FERMI SURFACE OF THE ONE-DIMENSIONAL HUBBARD MODEL: FINITE-SIZE EFFECTS

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The results reported here, using a standard numerical algorithm and a simple low temperature extrapolation, appear consistent with numerical results of Sorella et al. for the one-dimensional Hubbard model in the half-filled and quarter-filled band cases. However, it is argued that the discontinuity at the Fermi level found in the quarter-filled case is likely to come from the zero-temperature finite-size dependence of the quasiparticle weight Z, which is also discussed here.

1. INTRODUCTION

One of the key questions on the two-dimensional Hubbard model in the context of superconductivity is whether, away from half filling, Fermi liquid concepts are applicable, or if a whole new description with new kinds of elementary excitations is necessary. To test the validity of numerical approaches to this problem, we first consider a case where we think the answer is known, namely in one dimension.

2. METHOD AND MODEL

We are studying the Hubbard model

\[ H = -t \sum_{\langle i, j \rangle} (c_{i\sigma}^+ c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i \uparrow} n_{i \downarrow} - \mu \sum_i n_{i \sigma} \]

where \( \sigma \) is the spin label and \( \langle i, j \rangle \) denotes a sum over nearest-neighbors on a one-dimensional lattice. We take periodic boundary conditions and consider the case \( U/t = 4 \) with average site occupations \( \rho = 1 \) and \( 1/2 \). We use the BSSH algorithm. Improvements of this algorithm have been announced after this work was completed.

3. RESULTS

3.1. Half filling, \( \rho = 1 \)

In the half-filled case, \( \rho = 1 \), our lowest temperature results (not shown here) are consistent with the zero-temperature results of Ref. 4. Clearly then, this confirms that there is no Fermi surface in this case, in agreement also with results obtained from \( t/U \) expansions.

3.2. Quarter Filling, \( \rho = 1/2 \)

The large \( \ell \) solution of the renormalization group equations is \( Z(\ell) = C (E_{c}(\ell)/E_{c})^{\theta} \) where \( C \) contains various constants of integration, \( E_{c} \) is the bare-bandwidth cutoff, \( E_{c}(\ell) \) the length-scale dependent cutoff, and \( \theta \) is an exponent which is a function of the fixed point value of the coupling constants.

As the cutoff goes to zero, the quasiparticle weight also vanishes, as expected. However, finite temperature, or finite frequencies set a minimal value of the cutoff. Under these conditions, one has a non-vanishing quasiparticle weight. In the present case, we are working in the limit

\[ \Delta \ell = 2t \sin k_{F} \Delta k > \beta^{-1} \]

(1)

where \( \Delta k \) is the difference between the last wave vector which can be eliminated and the Fermi wave vector, namely, \( \Delta k = 2\pi/\text{L} \) where \( \text{L} = 32 \). The important conclusion, then, is that at sufficiently low temperatures, as defined by Eq. (1), the cutoff becomes \( E_{c}(\ell) = \Delta \ell \) instead of temperature and hence the quasiparticle weight \( Z \) is determined by the system size, namely,

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\( Z \propto L^\theta \). The condition (1) also has another physically interesting interpretation in terms of length, namely, it can be rewritten as \( \xi \propto L \), where \( \xi = 2\pi v_\beta / \beta \) is the thermal de Broglie wavelength.

We use these results to interpret our simulations in the quarter-filled case, \( \rho = 1/2 \), through a fit of the limiting low-temperature dependence of the momentum distribution to a quasiparticle-plus-background functional form.

The results for \( \xi_k \) are illustrated by circles in Fig. 1. The full line is the curve, 
\[
\xi_k = -2t^* \cos k + \xi_0 \text{ with } \xi_0 = 0.31 \text{ and } t^* = 0.79.
\]
Note that the full circle in Fig. 1 is, as one would expect from a simple quasiparticle model, simply at the coordinates \( k_F = \pi/4 \) and \( \xi_k = \mu \) with \( \mu \) the limiting low-temperature value of the chemical potential used in the simulation.

Solely from the fit, the uncertainties on the parameters are of order \( \Delta \xi_0 = \pm 0.05 \) and \( \Delta t^* = \pm 0.02 \). However, \( t^* = 0.79 \pm 0.02 \) should not be used to estimate the renormalized Fermi velocity \( v_F^* \). A more realistic estimate would yield, using only points near the Fermi surface, 
\[
v_F^* = (0.85 \pm 0.15)v_F.
\]

While the relative errors for \( \xi_k \) are quite small, the errors in \( v_F^* \) are much larger since they involve taking a derivative. For \( Z_k \) and \( \Gamma_k \), errors from the fit itself are large. We can estimate \( \Gamma_k = 0.03 \pm 0.02 \) and \( Z_k = 0.95 \pm 0.05 \), with a \( k \) dependence which is within the uncertainty. We cannot evaluate \( \Gamma_k \) at the Fermi surface itself.

4. DISCUSSION

One should note that Sorella et al. also obtained a large \( Z \) at quarter filling, even for systems of size 200. While that may seem surprising at first, this is in fact a consequence of the combined effect of the finite-size dependence of \( Z \) and the smallness of the exponent \( \theta \), a possibility which they also suggested.

Indeed, from above, we see that \( Z(\text{L}=200)/Z(\text{L}=32) = (32/200)\theta \). A very rough estimate for this exponent is obtained by setting \( g_\theta^0 = g_\theta^0 = U \) and \( v_F = 2t \sin k_F \) from which one obtains \( \theta = 0.05 \). However, even for \( \theta \) twice as large, \( \theta = 0.1 \), we obtain \( Z(\text{L}=200)/Z(\text{L}=32) = 0.83 \), consistent with our \( Z(\text{L}=32) \approx 0.95 \) and with \( Z(\text{L}=200) \approx 0.8 \).

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