Correlation Exponents and the Metal-Insulator Transition in the One-Dimensional Hubbard Model

H. J. Schulz
Laboratoire de Physique des Solides, Université Paris-Sud, 91405 Orsay, France
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The long-distance decay of correlation functions in the one-dimensional Hubbard model is determined for arbitrary band filling and correlation strength, using the exact solution of Lieb and Wu. In particular, for either infinitely strong on-site repulsion U, or in the close proximity of half filling for any U, spin-spin correlations decay like $\cos(2k_F x)x^{-3/2}\ln^{1/2}(x)$. For infinite U the results are generalized to the case of nonzero nearest-neighbor interaction. The behavior of the frequency-dependent conductivity is also discussed, in particular in the proximity of the metal-insulator transitions occurring for half and quarter filling.

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A theoretical understanding of interacting fermion systems in one dimension is important for a number of reasons. On the one hand, in the physics of quasi-one-dimensional organic conductors[1] or of conducting polymers,[2] interaction effects play a major role. On the other hand, one-dimensional models can be easier to understand than their higher-dimensional versions, or even exactly solvable, as is the case with the prototypical model of correlated fermions, the Hubbard model.[3] They therefore can provide valuable information on the role of correlation effects in higher dimensions, e.g., on the physics of correlated fermions in two dimensions, which is thought to be at the origin of the many interesting properties of high-temperature superconductors.[4]

The theory of one-dimensional interacting fermions has made progress along two somewhat separate lines: (i) Perturbative renormalization-group calculations have shown that different correlation functions [see, e.g., Eqs. (5) and (6) below] have long-range power-law behavior, with interaction-dependent exponents.[5,6] These exponents in turn determine a number of physical properties: temperature dependence of the NMR relaxation rate[7] or x-ray scattering intensities,[8] effect of impurities,[9] or possible low-temperature ordered states in systems of coupled chains. (ii) Specific lattice models like the Hubbard model and its generalizations have been studied numerically to obtain correlation functions[10] and the energetics of ground and excited states.[11,12]

In the present paper, I shall describe a way to obtain precise information about correlation exponents from energies alone *without the explicit calculation of correlation functions.* The reasoning used is a straightforward generalization of arguments due to Haldane[13] to the case of spin-$\frac{1}{2}$ fermions. I will illustrate the method using the Hubbard model, where exact energies can be obtained even in the thermodynamic limit. Even then the eigenfunctions are so complicated that the direct calculation of correlation functions like (5) and (6) is hard even for very small systems.[14] The present calculation then provides a rather detailed description of the crossover between weak and strong correlation and of the metal-insulator transition occurring when the average particle number per site n approaches unity. It will be seen that the method can also give rather reliable results in cases where only small finite systems can be solved exactly.

The low-energy, large-distance behavior of a one-dimensional fermion system with spin-independent interactions is described by the Hamiltonian[5,6]

$$H=H_\rho+H_\sigma+\frac{2g_1}{(2\pi\alpha)^2}\int dx\cos(\sqrt{8}\phi_\sigma)\,. \tag{1}$$

Here α is a short-distance cutoff, g_1 is the backward-scattering amplitude, and for $\nu=\rho,\sigma$

$$H_\nu=\int dx\left[\frac{\pi u_\nu K_\nu}{2}\Pi_\nu^2+\frac{u_\nu}{2\pi K_\nu}(\partial_x\phi_\nu)^2\right]. \tag{2}$$

The phase fields are[15]

$$\phi_\nu(x)=-\frac{i\pi}{L}\sum_{p\neq 0}\frac{1}{p}e^{-\alpha|p|x/2-ipx}[\nu_+(p)+\nu_-(p)] -N_\nu\frac{\pi x}{L}\,, \tag{3}$$

$$\Pi_\nu(x)=\frac{1}{L}\sum_{p\neq 0}e^{-\alpha|p|x/2-ipx}[\nu_+(p)-\nu_-(p)] +\frac{J_\nu}{L}\,. \tag{4}$$

Here $\rho_r(p)$ [$\sigma_r(p)$] are the Fourier components of the charge- [spin-] density operator for right- ($r=+$) and left- ($r=-$) going fermions. Introducing the *total* number operators (measured with respect to the ground state) N_{rs} for right- and left-going particles ($r=\pm$) of spin s, the (charge and spin) number and current operators are

$$N_\nu=[(N_{+\uparrow}+N_{-\uparrow})\pm(N_{+\downarrow}+N_{-\downarrow})]/\sqrt{2}\,,$$

$$J_\nu=[(N_{+\uparrow}-N_{-\uparrow})\pm(N_{+\downarrow}-N_{-\downarrow})]/\sqrt{2}\,,$$

where the upper and lower sign refer to charge and spin, respectively.

The operators ϕ_ν and Π_ν in (1) obey Bose-like commutation relations: $[\phi_\nu(x),\Pi_\mu(y)]=i\delta_{\nu\mu}\delta(x-y)$, and con-

sequently, at least for $g_1=0$, (1) describes independent long-wavelength oscillations of the charge and spin density, with linear dispersion relation $\omega_\nu(k)=u_\nu|k|$, and the system is conducting.[16] The only nontrivial interaction effects in (1) come from the cosine term. However, for repulsive interactions ($g_1>0$), this term is renormalized to zero in the long-wavelength limit, and at the fixed point one has $K_\sigma^*=1$. The three remaining parameters in (1) then completely determine the long-distance properties of the system, and, in particular, K_ρ determines the long-distance decay of all the correlation functions of the system. For example, the charge and spin-correlation functions are[17,18]

$$\langle n(x)n(0)\rangle = K_\rho/(\pi x)^2 + A_1\cos(2k_F x)x^{-1-K_\rho}\ln^{-3/2}(x) + A_2\cos(4k_F x)x^{-4K_\rho}, \quad (5)$$

$$\langle \mathbf{S}(x)\cdot\mathbf{S}(0)\rangle = 1/(\pi x)^2 + B_1\cos(2k_F x)x^{-1-K_\rho}\ln^{1/2}(x), \quad (6)$$

with the model-dependent constants A_i, B_i. Similarly, K_ρ determines the singularity of the momentum distribution function close to k_F:

$$n_k \approx \tfrac{1}{2} - \mathrm{sgn}(k-k_F)|k-k_F|^\alpha, \quad (7)$$

and of the single-particle density of states $N(\omega)\approx|\omega|^\alpha$, with $\alpha=(K_\rho+1/K_\rho-2)/4$. Note that for any $K_\rho\neq 1$ the momentum distribution function and the density of states have power-law singularities at the Fermi level, quite unlike a standard Fermi liquid.

For the Hubbard model, K_ρ and u_ν can be determined perturbatively, e.g.,

$$K_\rho = 1 - U/\pi v_F + \cdots, \quad (8)$$

where $v_F=2t\sin(\pi n/2)$ is the Fermi velocity. For larger U, higher operators appear in the continuum Hamiltonian (1). These operators are irrelevant, i.e., they renormalize to zero and do not qualitatively change the long-distance properties, but they do lead to nontrivial corrections to the coefficients u_ν, K_ρ. These corrections can be treated order by order in perturbation theory. However, this approach is obviously unpractical for large U, and moreover, for sufficiently large U, perturbation theory will almost certainly fail. To obtain the exponents for arbitrary U a different approach is necessary. I note three points: (i) In the small-U perturbative regime, interactions renormalize to the weak-coupling fixed point $g_1^*=0$, $K_\sigma^*=1$; (ii) the exact solution[3] does not show any singular behavior at nonzero U, i.e., large U and small U are the same phase of the model, so that the long-range behavior even of the large-U case is determined by the fixed point $g_1^*=0$; (iii) the gradient of the phase field ϕ_ρ is proportional to the particle density, and, in particular, a constant slope of ϕ_ρ represents a change of total particle number. Consequently, the coefficient u_ρ/K_ρ in Eq. (2) is proportional to the variation of the ground-state energy E_0 with particle number[19]

$$\frac{1}{L}\frac{\partial^2 E_0(n)}{\partial n^2} = \frac{\pi}{2}\frac{u_\rho}{K_\rho}. \quad (9)$$

This equation now allows the direct determination of K_ρ: $E_0(n)$ can be obtained solving (numerically) Lieb and Wu's[3] integral equation, and u_ρ is obtained from the low-momentum limit of the charge-oscillation excitations, which can be identified with what Coll[20] calls (somewhat misleadingly) "particle-hole excitations." The resulting U dependence of K_ρ is shown in Fig. 1(a) for different particle densities. For small U one finds in all cases agreement with the perturbative expression, Eq. (8). The large-U limit, $K_\rho\to\frac{1}{2}$, is more apparent in Fig. 1(b), where K_ρ is plotted as a function of particle density at constant U. The limiting behavior for large U can be understood by noting that for $U=\infty$ the charge dynamics of the system can be described by noninteracting *spinless* fermions (the hard-core constraint is then satisfied by the Pauli principle) with k_F replaced by $2k_F$. Consequently, one finds a contribution proportional to $\cos(4k_F x)x^{-2}$ in the density-density correlation function, which from Eq. (5) implies $K_\rho=\frac{1}{2}$. One then finds an asymptotic decay like $\cos(2k_F x)x^{-3/2}\ln^{1/2}(x)$ for the spin-spin correlations, Eq. (6), and an exponent $\alpha=\frac{1}{8}$ in the momentum distribution function.[21] Ogata and Shiba's numerical results[14] are quite close to the exact values.

As is apparent from Fig. 1(b), the strong-coupling value $K_\rho=\frac{1}{2}$ is also reached in the limits $n\to 0,1$ *for any positive* U. For $n\to 0$ this behavior is easily understood: The effective interaction parameter is U/v_F, but v_F goes to zero in the low-density limit (corresponding to the diverging density of states). The limit $n\to 1$ is more subtle: In this case nearly every site is singly occupied,

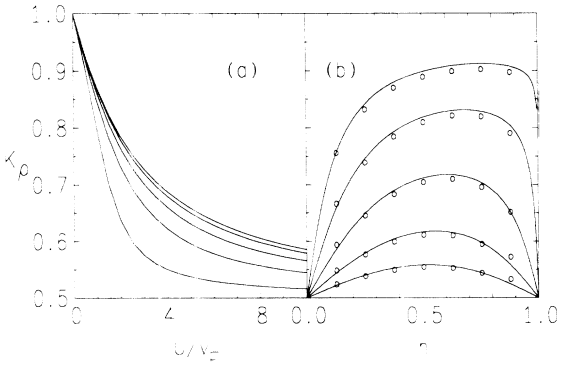

FIG. 1. The correlation exponent K_ρ (a) as a function of the effective interaction parameter U/v_F for different values of the band filling ($n=0.1$, 0.3, 0.5, 0.7, and 0.9 for the top to bottom curves) and (b) as a function of the band filling n for different values of U ($U/t=1$, 2, 4, 8, and 16 for the top to bottom curves). Note the rapid variation near $n=1$ for small U. The circles are results obtained for a sixteen-site chain.

with a very low density of holes. The only important interaction then is the short-range repulsion between holes, which can be approximated by treating the *holes* as a gas of spinless noninteracting fermions. Using (9), one then again finds $K_\rho = \frac{1}{2}$.

The exact solution of Lieb and Wu can also be combined with the long-wavelength effective Hamiltonian (1) to obtain some information on the frequency-dependent conductivity $\sigma(\omega)$. On the one hand, the total oscillator strength is proportional to the kinetic energy[22]

$$\sigma_{\rm tot} = \int_{-\infty}^{\infty} \sigma(\omega) d\omega = -\pi \langle H_{\rm kin} \rangle / L . \quad (10)$$

On the other hand, from Eq. (1) one obtains a contribution $\sigma_0 \delta(\omega)$ to the conductivity, with $\sigma_0 = 2u_\rho K_\rho$. Consequently, the relative weight of the dc peak in the total conductivity can be obtained and is plotted in Fig. 2. As expected, far from half filling, all the weight in $\sigma_{\rm tot}$ is in the dc peak. For exactly half filling the dc conductivity vanishes, due to the existence of a gap for charge excitations Δ_c created by umklapp scattering, and all the weight is at $\omega > \Delta_c$. Figure 2 then shows that as $n \to 1$, umklapp scattering progressively transfers weight from zero to high frequency. The crossover is very sharp for small or large U, but rather smooth in intermediate cases ($U/t \approx 16$). This nonmonotonic behavior as a function of U can be understood noting that initially with increasing U umklapp scattering plays an increasingly important role. Beyond $U/t \approx 16$, however, the spinless-fermion picture becomes more and more appropriate, and at $U = \infty$ one again has all the weight in the dc peak. The linear vanishing of σ_0 as $n \to 1$ implies a linear variation of the effective carrier density with "doping."

For more complicated models, e.g., the "extended Hubbard model,"

$$H = -t \sum_{\langle i,j \rangle, s} (a_{is}^\dagger a_{js} + a_{js}^\dagger a_{is}) + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle i,j \rangle} n_i n_j , \quad (11)$$

exact eigenvalues cannot be obtained in the thermodynamic limit. The parameters in Eq. (9) can, however, be calculated reliably for finite systems, and this gives rather good results, as can be seen Fig. 1(b): The circles represent results from the solution of a chain of sixteen sites (with $V=0$), in excellent agreement with the thermodynamic limit over the whole range of parameters. I thus expect that reliable estimates of K_ρ can be obtained from finite-size diagonalization also for models more complicated than the Hubbard model.

Exact exponents can be obtained for the model (11) in the limit $U \to \infty$: Then one has effectively spinless fermions (with $k_F \to 2k_F$) with nearest-neighbor interaction, a model which can be exactly solved using the Jordan-Wigner transformation into the XXZ spin chain. In particular, the $4k_F$ component of (5) is related to the correlation function of S_z. From the known results[23] one obtains, for a quarter-filled band ($n = \frac{1}{2}$), $K_\rho = 1/[2 + (4/\pi)\sin^{-1}(v)]$, $u_\rho = \pi t (1 - v^2)^{1/2} / \cos^{-1}(v)$, with $v = V/2|t|$. Now $K_\rho < \frac{1}{2}$ is possible. For $v > 1$ the system is in a dimerized insulating state. Approaching the insulating state from $v < 1$ both K_ρ and u_ρ remain finite, i.e., σ_0 jumps to zero at $v = 1$. For $n \neq \frac{1}{2}$ the parameters u_ρ, K_ρ can be obtained from numerical results.[13] Quite generally, one has $K_\rho > \frac{1}{8}$, but $K_\rho = \frac{1}{2}$ for $n \to 0, 1$, independent of v. On the other hand, $u_\rho \to 0$ as $n \to \frac{1}{2}$ for $v > 1$; i.e., in that case the weight of the dc conductivity goes to zero continuously, the point $(v, n) = (1, \frac{1}{2})$ is thus highly singular. The same type of singularity also occurs at $U = 0$, $n = 1$ in the Hubbard model. Also note that the singularities in u_ρ and K_ρ at $v = -1$ (attractive interaction) represent a point of phase separation.

The present results place some constraints on the way experimental systems can be modeled. For example, in the quasi-one-dimensional organic compound tetrathiafulvalene tetracyanoquinodimethane (TTF-TCNQ), one observes strong diffuse x-ray scattering at $4k_F$.[8] From Eq. (5) one then concludes that $K_\rho < \frac{1}{2}$, and therefore the Hubbard model alone cannot be sufficient to describe correlation effects in this compound. The experimentally determined exponents in a number of other compounds[7,8] also imply $K_\rho < \frac{1}{2}$; i.e., finite-range interactions seem to be rather important in many cases.

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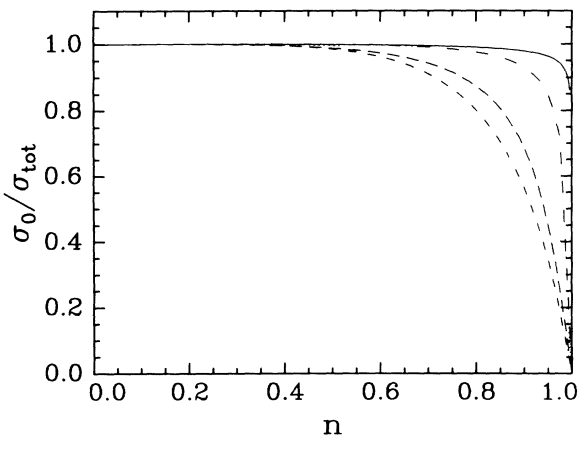

FIG. 2. Variation of the relative weight of the dc peak in the total conductivity oscillator strength as a function of the band filling n for different values of U: $U/t = 1$ (solid line), 4 (dashed line), 16 (dash-dotted line), 64 (dotted line), and 256 (dash-double-dotted line).

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