Interaction-Induced Collapse of a Section of the Fermi Sea in the Zigzag Hubbard Ladder

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Using the next-nearest-neighbor (zigzag) Hubbard chain as a one-dimensional model, we investigate the influence of interactions on the position of the Fermi wave vectors with the density-matrix renormalization-group technique. For suitable choices of the hopping parameters we observe that electron-electron correlations induce very different renormalizations for the two different Fermi wave vectors, which ultimately lead to a complete destruction of one section of the Fermi sea in a quantum critical point.

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Introduction.—Many aspects of the low-energy physics of an electronic system are influenced by the shape of its Fermi surface and the occupation of nearby states. Associated observables may vary strongly with the temperature and the strength of the interaction of the electrons. Changes in the Fermi-surface geometry induce magnetic and other instabilities. Electron-electron interactions induce a momentum dependent softening of the Fermi surface, which is responsible for a wide variety of phenomena, such as the loss of magnetic order or high-temperature superconductivity. In systems where the Fermi surface is not simply connected, interactions may lead to a partial or total collapse of parts of the Fermi surface at a quantum critical point and an associated drastic change in the physical properties of the system. It is therefore important to study the renormalization of the individual Fermi surface sections under the influence of electron-electron correlations in competition with frustrating interactions.

Recent investigations suggested a spontaneous, interaction-induced deformation of the Fermi surface of the 2D t-J model [1] as well as of the (extended) Hubbard model [2–5]. Because the effect of strong electronic interactions is difficult to study in two- or three-dimensional systems, these studies either are confined to the weak coupling limit or involve extensive numerical studies of effective lattice models. Many aspects regarding the Fermi surface renormalization for strong interactions remain presently unclear.

The development of the density matrix renormalization group now offers a reliable—though numerically involved—approach to rigorously study the effect of strong interaction in one dimension. In this Letter we report a study of the renormalization of the Fermi wave vector, or Fermi point, in the Hubbard chain with next-nearest-neighbor hopping matrix elements as a one-dimensional model for Fermi surface renormalization. We confirm results of a recent renormalization group (RG) analysis for the Fermi point renormalization in weak coupling. Fermi points close to a saddle point of the momentum-distribution function $n(k)$ are predicted to shift towards the van Hove singularity. A similar renormalization has been suggested for two-dimensional systems [1,4]. For strong interactions, the pocket of the Fermi sea near the saddle point may be emptied completely, a hypothesis [6] which cannot be verified in weak coupling. In order to study this prediction rigorously, we have performed a density-matrix renormalization-group (DMRG) study of the t_1-t_2 Hubbard model for rings with periodic boundary conditions, evaluating the momentum-distribution function $n(k)$ directly for rings with up to 80 sites. For larger interaction strength we find a novel interaction-induced quantum critical point that is associated with the collapse of a Fermi sea pocket. This phenomenon is analogous to the opening of a pseudogap, found experimentally in the high-T_C cuprates [7], near the saddle point of the electronic dispersion.

The Hamiltonian of the zigzag Hubbard ladder (see Fig. 1, top) is given as

$$H = \sum_{\substack{n,\sigma \\ \Delta n=1,2}} t_{\Delta n}(c^\dagger_{n+\Delta n,\sigma} c_{n,\sigma} + \text{H.c.}) + U \sum_n c^\dagger_{n,\uparrow} c_{n,\uparrow} c^\dagger_{n,\downarrow} c_{n,\downarrow}\,, \quad (1)$$

where the $c^\dagger_{n,\sigma}$ ($c_{n,\sigma}$) are fermion-creation (destruction) operators on site n and spin $\sigma = \uparrow, \downarrow$. For appropriate choices of the parameters this model describes either the low-energy properties of Hubbard ladders [6] or half-filled edge-sharing double-chain materials like $SrCuO_2$ [8] or LiV_2O_5 [9] for which the next-nearest-neighbor hopping t_2 is expected to be substantial.

Generically, the variation of the two hopping parameters ($t_{1,2}$) allows changes in the position of the Fermi point in the noninteracting limit. When the hopping t_2 is large enough, the Fermi sea will split into two separate parts; see Fig. 1. According to a recent RG analysis for the case of two separate Fermi seas [6] the Fermi points $k_F^{(i)}$ ($i = 1, 2$) are renormalized as

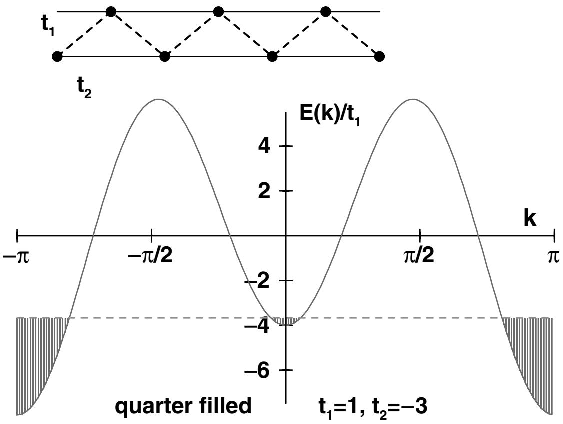

FIG. 1. Top: Illustration of the t_1-t_2 zigzag ladder, the dashed/full lines correspond to t_1/t_2 bonds. Bottom: Illustration of the $U = 0$ dispersion relation $E(k) = 2t_1 \cos(k) + 2t_2 \cos(2k)$ for the case $t_1 = 1$, $t_2 = -3$. Also shown (horizontal dashed line) is the Fermi energy $E_f = -3.6736t_1$ for the quarter-filled case.

$$-\Delta k_F^{(1)} = -\Delta k_F^{(2)} = \Delta k \simeq \frac{U^2}{2\pi^2} \frac{v_2 - v_1}{(v_1 + v_2)^2} \frac{\Lambda_0}{v_1 v_2}. \tag{2}$$

In weak coupling, the Fermi point shift Δk depends only on the respective Fermi velocities v_i and on the initial momentum cutoff Λ_0. Equation (2) is rigorous in the weak-coupling limit.

DMRG.—The evaluation of $n(k)$ as the Fourier transform of the correlation function,

$$n_\sigma(k) = \frac{2}{L} \sum_{n,n'=1}^{L} \cos[k(n - n')] \langle c_{n,\sigma}^\dagger c_{n',\sigma} \rangle, \tag{3}$$

is numerically difficult and costly in the framework of the DMRG [10,11], in particular for periodic boundary conditions [12]. For large interaction strength, the suppression of double occupancy reduces the size of the relevant Hilbert space and improves the convergence properties of the DMRG procedure [13]. We have therefore decided to study the case of quarter-filling, where the renormalization of the Fermi point occurs at relatively large values of the interaction U. We chose $t_2/t_1 = -3$ as a good set of parameters to observe the Fermi point renormalization effects at quarter-filling, since one of the Fermi seas is small for this case (see Fig. 1) and since the weak-coupling RG predicts gapless Luttinger-liquid behavior for these parameters [6].

We checked for both the convergence of the variational energy and of the correlation functions by increasing the number of DMRG states m and found reasonable choices for the desired accuracy. The weight of the discarded fraction of the density matrix varies between 1×10^{-4} to 2×10^{-5} depending on the choice of system size and the number of states. Figure 2 demonstrates the convergence

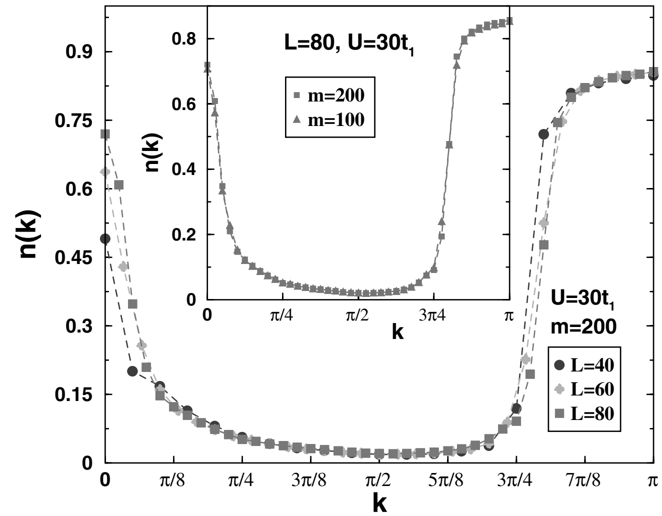

FIG. 2. Convergence of the correlation function $n(k)$ compared for different chain lengths L and DMRG states m (inset shows $L = 80$) for a quarter-filled system with $t_1 = 1$, $t_2 = -3$. The lines are guides to the eye.

of $n(k)$ both as a function of lattice size and of the number of states m in the DMRG procedure. Additionally, we performed calculations for open chains and verified that the behaviors of the real-space correlation function is consistent with those for periodic systems.

Results.—Depending on the relative strength of the hopping parameters t_2/t_1 and interaction strength U/t_1, the ground-state phase diagram of the t_1-t_2 model exhibits various instabilities towards the formation of states with spin and/or charge gap [14,15]. We have therefore investigated the possibility of instabilities towards ferromagnetism and phase separation by evaluating $\Delta E_F = E(N_\uparrow + 1, N_\downarrow - 1) - E(N_\uparrow, N_\downarrow)$, where $E(N_\uparrow, N_\downarrow)$ is the ground-state energy of the quarter-filled system, and $\Delta E_{ph} = E(N_\uparrow + 1, N_\downarrow + 1) + E(N_\uparrow - 1, N_\downarrow - 1) - 2E(N_\uparrow, N_\downarrow)$. For the parameters considered here no tendency towards an instability was found for any interaction strength, in accordance with Ref. [15].

In Fig. 3 we present results for the momentum distribution function for $U/t_1 = 1, 30, 100$. For $t_2 = -3t_1$, there is quarter filling. For $U = 0$, the two Fermi wave vectors are $k_F^{(1)} = 0.055\pi$ and $k_F^{(2)} = 0.805\pi$. The parameter $\alpha = (v_F^{(1)} + v_F^{(2)})/(2v_F^{(1)}) = 5.53$ entering the weak-coupling RG equations [6] indicates a gapless Luttinger-liquid phase at small couplings.

For small U we clearly observe the existence of two Fermi points $k_F^{(1)}$ and $k_F^{(2)}$ (see Fig. 3), which are substantially renormalized with growing interaction strength.

It is evident from the data presented in Fig. 3 that the magnitude of the momentum distribution function inside the smaller Fermi sea is reduced substantially stronger by the interaction than the one inside the large Fermi point. This is a consequence of the very different values for the respective Fermi velocities, $v_1 = 0.658t_1$ and

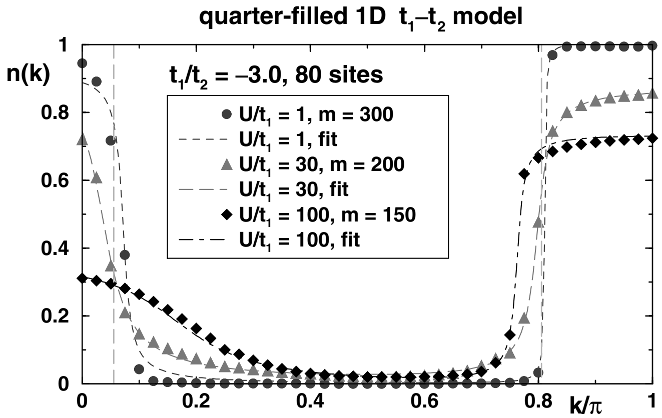

FIG. 3. The DMRG results (symbols) for the momentum-distribution function for a quarter-filled 80-site system with periodic boundary conditions. The parameters are $t_1 = 1$, $t_2 = -3$, and $U = 1$ and $U = 30$, respectively. The lines through the DMRG data are fits by Eq. (4). The dashed vertical lines indicate the $U = 0$ positions of the two Fermi points.

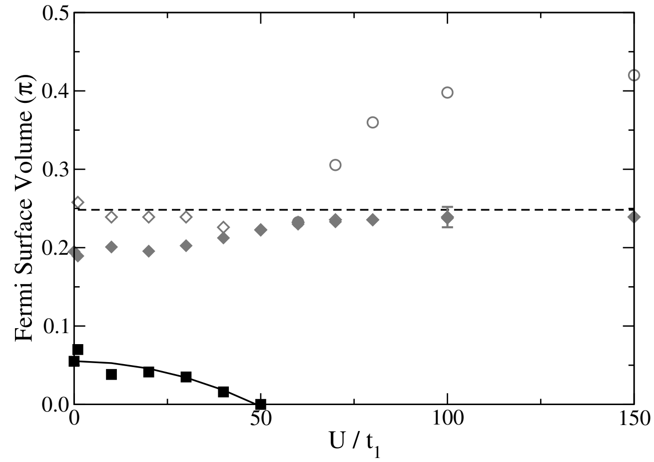

FIG. 4. The DMRG results for the volume of the small ($k_F^{(1)}$, filled squares, the line is a guide to the eye) and large ($\pi - k_F^{(2)}$, filled diamonds) Fermi sea and the total (open diamonds) volume of the Fermi sea (FSV). The latter is identical with the volume of the remaining Fermi sea for $U > 50$. The dashed line indicates the analytical value of the total FSV at $U = 0$ (quarter-filling). The open circles indicate the total FSV under the assumption that a small Fermi point persists for $U > 50$.

$v_2 = 6.620t_1$, which differ by 1 order of magnitude. The energies of particle-hole excitations are $\sim v_F \Delta k$; many more particle-hole excitations are therefore created for the Fermi sea pocket, which has the smaller $v_F = v_1$, resulting in a substantial reduction in the occupation numbers $n(k)$ for $k < k_F^{(1)}$.

In order to quantify the results of Fig. 3 we analyze the Fermi point position as the point where the slope of the momentum-distribution function is maximal. We find that our finite-lattice data for the momentum distribution function $n(k)$ is approximated well by two washed-out step functions:

$$n(k) = a_0 + a_1 \arctan \frac{k - k_F^{(1)}}{p_1} + a_2 \arctan \frac{k - k_F^{(2)}}{p_2} . \quad (4)$$

The quality of this fit is illustrated by the lines in Fig. 3.

Figure 4 shows the dependence of $k_F^{(1/2)}$ as well as the total volume of the Fermi sea (in units of π) as a function of U. The data clearly indicate the presence of a quantum-critical point with $U_c \approx 50t_1$, for which the smaller Fermi sea collapses. The fit-parameter $k_F^{(1)}$ entering (4) denotes a locus of maximal slope in $n(k)$, which corresponds to the Fermi-point position for $U < U_c$. As the calculations were done for fixed particle density, we expect the Fermi sea volume to be independent of the interaction-strength U (Luttinger's theorem [16]). From Fig. 4 we see that this expectation is approximatively fulfilled if we take $(\pi - k_F^{(2)}) + k_F^{(1)}$ for the volume of the Fermi sea for $U < U_c$ [open diamonds in Fig. 4] and $\pi - k_F^{(2)}$ for $U > U_c$. Some numerical uncertainty is observed as usual in numerical simulations, near the critical point. The error bar in the figure denotes the lattice-induced finite-size error on the Fermi point position. Within this error all data are compatible with the exact result in the noninteracting limit.

As the data for $U = 100$ in Fig. 3 indicates, we also have maxima in the slope of $n(k)$ corresponding to the remainder of the small Fermi sea for $U > U_c$. To distinguish between incoherent excitations and a sharp Fermi point we have plotted the hypothetical total Fermi sea volume (open circles in Fig. 4) under the assumption that these inflection points also correspond to Fermi points. As the figure indicates, this would lead to a massive violation of the Luttinger theorem for all $U > U_c$. We thus conclude that $n(k)$ for small k and $U > U_c$ can be consistently associated with contributions from incoherent excitations to the momentum-distribution function.

Conclusions.—In a one-dimensional model we have analyzed the stability of Fermi sea pockets with respect to electron-electron interactions and found that sufficiently strong repulsive interactions lead to a novel quantum critical point at which the one Fermi sea pocket is destroyed altogether. We studied this quantum-phase transition within the t_1-t_2 zigzag ladder as a prototypical model. We estimate the value of $U_c/t_1 \approx 50$ for $t_2 = -3t_1$ in a quarter-filled system. We note that the nature and existence of this transition does not depend on the specific choice of t_1, t_2 and the filling, but that a manifold of transitions exist for appropriate choices of these parameters. The conditions of the existence of the transition are the existence of two different pockets of the Fermi sea with a significantly lower Fermi velocity at the Fermi point of the smaller pocket. In our study we have chosen the values of the parameters such that the transition becomes amenable to quantitative treatment with the DMRG, which converges progressively worse near half-filled systems. This leads to a critical U_c that seems to be too large to be relevant for experimental realizations of (1), but we point out that at least two effects are likely to dramatically reduce the critical U_c.

(i) At half-filling the t_2-t_1 model undergoes a Mott-Hubbard transition for $t_2 > t_1/2$. For $t_2 \rightarrow t_1/2$ the critical $U_c \rightarrow 0$. It has been estimated [6] that the RG estimate for the critical U_c obtained from Eq. (2) is in agreement with numerical results [17,18]. We therefore expect the critical U_c for the destruction of the small Fermi-surface pocket to reduce drastically near half-filling. Here we did not investigate this region due to numerical difficulties.

(ii) In realistic systems the Coulomb interaction will be longer ranged than the on-site form assumed in the present study. It is known that longer-range contributions to the interaction increase substantially the effect of the interaction on the Luttinger-liquid parameters in the one-dimensional electron gas [19,20]. We expect a similar enhanced influence on the renormalized position of the Fermi points.

We believe our rigorous findings for the one-dimensional case to be relevant for two dimensions. We note that the Fermi-surface instability observed in the present study is qualitatively different from the Pomeranchuk instability observed in weak coupling [21] for the 2D Hubbard model, since the Pomeranchuk instability corresponds to a spontaneous breaking of the tetragonal (C_4) symmetry due to enhanced scattering from one saddle point to another. The Fermi surface instability observed in the present study is driven, on the other hand, by scattering between "normal" and flat parts of the Fermi surface.

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