Quasiparticle structure in the vicinity of the Heisenberg model in one and higher dimensions

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We study quasiparticle structure in the vicinity of the Heisenberg model. At first, we focus on the model in one dimension and show how solitonic quasiparticles (and their bound states) emerge. Further we discuss its anlaog in higher dimensions. Related to this subject, numerical data are presented and a discussion is given for the quasiparticles in the two-dimensional Hubbard model at half filling on a triangular-type lattice.

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I. INTRODUCTION

It is a fundamental issue in modern condensed matter physics to elucidate the fate of quasiparticles (if they are well defined), when the system approaches to the Mott insulator. In other words, how the quasiparticles are reconstructed and the "Fermi surface" collapses in the passage to the Mott insulator. There are several ways to get there. For example, when the temperature is lowered, one can approach to it in the two-dimensional (2D) Hubbard model at half filling on a square lattice. In this model, anisotropic suppression of the charge excitation has been discovered recently,[1,2] where the temperature is in the intermediate regime and the antiferromagnetic correlation is short ranged. The result has been confirmed both in the strong-coupling[1] and the weak-coupling region.[2] It imposes a severe constraint on possible quasiparticle structure near the 2D Mott insulator.

Related to the above subject, it would be valuable to pursue quasiparticle structure in the vicinity of the Heisenberg model (a low-energy model of the Mott insulator). Our focus is on the case when the antiferromagnetic correlation is suppressed. In the beginning, we shall study the model in one dimension and reveal the quasiparticle structure. It is closely related to a basic model, $d=2$ Ashkin-Teller classical statistical model,[3] and it is important to shed light on the quasiparticle structure. This problem is also discussed in a more recent context, e.g., in Ref. 4. Further we shall discuss its anlaogue in higher dimensions. Finally, related to this suject, numerical data are presented and a discussion is given for the quasiparticles in the 2D Hubbard model at half-filling on a triangular-type lattice.

II. IN ONE DIMENSION

A. Model, continuum limit, and the quasiparticle structure

Our model is defined on a chain with its length L and the Hamiltonian is

$$H=\sum_{i\in\mathrm{odd}} -2J_1(S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+\Delta S_i^zS_{i+1}^z) + \sum_{i\in\mathrm{even}} -2J_2(S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+\Delta S_i^zS_{i+1}^z), \quad (1)$$

where periodic boundary condition is imposed, $J_{1(2)}$ is set to be negative, and focus is on the sector $S_z=0$. In the following, we limit ourselves to the properties at zero temperature.

In the uniform case ($\beta=J_2/J_1=1$) and $\Delta=1$, it reduces to the Heisenberg model. Moreover, as discussed in Ref. 3, it is a transfer matrix of the $d=2$ Ashkin-Teller model. When $\beta=1$, the antiferromagnetic correlation decays algebraically for $0\leqslant\Delta\leqslant1$. But it is generically short-ranged away from it ($\beta\neq1$, $0\leqslant\Delta$).

Applying the Jordan-Wigner transformation, this quantum spin model is mapped into a fermionic model

$$H=\sum_{i\in\mathrm{odd}} -t_1(f_i^\dagger f_{i+1}+f_{i+1}^\dagger f_i)+V_1(f_i^\dagger f_i-1/2)(f_{i+1}^\dagger f_{i+1}-1/2) + \sum_{i\in\mathrm{even}} -t_2(f_i^\dagger f_{i+1}+f_{i+1}^\dagger f_i) + V_2(f_i^\dagger f_i-1/2)(f_{i+1}^\dagger f_{i+1}-1/2), \quad (2)$$

where $f_i^\dagger/f_i$ creates/annihilates a spinless fermion at the site i. The $V_{1(2)}$ denotes repulsive interaction between the fermions, which we set to be positive. The total fermion number N is set to be half filled ($N=L/2$), and the boundary condition is (anti)periodic when N is odd(even). The relation between the parameters is $t_2/t_1=V_2/V_1=\beta$ and $V_1/t_1=V_2/t_2=2\Delta$. In the uniform case ($\beta=1$) and $0\leqslant\Delta\leqslant1$, the system belongs to the universality class of the Tomonaga-Luttinger liquid and the physical degree of freedom can be represented in terms of a free real boson in the continuum limit. On the other hand, with a sufficiently strong interaction ($\Delta>1$), crystallization of the fermions occurs with a Z_2 symmetry breaking and it can be identified with the Mott insulator. In the following, we also use this kind of "fermionic" terminology ("Mott insulator," etc.) even in the context of quantum spin model.

Now let us derive a continuum model for $0\leqslant\Delta\leqslant1$. The starting point is the uniform case $\beta=1$. It has been established that, apart from the (marginally) irrelevant operators, the low-energy degree of freedom can be represented in terms of a free real boson ϕ with its Lagrangian density

$$\mathcal{L}=\frac{1}{2}[(\partial_t\phi)^2-(\partial_x\phi)^2], \quad (3)$$

where the velocity is set equal to 1 and ϕ is "compactified" as $\phi\sim\phi+2\pi R$ ($R=1/\sqrt{2\pi}$ at $\Delta=1$ and $1/\sqrt{4\pi}\leqslant R$

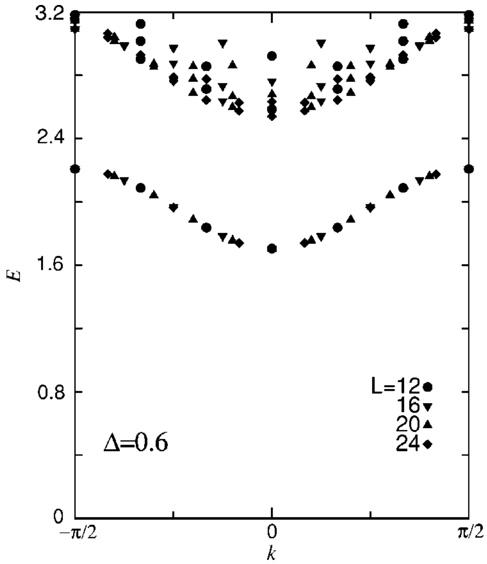

FIG. 1. Excitation spectrum at $J_1=-1$, $J_2=-0.3$, $\Delta=0.6$, $L=12,16,20,24$.

$\leqslant 1/\sqrt{2\pi}$ when $0\leqslant\Delta\leqslant 1$). And $\bar{\phi}$ is the "dual" boson. In this language, the staggered parts of the spin operators are expressed as

$$S_j^z \sim A(-1)^j \cos\left(\frac{\phi}{R}\right)$$

and

$$S_j^- \sim C(-1)^j \exp(i2\pi R\bar{\phi}),$$

where A, C are nonuniversal constants. Away from the uniform case ($\beta\neq 1$), the perturbation $(-1)^i\mathbf{S}_i\cdot\mathbf{S}_{i+1}$ breaks the translational symmetry by single lattice spacing ($\phi\to\phi+\pi R$) and it should generate a relevant term $\cos(\phi/R)$. It causes a gap which is adiabatically connected to the "band gap" at $\Delta=0$ and we say that the system belongs to the "band insulator." To summarize, the Lagrangian density becomes the Sine-Gordon model[5,6]

$$\mathcal{L} = \frac{1}{2}[(\partial_t\phi)^2 - (\partial_x\phi)^2] + g_1\cos(\phi/R), \tag{4}$$

where we limit ourselves to the region near the uniform case with $0\leqslant\Delta\leqslant 1$.

The above continuum model is integrable and exact data are available.[7,8] The basic quasiparticles are a soliton of the boson field and its counterpart (antisoliton). The soliton has a mass (energy gap) M_0. Moreover there exists a family of

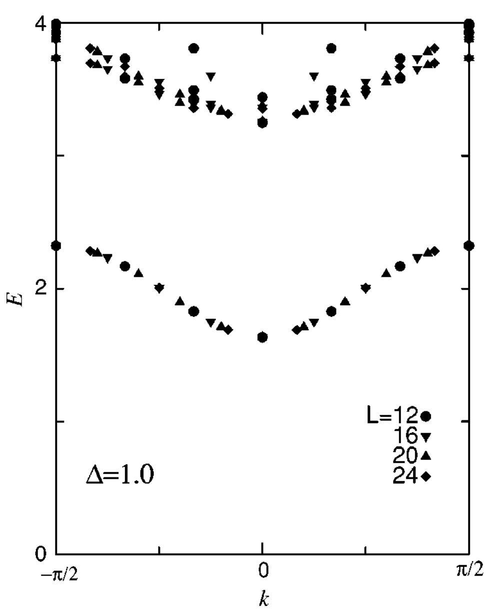

FIG. 2. Excitation spectrum at $J_1=-1$; $J_2=-0.3$, $\Delta=1$, $L=12,16,20,24$.

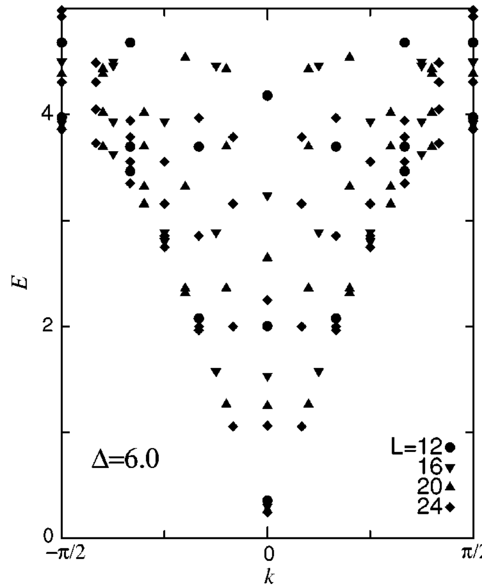

FIG. 3. Excitation spectrum at $J_1=-1$, $J_2=-0.3$, $\Delta=6$, $L=12,16,20,24$.

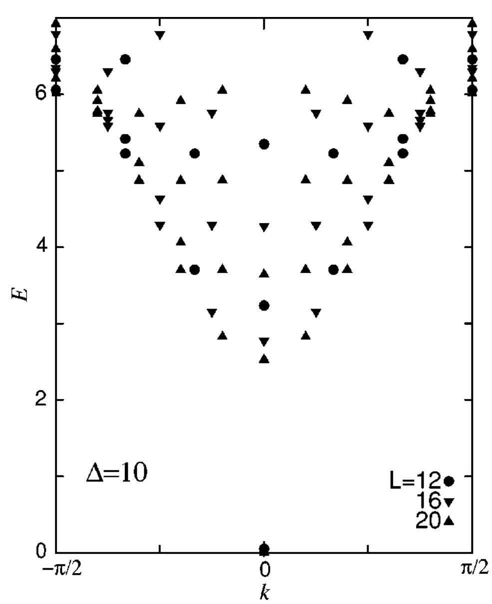

FIG. 4. Excitation spectrum at $J_1=-1$, $J_2=-0.3$, $\Delta=10$, $L=12,16,20$. The charge is ordered. The ground state is twofold degenerate in the thermodynamic limit.

bound state of the soliton-antisoliton. The "lightest" one has a mass $2M_0 \sin[\pi/(16\pi R^2-2)]$, which is M_0 at the SU(2) symmetric point ($\Delta=1$ and $R=1/\sqrt{2\pi}$). The low-lying neutral excitation (which does not change the total fermion number) consists of two elements: (1) the branch (bound state of the soliton-antisoliton) $\epsilon_b(k)$ and (2) the continuum (scattering state of the soliton-antisoliton) whose lower edge is represented by that of $\epsilon_c(k)=\Sigma_q[\epsilon(k-q)+\epsilon(q)]$. Here $\epsilon_b(k)$ shows a different dispersion than $\epsilon(k)[\epsilon_b(k)\neq\epsilon(k)]$. Then the structure of the continuum clearly shows the existence of quasiparticle other than the bound state.

B. Comparison with numerics

Let us discuss quasiparticle structure in the above lattice model, based on our numerical data. We have diagonalized the finite-size Hamiltonian numerically through the Lanczos method up to $L=24$ in the subspace with a fixed momentum k. We show figures for $\beta=0.3$ as a typical example (Figs. 1–4). The excitation spectrum E is obtained for the low-lying excitations as a function of momentum k. As seen in the Figs. 1 and 2 (they correspond to the discussion in the continuum limit), the excitation spectrum consists of the branch and continuum. Genereally speaking, "resiudal" interaction is irrelevant in the continuum. In other words, the lower edge of the continuum should be represented by that of $\epsilon_c(k)\sim\Sigma_q[\epsilon(k-q)+\epsilon(q)]$. Actually, in the continuum limit, this relation becomes exact.

Further, let us discuss the mass ratio. It is a ratio between the gap for the branch and the continuum. In the case with SU(2) symmetry, it is 2.0 in the therodynamic limit for $\beta=0.3$ and $\Delta=1$ (see Fig. 2). On the other hand, it is fragile to the SU(2)-breaking perturbation. Actually it is 1.5 for $\beta=0.3$ and $\Delta=0.6$ (see Fig. 1). And it decreases toward 1, as one comes close to $\Delta=+0$. Then we consider that the continuum consists of a scattering state of a quasiparticle (and hole) whose dispersion is generally independent of that of the quasiparticle for the branch. Actually, this is the picture established in the Sine-Gordon model.

Now we have confirmed the quasiparticle structure for this model and let us discuss a passage to the Mott insulator. We set the system away from the uniform case and it belongs to the band insulator with weak interaction (small Δ), as discussed above. For suffciently strong interaction (large Δ), it is natural to expect a charge ordering (Mott insulator). It implies that the system shows a transition from the band insulator to the Mott insulator, which is driven by the interaction. In fact, as seen in Figs. 1–3, the gap decreases with increasing Δ and finally the lower edge of the continuum touches at the ground state ($\Delta=\Delta_c$). When $\Delta>\Delta_c$, it leads to twofold degenerate ground states in the thermodynamic limit and a finite gap exists above it (see Fig. 4). We assign it to the Z_2 symmetry breaking. Actually we confirmed that the ground state is adiabatically connected to the case $\beta=1$, where exact results from the Bethe ansatz tell us that the Z_2 symmetry does break.

III. ANALOG IN HIGHER DIMENSIONS

A. In the vicinity of the 2D Heisenberg model

In the above, we have discussed quasiparticle structure in the vicinity of the 1D Heisenberg model, where solitonic excitations play a crucial role. The branch in the excitation spectrum corresponds to a bound state of the soliton-antisoliton, and the continuum corresponds to a scattering state of them.

There are some proposals on solitonic (topological) excitations in quantum spin models in higher dimensions.[9–12] However, when the ground state is antiferromagnetically ordered, a crossover should occur toward the $O(3)$ nonlinear σ model in $(2+1)$-dimensions in the long-wavelength and low-energy limit, as has been well established in the 2D Heisenberg model on a square lattice.[13] On the other hand, it is recently suggested that there exists the Mott insulator without any long-range order (in the quantum spin model[14] and also in the Hubbard model[15]). In this section, we want to discuss a possible scenario for the quasiparticle dynamics in such a phase, based on an analogy with one dimension.

Let us focus on the 2D antiferromagnetic quantum spin model

$$H=\sum_{\langle j,k\rangle\in A} J_A \mathbf{S}_j\cdot\mathbf{S}_k+\sum_{\langle j,k\rangle\in B} J_B \mathbf{S}_j\cdot\mathbf{S}_k, \tag{5}$$

where we set the model so that it can be deformed continuously into the Heisenberg model on a square lattice by tuning J_A and J_B. Further, we limit ourselves to the case without any long-range order. A possible example of this type of model has been discussed in Ref. 14, which is defined on a triangular-type lattice in two dimensions.

Here we *assume* that a fermionic soliton with spin-1/2 is well-defined in the above model and the continuum corresponds to a scattering state of the soliton-antisoliton. Then we introduce the fermion $f_{l\sigma}$ which represents the soliton on a lattice. In order to describe the dynamics of them, the effective Hamiltonian on a lattice is set to be

$$\begin{aligned} H=&\sum_{\langle l,m\rangle\in a}(f^\dagger_{l\sigma}t^a_{lm}f_{m\sigma}+f^\dagger_{m\sigma}t^a_{ml}f_{l\sigma})\\ &+\sum_{\langle l,m\rangle\in b}(f^\dagger_{l\sigma}t^b_{lm}f_{m\sigma}+f^\dagger_{m\sigma}t^b_{ml}f_{l\sigma}),\end{aligned} \tag{6}$$

where $t^{a(b)}_{lm}/|t^{a(b)}_{lm}|=\exp(2\pi i a_{lm})$, $a_{lm}=-a_{ml}$, and the effective "flux" is defined by Σa_{lm} where the summation is over each cycle (see, e.g., Ref. 11 for the "derivation"). Here the filling is set to be half filled ($\nu=1/2$) and a_{lm} is introduced so that ϕ is $1/2$ around every elementary plaquette. (For example, in the case of triangular-type lattice in two dimensions, $\phi=1/2$ per plaquette implies $\phi=1/4$ per triangle.) It is to be noted that we do *not* assume that the "flux phase" is long-range ordered. But we only focus on how to describe the continuum and the spectrum below it is beyond the scope. Now, to be explicit, we set the geometry to be triangular-type in two dimensions. It is constructed by deforming a square lattice. Set the hopping in the $x(y)$ direction [(1,0) and (0,1)] to be t. Then the triangular lattice is constructed by adding the next nearest-neighbor hopping t' in the direction $(1,1)$. The energy spectrum of this model is "anisotropic" in the $\mathbf{k}$ space, which is $\epsilon_\pm(\mathbf{k})=\pm[A(\mathbf{k})^2+|B(\mathbf{k})|^2]^{1/2}$ with $A(\mathbf{k})=2t\cos(k_x)$, $B(\mathbf{k})=2t\cos(k_y)+2it'\cos(k_x+k_y)$ and $(k_x,k_y)\in[0,\pi)\times[0,2\pi)$. Remarkably it has a small gap around $(\pi/2,\pi/2)$ which is in contrast with a large gap around $(k_x,k_y)=(\pi,0),(0,\pi)$.

Then the lower edge of the continuum should be represented by that of $\epsilon_c(\mathbf{k})\sim\Sigma_q[\epsilon_+(\mathbf{k}-\mathbf{q})+\epsilon_+(\mathbf{q})]$. Moreover, there can exist bound states as in the case in 1D. The scattering and bound states are basically independent of each other and both of them can appear in the low-energy regime and become overlapped. Related to our discussion in one dimension, a comment is in order. In the model discussed above, there can exist a "branch" below the continuum in the energy spectrum. It is conventional to apply the so-called magnon picture in such a case. But it is not always so, as has been confirmed in the case of one dimension.

B. Extension to the 2D Hubbard model

In this section, based on the above scenario, we shall analyze data on the 2D Hubbard model at half filling $\langle n_j\rangle=1$:

$$H=-\sum_{\langle j,k\rangle\in A,\sigma} t_A c_{j\sigma}^\dagger c_{k\sigma}-\sum_{\langle j,k\rangle\in B,\sigma} t_B c_{j\sigma}^\dagger c_{k\sigma} + U\sum_j (n_{j\uparrow}-1/2)(n_{j\downarrow}-1/2), \qquad (7)$$

where $c_i^\dagger/c_i$ creates/annihilates a fermion with spin-1/2 at the site i and $n_{i\sigma}=c_{i\sigma}^\dagger c_{i\sigma}$. Since this reduces to the 2D antiferromagnetic quantum spin model in the large-U limit, we shall apply the scenario in the previous subsection. See, e.g., Ref. 11 which shares the picture with us. What we aim at in this paper is to offer the *first* (so far as we know) approximation-free results to support that picture. The geometry is set to be triangular type in two dimensions. It is constructed by deforming the square-lattice model as described in the previous subsection. It is to be noted that antiferromagnetic correlation is suppressed in this model down to sufficiently low temperature (or zero temperature), as discussed in Ref. 15 (see also Refs. 16–20 for previous studies on this model).

If the quasiparticle picture in the previous subsection is realized in this model, the anisotropic dispersion should give drastic effects in the **k**-dependent observables, as we have discussed. Here we shall focus on the **k**-resolved charge compressibility $\kappa(\mathbf{k})=d\langle n(\mathbf{k})\rangle/d\mu$ where $\langle n(\mathbf{k})\rangle=\langle c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}\rangle$ and μ is the chemical potential.[1,2] It has been confirmed in Ref. 1 that this observable tells us a fine structure of the quasiparticles.

Then, applying the finite temperature auxiliary-field quantum Monte Carlo method,[21–23] we have obtained $\kappa(\mathbf{k})$ (see Fig. 5). In the data, we set t to be unit energy scale $(t=1)$ and $U/t=4$. The system size is 12×12 and the slice size in imaginary time is $\Delta\tau=0.1/t$. We performed 5000 Monte Carlo sweeps in order to reach a thermal equilibrium followed by 10 000 sweeps for the measurement. The temperature is set to be $T=0.2t\sim J\sim t^2/U\ll U$ and we have confirmed that the charge compressibility is strongly suppressed due to interaction and shows a thermally activated behavior.

Now let us focus on the line $k_x+k_y=\pi$ in $[0,\pi)\times[0,\pi)$. In the absence of interaction $(U/t=0)$, the $\kappa(\mathbf{k})$ on this line is constant in this model. The question is which part on this line

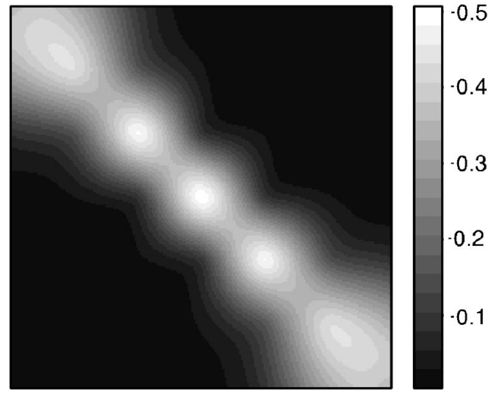

FIG. 5. **k**-resolved charge compressibility $\kappa(\mathbf{k})$ at $t'/t=0.5$, $U/t=4$ for $[0,\pi)\times[0,\pi)$. In the absence of interaction $(U/t=0)$, the $\kappa(\mathbf{k})$ on $k_x+k_y=\pi$ is constant in this window. The result shows that finite interaction makes the system compressible around $(\pi/2,\pi/2)$ more than $(k_x,k_y)=(\pi,0),(0,\pi)$.

is more compressible than others in the presence of interaction. The results show that finite interaction makes the system compressible around $(\pi/2,\pi/2)$ more than $(k_x,k_y)=(\pi,0),(0,\pi)$. By varying t'/t, we confirmed that the effects are not suppressed against the disordering of the antiferromagnetic order in the ground state. This is what we expect from the scenario in the previous subsection, as seen in the energy dispersion of the quasiparticles (see also the discussion in Ref. 1). This kind of anisotropic effects due to interaction is in contrast with, for example, the results in infinite dimensions[24] and we consider that it is important in itself. We also studied the temperature effects in a systematic way. As temperature is raised, the charge compressibility becomes enhanced and the anisotropy is washed out. In other words, the anisotropoic behavior is a manifestation of the nontrivial low-energy physics. Although it needs further study to identify the origin, we consider that the above quasiparticle picture is one of the candidates.

IV. SUMMARY AND DISCUSSION

In this paper, we have studied quasiparticle structure in the vicinity of the Heisenberg model. In one dimension, we have confirmed solitonic quasiparticles in the model. Further, we discussed its analog in higher dimensions. To be concrete, we proposed several consequences from solitonic excitations in two dimensions. In particular, it should lead to "anisotropy" in the **k** space. In that context, we numerically studied **k**-resolved charge compressibility $\kappa(\mathbf{k})$ and discussed a scenario for the quasiparticles in the 2D Hubbard model at half filling on a triangular-type lattice.

For further progress, it is crucial to collect bias-free data on the energy spectrum, dynamical correlation function, etc., through approximation-free approach. It should clarify when the solitons become *real* in higher dimensions.

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