pi\rho-k_0-\gamma\sin k_0,$$
$$j=2\{\sin\pi\rho-\sin(\pi\rho-p)+\gamma[\sin\pi\rho(\sin\pi\rho-\sin(\pi\rho-p))/\pi\rho-{}^1/_2\sin 2\pi\rho+{}^1/_2\sin 2(\pi\rho-p)]\},\quad \gamma=4\rho u^{-1}\ln 2. \tag{23}$$

We shall determine the excitation velocity from Eq. (23) accurate to within $O(1/u)$:

$$v=2[\sin(\pi\rho-p)-\gamma\sin 2(\pi\rho-p)], \tag{24}$$

so that the charge is now given by

$$q=\frac{\sin\pi\rho-\sin(\pi\rho-p)}{\sin(\pi\rho-p)}+\frac{\gamma}{\sin(\pi\rho-p)}\left\{\frac{\sin\pi\rho}{\pi\rho}[\sin\pi\rho-\sin(\pi\rho-p)]+\sin p\right\}. \tag{25}$$

It follows from Eq. (25) that in the general case of $q\neq 1$ we find that in the limit $k_0\to Q$ the charge becomes $q\to 0$. It should be stressed once again that these excitations occur in a system with $\rho\neq 1$, i.e., when $Q\neq\pi$.

b) Particle states are obtained if a particle with a quasimomentum $k_N=Q$ is in a state with $k_0>Q$. Subtracting from Eqs. (2) and (3) the equations for the ground state of N particles, we find from Eq. (7) that

$$2\pi\tilde{\rho}(k)=\int_{-\infty}^{\infty}\frac{8u\tilde{\sigma}(\lambda)\,d\lambda}{u^2+16(\sin k-\lambda)^2}, \tag{26}$$

$$\int\frac{8u\cos k\tilde{\rho}(k)\,dk}{u^2+16(\sin k-\lambda)^2}=2\pi\tilde{\sigma}(\lambda)+\int\frac{4u\tilde{\sigma}(\lambda')\,d\lambda'}{u^2+4(\lambda-\lambda')^2}+2\,\mathrm{arctg}\frac{4(\lambda-\sin k_0)}{u}-2\,\mathrm{arctg}\frac{4(\lambda-\sin Q)}{u}, \tag{27}$$

where $\tilde{\rho}(k)$, $\tilde{\sigma}(\lambda)$ are defined as in Eq. (9). Equations (26) and (27) yeild the following expressions for $\tilde{\rho}(k)$, $\tilde{\sigma}(k)$:

$$\tilde{\rho}(k)=\int_{Q}^{k_0}\frac{4}{u}R\left(\frac{4}{u}[\sin k-\sin k']\right)\cos k'\,dk'+\int_{-Q}^{Q}\frac{4}{u}R\left(\frac{4}{u}[\sin k-\sin k']\right)\tilde{\rho}(k')\cos k'\,dk', \tag{28}$$

$$\tilde{\sigma}(\omega)=-\frac{\exp(-i\omega\sin k_0)-\exp(-i\omega\sin Q)}{i\omega\,\mathrm{ch}(\omega u/4)}+\frac{\int d\omega'\tilde{\sigma}(\omega')\exp(-|\omega'|u/4)}{2\pi\,\mathrm{ch}(\omega u/4)}\frac{\sin[(\omega-\omega')\sin Q]}{\omega-\omega'}$$
$$\tilde{\sigma}(\omega)=\int\sigma(\lambda)e^{-i\omega\lambda}d\lambda. \tag{29}$$

We can easily see that equations for $\tilde{\rho}(k)$, $\tilde{\sigma}(\omega)$ differ only by the sign of the free term from the equations for the distribution functions $\tilde{\rho}(k)-\theta(k-k_0)$ and $\tilde{\sigma}(\omega)$ of the hole states. Therefore, the expressions for the energy, momentum, and charge will differ only in sign from the corresponding expressions given by Eqs. (23) and (24) and applicable to the hole states, on condition that these states are characterized by $|k_0|<Q$, whereas in the case of the particle states we have $|k_0|>Q$. A combination of the particle and hole states represents a particle-hole excitation formed on transfer of an electron from a state with a quasimomentum $|k_1|<Q$ to a state with a quasimomentum $|k_2|>Q$. The expressions for the energy, momentum, and current are trivial combinations of expressions of the type given by Eq. (23).

3. Excitations with a gap described by complex wave numbers

Such excitations have been investigated in Ref. 14, where the band structure was found. We shall assume that there is a state with a pair of complex quasimomenta $k_{j_0}=\varkappa\pm i\chi$. Then, Eq. (2) for $j=j_0$ becomes

$$N_a(\varkappa\pm i\chi)=2\pi I+\sum_{\beta=1}^{N/2-1}\theta(2[\sin(\varkappa\pm i\chi)-\lambda_\beta])+\theta(2[\sin(\varkappa\pm i\chi)]-\Lambda). \tag{30}$$

In Eq. (30) it is assumed[14] that all the values of λ_β, apart from one, shift by $O(1/N)$ relative to the values for the ground state. It is found in Ref. 14 that

$$\sin(\varkappa\pm i\chi)=\Lambda\pm iu/4+O(e^{-\eta N}),\quad \eta=O(1), \tag{31a}$$
$$\varkappa=\arcsin\{{}^1/_2[(u/4)^2+(\Lambda+1)^2]^{1/2}+{}^1/_2[(u/4)^2+(\Lambda-1)^2]^{1/2}\},\quad \cos\varkappa<0, \tag{31b}$$
$$\chi=\mathrm{arcch}\{{}^1/_2[(u/4)^2+(\Lambda+1)^2]^{1/2}+{}^1/_2[(u/4)^2+(\Lambda-1)^2]^{1/2}\},\quad \chi>0, \tag{31c}$$

$$N_ak_j=2\pi I_j+\sum_{\beta=1}^{N/2-1}\theta(2[\sin k_j-\lambda_\beta])+\theta(2[\sin k_j-\Lambda]), \tag{32a}$$
$$\theta(2[\sin k_j-\lambda_\alpha])=2\pi J_\alpha-\sum_{\beta=1}^{N/2-1}\theta(\lambda_\alpha-\lambda_\beta), \tag{32b}$$
$$I_{j+1}-I_j=1+\delta_{j,j_l}+\delta_{j,j_m}, \tag{32c}$$

where I_j is a set of values for the ground state of N particles with two holes and J_α is the set of values for the ground state of $N-2$ particles. The numbers J_α are selected so as to separate excitations associated only with the excitation of the electric charge and not of the spin. In the case of states k_j in the continuous spectrum, λ_α can be obtained by analogy with the treatments given in the preceding sections and equations for $\tilde{\rho}(k)$, $\tilde{\sigma}(\lambda)$ are

$$2\pi\rho(k)=-2\pi+2\pi[\theta(k-k_l)+\theta(k-k_m)] - 2\,\mathrm{arctg}\frac{4(\sin k-\Lambda)}{u}+\int\frac{8u\tilde{\sigma}(\lambda)\,d\lambda}{u^2+16(\sin k-\lambda)^2},$$

$$\int_{-Q}^{Q}\frac{8u\tilde{\rho}(k)\cos k\,dk}{u^2+16(\sin k-\lambda)^2}=2\pi\tilde{\sigma}(\lambda)+\int\frac{4u\tilde{\sigma}(\lambda')\,d\lambda'}{u^2+4(\lambda-\lambda')^2}, \tag{33}$$

and hence we find that $\tilde{\rho}(k)$ is described by

$$\tilde{\rho}(k)=-1+\theta(k-k_l)+\theta(k-k_m)-\frac{1}{\pi}\mathrm{arctg}\frac{4(\sin k-\Lambda)}{u} + \int\cos k'\rho(k')\frac{4}{u}R\left(\frac{4}{u}[\sin k-\sin k']\right)dk'. \tag{34}$$

We shall find the current carried by excitations. Using Eq. (34) we obtain

$$j=2\int\tilde{\rho}(k)\cos k\,dk+4\Lambda. \tag{35}$$

The value of Λ corresponding to $\rho=1$ is defined in Ref. 14:

$$\Lambda=(\sin k_l+\sin k_m)/2. \tag{36}$$

Equation (34) corresponding to $\rho=1$ can be solved exactly:

$$\tilde{\rho}(k)=-1+\theta(k-k_l)+\theta(k-k_m)-\frac{1}{\pi}\mathrm{arctg}\frac{4(\sin k-\Lambda)}{u} +\left(\int_{\sin k_l}^{\sin Q}+\int_{\sin k_m}^{\sin Q}\right)\frac{4}{u}R\left(\frac{4}{u}[\sin k-t]\right)dt.$$

The energy and momentum are defined in Ref. 14. In the case of the current we find from Eqs. (34)–(36) that if $\rho=1$, then integration of Eq. (34) with a weighting factor $\cos k$ yields $j=0$. For an arbitrary value of ρ in the limit of high u it follows from Eqs. (34)–(36) that

$$\tilde{\rho}(k)=\theta(k-k_l)+\theta(k-k_m)-1-4[\sin k-\Lambda +(\sin k_l+\sin k_m)\ln 2]/\pi u. \tag{37}$$

The energy, momentum, and current are then found from Eqs. (30)–(35) and (37):

$$\varepsilon=u+2(\cos k_l-\cos Q)+2(\cos k_m-\cos Q) +4\sin(2Q)/\pi u+8(1-Q/\pi)/u,$$
$$p=-k_l-k_m+8\Lambda(Q/\pi-1)/\pi-4(\ln 2)Q(\sin k_l+\sin k_m)/\pi u, \tag{38}$$
$$j=-2\sin k_l-2\sin k_m+4\Lambda +8\sin Q[2\Lambda-(\sin k_l+\sin k_m)\ln 2]/\pi u.$$

The parameter Λ can be found with the aid of the results in Ref. 14:

$$\Lambda=(\sin k_l+\sin k_m)/(N_a-N+2). \tag{39}$$

The expression (39) is derived from the exact equations in the limit of high u and for $\rho=1$, we obtain Eq. (36) whereas for $\rho\neq 1$ ($N_a-N\gg 1$) it follows that $\Lambda\to 0$.

4. Excited states of a system of $N+1$ particles

a. Introduction of an additional particle into a system of N particles may give rise to excited states of two types. We shall first consider a system with $\rho<1$ and find the effects of introduction of a particle with a quasimomentum k_0 ($|k_0|>Q$) and a spin $\sigma=\uparrow$. States of this kind differ from the ground distribution of electrons between the quasimomenta and are similar to the particle excitations discussed in subsection 2b of the present section. The numbers I_j and J_α are related to the numbers I_j^0 and J_α^0 for the state of a system of N particles:

$$I_j=I_j^{(0)},\quad j=1,\dots,N;\quad I_{N+1}>I_N;\quad J_\alpha=J_\alpha^0. \tag{40}$$

Subtracting from Eqs. (2) and (3) the equations for the ground states of a system of N particles and using Eq. (40), we find equations for the functions $\tilde{\rho}(k)$, $\tilde{\sigma}(\lambda)$ defined in Eq. (9):

$$2\pi\rho(k)=\int\frac{8u\tilde{\sigma}(\lambda)\,d\lambda}{u^2+16(\sin k-\lambda)^2}, \tag{41}$$
$$\int\frac{8u\tilde{\rho}(k)\cos k\,dk}{u^2+16(\sin k-\lambda)^2}=2\pi\tilde{\sigma}(\lambda) +\int\frac{4u\tilde{\sigma}(\lambda')\,d\lambda'}{u^2+4(\lambda-\lambda')^2}+2\,\mathrm{arctg}\frac{4(\Lambda-\sin k_0)}{u}.$$

Equation (41) and the Fourier transformation can be used to find the following equation for $\tilde{\rho}(k)$:

$$\tilde{\rho}(k)=\int_k^{k_0}dk'\cos k'\frac{4}{u}R\left(\frac{4}{u}[\sin k-\sin k']\right) +\int_{-Q}^{Q}dk'\cos k'\tilde{\rho}(k')\frac{4}{u}R\left(\frac{4}{u}[\sin k-\sin k']\right). \tag{42}$$

Expanding Eq. (42) as a series in terms of $1/u$, we obtain

$$\tilde{\rho}(k)=2(\ln 2)(\sin k_0-\sin k)/\pi u. \tag{43}$$

The energy, momentum, current, velocity, and electric charge of excitations deduced from Eq. (23) are given by the following expressions deduced in the leading order in $1/u$:

$$\varepsilon=-2\cos p-2\gamma\sin^2 p-\gamma[1-\sin(2\pi\rho)/2\pi\rho],$$
$$p=k_0+\gamma\sin k_0,\quad j=2[1-\gamma\cos p+\gamma\sin(\pi\rho)/\pi\rho]\sin p, \tag{44}$$
$$v=2(1-2\gamma\cos p)\sin p,\quad q=1+\gamma\cos p+\gamma\sin(\pi\rho)/\pi\rho.$$

Depending on the values of ρ and p, the value of q can be greater or smaller than unity.

We can similarly consider the excited states obtained when one particle with a momentum $|k_0|<Q$ is removed from a system. The values of I_j and J_α are selected as follows:

$$I_j=I_j^0,\quad j=1,\dots,j_0-1;\quad I_j=I_{j+1}^0,\quad j=j_0,\dots,N-1;\quad J_\alpha=J_\alpha^0.$$

The equations for $\tilde{\rho}(k)$ and $\tilde{\sigma}(\lambda)$ differ from Eqs. (41) and (42) obtained for the case $|k_0|>Q$ only in respect of the sign of the free term. The expressions for the energy, momentum, current, and charge differ from Eq. (42) only in respect of the sign.

b. In addition to these excitations of a system with $\rho\neq 1$, the addition of a particle can give rise to excited states with a high energy (of the order of u or greater than u), which appear when an additional particle is placed at an occupied lattice site. Such excitations, which occur for both $\rho = 1$ and $\rho \neq 1$, are described by complex wave vectors by analogy with subsection 3, so that we shall now use the results obtained in that subsection.

We shall consider an excited state with one pair of complex quasimomenta formed when an additional particle with a spin $\sigma = \uparrow$ is introduced into a system with $N-1$ particles. Equations (31)–(34) are modified slightly and the terms containing k_m disappear; the set of numbers I_j is obtained from the I_j^0 sequence of numbers for the ground state of a system of $N-1$ particles by removing one value I_l, modifying Eq. (32) by the substitution of $j = 1, \dots N-2$, and altering Eq. (33) so that instead of the free term -2π there is $-\pi$.

In the case of $\tilde\rho(k)$ we now have the following equation:

$$\tilde\rho(k) = \theta(k-k_l) - \frac{1}{2} - \frac{1}{\pi}\operatorname{arctg}\frac{4(\sin k - \Lambda)}{u} + \int_{-Q}^{Q} dk' \cos k' \rho(k') \frac{4}{u} R\left(\frac{4}{u}[\sin k - \sin k']\right). \quad (45)$$

If $\rho = 1$, the equation can be solved exactly:

$$\rho(k) = \theta(k-k_l) - \frac{1}{2} - \frac{1}{\pi}\operatorname{arctg}\frac{4(\sin k - \Lambda)}{u} - \int_0^{\sin k_l} dt' \frac{4}{u} R\left(\frac{4}{u}[\sin k - t']\right), \quad (46)$$

where $\Lambda = \sin k_l$ is found with the aid of Ref. 14. In the case of $\rho = 1$ we can write down the exact expressions for the momentum, energy, current, and charge of excitations:

$$p = \int \tilde\rho(k)\,dk + \varkappa, \quad \varepsilon = 2\int \tilde\rho(k) \sin k\, dk - 4\cos k \operatorname{ch}\chi + \mu_-,$$
$$j = 4\sin k_l + 2\int \tilde\rho(k)\cos k\, dk = 2\sin k_l, \quad (47)$$
$$q = j/v, \quad v = d\varepsilon/dp,$$

where $\tilde\rho(k)$ is given by Eq. (46); $\varkappa$ and χ are defined by Eq. (31); μ_- is the chemical potential given in Ref. 11:

$$\mu_- = E_0(N=N_a) - E_0(N=N_a-1).$$

For an arbitrary ρ, we obtain expressions for $\tilde\rho(k)$, energy, momentum, current, and velocity in the leading order in respect of $1/u$:

$$\tilde\rho(k) = \theta(k-k_l) - {}^1/_2 - 4(\sin k - \Lambda + {}^1/_2 \sin k_l \ln 2)/\pi u,$$
$$\Lambda = \begin{cases} \sin k_l, & \rho = 1 \\ 0 & \rho < 1 \end{cases} \quad p = -k_l - \gamma \sin k_l,$$
$$\varepsilon = u + \mu + 2[\cos p - \cos \pi\rho + \gamma(\sin^2 p - \sin^2 \pi\rho)],$$
$$\mu = dE_0/dN = 2\cos[\pi(1-\rho)] - \gamma[2 - \cos(2\pi\rho) - \sin(2\pi\rho)/2\pi\rho], \quad (48)$$
$$j = \begin{cases} -2(1-\gamma\cos p)\sin p, & \rho = 1, \\ 2[1 - \gamma\cos p + \gamma\sin(\pi\rho)/\pi\rho], & \rho < 1, \end{cases}$$
$$v = -2(1 - 2\gamma\cos p)\sin p.$$

The electric charge is given by

$$q = \begin{cases} 1 + \gamma\cos p, & \rho = 1, \\ -[1 + \gamma\cos p + \gamma\sin(\pi\rho)/\pi\rho], & \rho < 1. \end{cases} \quad (49)$$

It is interesting to note that the charge of Eq. (49) is identical, in the $\rho \neq 1$ case, with the charge of hole excitations of Eq. (44), indicating that in this case the current is mainly due to holes.

We shall conclude by noting that the expression for the electric current given by Eq. (8) can be derived from the general expression $j = -\langle \delta H / \delta A \rangle$, where H is the Hamiltonian and A is the potential of the electric field. We can easily see that introduction of a constant vector potential A gives an expression for the energy $E = -2\Sigma \cos(k_j - eA)$, which can be differentiated with respect to A to give $j = 2\Sigma \sin k_j$. The velocity of excitations is

$$v = -dE/dp = 2\sum_j \sin k_j\, dk_j \Big/ \sum_i dk_i$$

and it is not equal to $2\Sigma \sin k_j$, because the differentials $dk_j = f(dI_1, \dots, dI_N, dJ_1, \dots, dJ_M)$ are not independent as a result of which we have in general $q = j/v \neq e$, which is a consequence of the fact that $E \neq E(p - eA)$ and that $E = \Sigma f(k_j - eA)$.

CONCLUSIONS

We calculated the electric current carried by various excitations in the Hubbard model. We considered excited states resulting from a redistribution of particles in a system or created by introduction of an additional particle or a hole. The former include quasicovalent excitations of the triplet type (spin waves), particle and hole states, and excitations with complex quasimomenta. We demonstrated that a spin wave in a system with an energy band which is not half-filled ($\rho \neq 1$) can carry an electric current [Eq. (13)]. The spin current carried by a spin wave was found for the case when $\rho = 1$ [Eqs. (18) and (19)]. According to the classification of Refs. 16, 17, and 12, all the excitations can be divided into quasicovalent and quasiionic. Quasicovalent excitations are those which do not exhibit ionic structures when the sites in a chain are moved apart ($U/t \to \infty$) and are eigenstates of the spin Heisenberg Hamiltonian. From the point of view of the exact solutions these quasicovalent excitations are associated with holes in the distribution of the numbers J_α, whereas the excitations associated with holes in the I_j distribution are known as quasi-ionic because (apart from spin waves) are of the quasi-ionic type.

We investigated zero-gap hole or particle states resulting from a redistribution of quasimomenta k_j of particles: in the case of a hole state a particle from a state with a quasimomentum $|k_0| < Q$ is located at the edge of an energy band in a state with the quasimomentum Q, whereas in the case of a particle state with a quasimomentum Q a particle is located in a state with a quasimomentum $|k_0| > Q$. Such excitations are possible for a system with $\rho \neq 1$. The current carried by such excitations is described by Eq. (23) and the charge, defined as the ratio of the current to the excitation rate, is given by Eq. (25). In the case of low momenta ($p \to 0$) we find that the current and the charge both approach zero (j, $q \to 0$).

We investigated excited states of a system with a gap in the spectrum ($\varepsilon \sim u$ in the limit of high u), described by complex quasimomenta and corresponding to the case when there are two particles at one site. We found that if $\rho = 1$, such excitations do not carry an electric current [Eq. (33)], whereas for $\rho \neq 1$ the value of the current is proportional to $|\rho - 1|/u$ [Eq. (38)].

We discussed excitations of the system resulting from introduction of an additional particle and calculated the spectrum, electric current, and charge of excitations in the limit of high u. We investigated two different states, one of which was obtained for $\rho \neq 1$ when an additional particle is located in a state with a quasimomentum $|k_0| > Q$, has an energy of the order of μ, carries the current described by Eq. (44), and has a fractional charge also described by Eq. (44). In the limit of high values of u the charge differs from unity by an amount of the order of the u^{-1}. The other state has a much higher energy ($\varepsilon \sim u$ in the limit of high u) and is described by complex quasimomenta. In the limit of high u such a state corresponds to a situation when there are two particles at one site. We derived the current [Eq. (48)] and the fractional charge [Eq. (48)] carried by an excitation. When the band occupancy is $\rho = 1$, such excitations are the only carriers of the current in the system among the excitations discussed above. If $\rho \neq 1$, then the current is carried by all the excitations discussed above: a spin wave, particle and hole states, and excitations with a gap obtained on introduction of additional particles or holes into the system.

We discussed the cases when a system has one excitation. We shall now consider a situation which arises when several excitations are present in a system. We can readily see that if $\rho = 1$, the additivity of the currents of excitations is no longer obeyed, i.e., the current is no longer equal to the sum of the current due to various excitations. This follows from the results in subsections 2, 3, and 4b of Sec. II. For example, an excitation described in subsection 4b may be regarded as the result of superposition of two excitations: an excitation with a gap (subsection 3) and a pair of complex quasimomenta, and holes I_l and I_m when a particle with the number I_m is added to the system. In this case the energy and momentum of an excitation are the sums of energies and momenta of the two excitations, but the current in the system is not equal to the sum of the currents, as demonstrated by Eqs. (23), (38), and (48). However, if $\rho \neq 1$, the additivity of the current is restored, at least for the leading orders in $1/u$, as demonstrated by the same expressions. If $\rho < 1$, the rule of superposition of the current is satisfied for excitations of the type described in subsections 1, 2, and 4b irrespective of the value of u. This conclusion follows in an elementary manner from the general form of the equations for the functions $\rho(k)$ which have the same structure: $\rho(k) = f(k) + \int \rho(k')K(k,k')dk'$. Formation of several excitations gives rise to additive terms in $f(k)$, so that the solution of $\rho(k)$ splits into a sum of terms due to different excitations. This ensures the additivity of the momentum, energy and current.

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[1)]As demonstrated by S. A. Brazovskiĭ, this method for the calculation of the charge of excitations was used earlier by Ovchinnikov and Ukrainskiĭ.[9]

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