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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

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

where σ 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.[1] Improvements of this algorithm have been announced[2] after this work was completed.

3. RESULTS

3.1. Half filling, $\rho = 1$

In the half-filled case, $\rho = 1$, our lowest temperature results[3] (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.[5]

3.2. Quarter Filling, $\rho = 1/2$

The large ℓ 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 θ 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

$$\Delta\varepsilon = 2t \sin k_F\, \Delta k \gtrsim \beta^{-1} \qquad (1)$$

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

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$Z \approx L^{-\theta}$. The condition (1) also has another physically interesting interpretation in terms of length, namely, it can be rewritten as $\xi \gtrsim L$, where $\xi = 2\pi v_F \beta$ 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 ε_k are illustrated by circles in Fig.1. The full line is the curve, $\varepsilon_k = -2t^* \cos k + \varepsilon_0$ with $\varepsilon_0 = 0.31$ 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 $\varepsilon_k = \mu$ with μ 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 $\Delta\varepsilon_0 = \pm 0.05$ 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 ε_k are quite small, the errors in v_F^* are much larger since they involve taking a derivative. For Z_k and Γ_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 Γ_k at the Fermi surface itself.

4. DISCUSSION

One should note that Sorella et al.[4] 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* θ, a possibility which they also suggested.

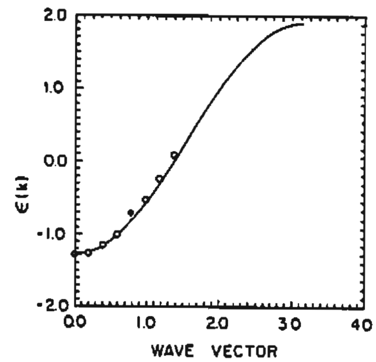

FIGURE 1
Quasiparticle energy-wave-vector relation. Circles are obtained from a fit of the Monte Carlo data of Fig.1.

Indeed, from above, we see that $Z(L=200)/Z(L=32) = (32/200)^{\theta}$. A very rough estimate for this exponent is obtained by setting $g_1^0 = g_2^0 = U$ and $v_F = 2t \sin k_F$ from which one obtains[3] $\theta = 0.05$. However, even for θ twice as large, $\theta = 0.1$, we obtain $Z(L=200)/Z(L=32) = 0.83$, consistent with our $Z(L=32) \cong 0.95$ and with[4] $Z(L=200) \cong 0.8$.

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