Exact elementary excitations with a complex wave vector in the one-dimensional Hubbard model

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(Received 10 December 1979)

Computer calculations of finite Hubbard chains indicate two peaks for the specific heat for a large Coulomb interaction U for band fillings less than 1/2. Even though the origin of this is physically obvious, no elementary excitations with a gap energy U have been explicitly demonstrated from the exact solution of the Hubbard model. We here demonstrate that there exists elementary excitation with a complex wave vector k for the $N-1$ spin-up case. These excitations with complex wave vectors have never been discussed previously. These results suggest similar excitations for the case with more general spin arrangements and may account for the specific-heat results.

I. INTRODUCTION

Recently there has been a lot of interest in the so-called one-dimensional materials.[1] Theoretically, there are three different approaches: (i) using the "exact" results of the Hubbard Hamiltonian,[1] (ii) doing computer calculations of finite Hubbard chains,[2] (iii) summing parquet diagrams, using an analytic renormalization-group technique,[3] and the exact results of the Tomonaga-Luttinger model. These calculations are complementary to each other and they should perhaps be synthesized to produce a more complete quantitative picture of the problem. The present work is motivated by these considerations.

Computer calculations of finite Hubbard chains[2] for the specific heat indicate two peaks separated by an energy of order U (the on-site Coulomb repulsion energy) in the limit of large U. These are usually interpreted as due to the fact that it takes an extra energy U to put two electrons on the same site, so that if U is much larger than the bandwidth a second peak should appear in the specific heat. While the above argument is extremely suggestive, it has not been demonstrated from the exact solutions of the Hubbard model. There have been calculations of the exact excitation spectrum of the one-dimensional Hubbard model but these have not included the possibility of excitations with complex wave vectors ("bound" states). While in the continuum limit no such bound states are possible for a repulsive Coulomb interaction,[4] such is not the case on a discrete lattice, as one can easily convince oneself by doing a two-body scattering problem.

The Hubbard model is described by a Hamiltonian:

$$H=\sum_{\sigma} C^{\dagger}_{i+1\sigma} C_{i\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} . \tag{1}$$

Here $C^{\dagger}_{i\sigma}$ is the creation operator for an electron of spin σ at site i. The hopping matrix element is set equal to one. We are interested in the limit of large U, in which case nearly all electrons are on different sites. The first excitation of energy U will arise from having only one doubly occupied site. Because of this, and for the sake of making the mathematics more accessible, we shall confine our interest in this paper to the case of $N-1$ electrons with spin up, 1 electron with spin down. This case would rule out the possiblity of spin-waves as well as that of having more than one doubly occupied site.

This paper is orgainzed as follows. The eigenvalues of these excited states are discussed in Sec. II. Then we discuss the corresponding wave functions in Sec. III. We conclude in the last section.

II. EXCITED STATES

Assuming that the lattice constant $a=1$, it is found[1,4] that the total energy E of an eigenstate of Eq. (1) is given by

$$E=-2\sum_{i}\cos k_i , \tag{2}$$

where the wave vectors k_i satisfy the relations

$$\sin k_j - \lambda = \tfrac{1}{4} U \cot(\tfrac{1}{2} N_a k_j) , \tag{3}$$

$$\sum_{j} k_j = \frac{2\pi n}{N_a} . \tag{4}$$

Here λ is a constant to be determined from the above equations, N_a is the total number of atoms, n is some integer.[1] To appreciate the significance of complex wave vectors k_j we write down the wave function in a region $x_1 \geq x_2 \geq \cdots \geq x_n$, where x_1 corresponds to the position of the spin-down electron. In this case

$$\psi(x_1 \cdots x_N) = \sum_P [P,1] \exp\, i \sum_{j=1}^{N} k_{pj} x_j \quad . \tag{5}$$

Here the summation indicates summing over all permutations of the N indices j. $[P,1]$ are just constant coefficients. Clearly complex wave vectors must occur in complex-conjugate pairs, otherwise E will not be real. A pair of complex wave vectors $(k_x \pm ik_y)$ will produce terms in the wave function (ψ) that are proportional to

$$\exp[-k_y|x_1 - x_j| + ik_x(x_1 + x_j)] \,, \tag{6}$$

indicating that the first and jth particle are sitting on top of each other and moving with a momentum k_x. This corresponds to the physical picture that we have been describing. We shall come back to the wave function in more detail in Sec. III, but now let us focus on the solution of (3) and (4), allowing for a pair of k_j's (say k_1 and k_2) to be complex.

For a complex k, Eq. (3) separates into two equations: one for the real part, the other for the complex part. Writing $k_1 = k_x + ik_y$, we get

$$(\sin k_x \cosh k_y - \lambda)\tan(\tfrac{1}{2}N_a k_x) - \cos k_x |\sinh k_y| = U/4 \,, \tag{7}$$

$$\cos k_x |\sinh k_y| + \cot(\tfrac{1}{2}N_a k_x)(\sin k_x \cosh k_y - \lambda) = -U/4 \,. \tag{8}$$

In deriving (7) and (8), we have made use of the fact that $|\sinh(\frac{1}{2}N_a k_y)| = \cosh(\frac{1}{2}N_a k_y)$, since N_a is very large and k_y is not infinitesimally small. Adding (7) and (8), we get

$$(\sin k_x \cosh k_y - \lambda)\frac{2}{\sin N_a k_x} = 0 \,.$$

We thus get

$$\sin k_x \cosh k_y = \lambda \,. \tag{9}$$

Substituting back, we get, in addition,

$$\cos k_x |\sinh k_y| = -U/4 \,. \tag{10}$$

From (10) we see that no solution exists unless $\cos k_x < 0$. This is quite reasonable because the energy due to this pair of complex wave-vector states will be

$$\delta E = -4 \cos k_x \cosh k_y \,, \tag{11}$$

so that if $\cos k_x$ is negative, δE is positive, indicating a high-lying state. Furthermore, note that in the large-U limit, we get for $\cos k_x = 1$, for example,

$$\sinh k_y \simeq \cosh k_y \simeq U/4 \,,$$

so that

$$k_y \simeq \ln(U/4) \,. \tag{12}$$

Substituting back into (6) we see that the probability amplitude that the two electrons hop from an "on-top" configuration to a nearest-neighbor configuration is down by a factor of $1/U$, consistent with first-order-perturbation results. δE can be expressed in a more transparent form. Expressing k_y in terms of k_x and U, and using (1) we get (on assuming that $\cos k_x < 0$)

$$\delta E = (U^2 + 16\cos^2 k_x)^{1/2} \,. \tag{13}$$

Thus $\delta E \geq U$ is consistent with our expectations. In particular, for U much greater than the bandwidth, we expect these excitations to form a separate band.

We now turn our attention to the evaluation of λ and the k_j's. From (9) and (10) we get

$$\tan k_x (\tfrac{1}{16}U^2 + \cos^2 k_x)^{1/2} = -\lambda \,. \tag{14}$$

For $j \neq 1, 2$, k_j satisfies Eq. (3). By our assumption $k_{1x} = k_{2x}$, Eq. (4) thus reduces to

$$2k_x + \sum_{j=3}^{N} k_j = \frac{2\pi n}{N_a} \,. \tag{15}$$

Analogous to the continuum case discussed by McGuire[4] the solution of Eq. (3) is given by

$$k_j = \pm\frac{2s\pi}{N_a} \pm \frac{2}{N_a}\cot^{-1}\left(\frac{4}{U}\sin\frac{2s\pi}{N_a} \pm \frac{4\lambda}{U}\right) \,, \quad s = 0,\ 1,\ 2\ldots, \tag{16}$$

as one can verify by direct substitution.

Substituting this back into (15) and assuming that the lowest $N-1$'s are occupied, we get, as a particular case

$$2k_x + \sum_{s=0}^{(N/2)-2} \frac{2}{N_a}\left[\cot^{-1}\left(\frac{4}{U}\sin\frac{2S\pi}{N_a} - \frac{4\lambda}{U}\right) - \cot^{-1}\left(\frac{4}{U}\sin\frac{2s\pi}{N_a} + \frac{4\lambda}{U}\right)\right] = \frac{2\pi n}{N_a} \,. \tag{17}$$

Converting the sum to an integral, we get

$$2k_x + \frac{2}{\pi}\int_0^{\bar{k}_F} dx \left[\cot^{-1}\left(\frac{4}{U}\sin 2x - \frac{4\lambda}{U}\right) - \cot^{-1}\left(\frac{4}{U}\sin 2x + \frac{4\lambda}{U}\right)\right] = \frac{2\pi n}{N_a} \,, \tag{18}$$

where $\bar{k}_F = (\frac{1}{2}N - 2)\pi/N_a$. Equation (18) can be easily solved on the computer but to gain some physical insight, let us consider the special case of $U \gg 4\lambda$, $\bar{k}_F \ll 1$. Under these assumptions, we get

$$\frac{2\pi n}{N_a} \simeq 2k_x - \frac{8\lambda}{\pi U}\cot^{-1}\left(\frac{4}{U}\bar{k}_F\right) , \tag{19}$$

and from (14)

$$k_x \simeq \pi/2 + 4\lambda/U .$$

Thus

$$\lambda = \frac{U}{4}\pi\left(\frac{2n}{N_a} - 1\right)\left(1 - \frac{2}{\pi}\cot^{-1}\frac{4\bar{k}_F}{U}\right)^{-1} . \tag{20}$$

Note that $4\bar{k}_F/U$ is a ratio of the bandwidth to U. Equation (2) provides a dependence of λ on the band filling. One can also calculate the change in energy ΔE of the $N-2$ particles with real k from the ground state ($\lambda = 0$) as a consequence of the creation of the bound pair by substituting (16) into (2). However, it is not particularly illuminating physically and thus will not be discussed here. This finishes our discussion of the eigenvalue spectrum; let us next turn to the wave function.

III. WAVE FUNCTION

Even though the wave function for a general spin configuration is quite complicated, the wave function for the present case is not. Indeed, in the notation of Eq. (5), the coefficients $[P,1]$ satisfy the following conditions.[1,4] Corresponding to a permutation $P = \binom{1\ 2\cdots N}{a\ b\cdots}$, let us denote $[P,1]$ by the symbol $[ab\cdots]_1$, then we get in the region $x_1 > x_2 > \cdots x_N$ the equations

$$\frac{[123\cdots N]_1}{[q23\cdots 1\cdots N]_1} = -\frac{(1-e^{ik_1L})}{(1-e^{ik_qL})} , \tag{21}$$

$$[123\cdots N]_1 = -[132\cdots N]_1, \ldots . \tag{22}$$

The first equation holds for all permutations involving the first (spin-down) electron. The second equation applies to permutations not involving the first electron. Recall that

$$k_1 = k_x + ik_y , \quad k_2 = k_x - ik_y , \quad k_y > 0 .$$

From (21) we get

$$\frac{[12\cdots N]_1}{[21\cdots N]_1} = -\frac{(1-e^{ik_xL}e^{-k_yL})}{(1-e^{ik_xL}e^{+k_yL})} \to +e^{-ik_xL}e^{-k_yL}, \quad L\to\infty . \tag{23}$$

This implies

$$[21\cdots N]_1 \gg [12\cdots N]_1 , \ [q12\cdots N]_1 \text{ for } q \geq 3 , \tag{24}$$

i.e., the wave function is equal to

$$\psi = \sum_{P'} [P',1] \exp i\left(k_2x_1 + \sum_{j=2}^{N} k_{P'j}x_j\right). \tag{25}$$

Here P' are permutations involving the $N-1$ indices not containing 2. Any term in the wave function not involving k_2x_1 in the exponent is equal to zero. Equation (25) can be rewritten as

$$\psi = \sum_{P'} [P',1] \exp[ik_x(x_1 + x_{P'-1_2}) - k_y(x_1 - x_{P'-1_2})] \times \exp\left(i\sum_{P'j\neq 2,1} k_{P'j}x_j\right). \tag{26}$$

Because $x_1 > x_2 > \ldots$, $x_1 - x_{P'-1_2}$ is always positive. Thus the above wave function is always exponentially damped. (k_y is also positive.) Any plane wave which is not exponentially damped does not contribute to the wave function. This is precisely what we have alluded to in the previous section. One can also work out the wave function in a different region. For example, in region 2 denoted by $x_2 > x_1 > x_3 \ldots$, the coefficients $[P,2]$ are related[1,4] to the coefficients $[P,1]$ by $[P,2] = \exp(ik_{P2}L)[P,1]$. Thus

$$[12\cdots]_2 = e^{ik_2L}[12\cdots]_1 = e^{ik_xL}e^{k_yL}[12\cdots]_1 .$$

$$[21\cdots]_2 = e^{ik_1L}[21\cdots]_1 = e^{ik_xL}e^{-k_yL}[21\cdots]_1 .$$

Thus

$$\frac{[12\cdots]_2}{[21\cdots]_2} = e^{2k_yL}\frac{[12\cdots]_1}{[21\cdots]_1} \to e^{-ik_xL}e^{+k_1yL} , \quad L\to\infty . \tag{27}$$

In this way we arrive at the fact that

$$[12\cdots]_2 \gg [21\cdots]_2 ; \ [1q\cdots]_2 , \quad q \geq 3$$

and

$$\psi = \sum_{\bar{P}} [\bar{P},2] \exp\left(ik_2x_2 + \sum_{j\neq 2} k_{\bar{P}j}x_j\right) = \sum_{\bar{P}} [\bar{P},2] \exp[ik_x(x_2 + x_{\bar{P}\text{-}1_1}) - ky(x_2 - x_{\bar{P}\text{-}1_1})] \times \exp\left(i\sum_{\bar{P}j\neq 1,2} k_{\bar{P}j}x_j\right). \tag{28}$$

Note that in the present case $x_2 - x_k$ is always positive so that once again the wave function has the desired property. The calculation for the remaining cases is now obvious and hence will not be explicitly carried out.

IV. CONCLUSION

In this paper we have demonstrated a new kind of excitation with a complex wave vector exactly for the one-dimensional model for the case with $N-1$ spins up and one spin down. The physical picture behind this is quite transparent. It is satisfying that indeed this can be reproduced from the exact solutions. As we discussed, we look at this particular spin configuration because this simplifies the mathematics considerably so that

the physics is much more transparent. The case of general spin configuration should be a tractable problem, but it has not been addressed in this paper.

ACKNOWLEDGMENTS

This work was started while the author was visiting the Central Research Institute in Hungary. I thank A. Zawadowskii for his hospitality. I also thank F. Woynarovich for arousing my interest in the exact solutions. He looked at the problem with complex quantum numbers (not k) for the magnetic excitations and found new results. He informed me that he also arrived at results for complex k's for the charge fluctuations similar to those reported here. This material is based upon work partially supported by the National Science Foundation under Grant No. DMR-7918697.

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