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Classical Linear-Chain Hubbard Model: Metal-Insulator Transition*

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The linear-chain Hubbard model with nearest-neighbor hopping parameter t is reexpressed in terms of pseudospin operators according to the Jordan–Wigner transformation. The resulting spin model is then treated classically. It is found that for a half-filled band there is a phase transition in the ground state as a function of t. The electrical conductivity is calculated and shown to vanish discontinuously at the critical value of $4t = U$ (Coulomb repulsion). A Josephson-type relation is obtained between the difference in azimuthal angles of adjacent spins and the potential difference between sites. It is also shown that a local magnetic moment exists in the insulating state. For the non-half-filled band, it is shown that the ground state is ferromagnetic for $4t < U$.

The one-dimensional Hubbard model[1] is written as

$$H = -t\sum_{i,\sigma}(C^\dagger_{i\sigma}C_{i+1\sigma}+\text{H. c.}) + U\sum_i n_{i\downarrow}n_{i\uparrow}\ . \qquad (1)$$

The hopping t is among nearest neighbors. $C^\dagger_{i\sigma}$ creates an electron on site R_i with spin σ; $n_{i\sigma} = C^\dagger_{i\sigma}C_{i\sigma}$. U is the intrasite Coulomb repulsion.

The Jordan–Wigner transformation[2] is applied to H. We define (with N = number of sites)

$$S_i^+ = C^\dagger_{i\uparrow}\exp\left[i\pi\left(\sum_{j=1}^{N} n_{j\downarrow} + \sum_{j=1}^{i-1} n_{j\uparrow}\right)\right]\ , \qquad (2)$$

$$T_i^+ = C^\dagger_{i\downarrow}\exp\left[i\pi\sum_{j=1}^{i-1} n_{j\downarrow}\right]\ . \qquad (3)$$

Here $S_i^+ = S_i^x + iS_i^y$, $T_i^+ = T_i^x + iT_i^y$, and it also follows that $S_i^z = n_{i\uparrow} - \frac{1}{2}$ and $T_i^z = n_{i\downarrow} - \frac{1}{2}$. The vector operators $\vec{S} = (S^x, S^y, S^z)$ and $\vec{T} = (T^x, T^y, T^z)$ are each spin-$\frac{1}{2}$ operators and satisfy the usual angular momentum commutator algebra. In terms of the spin operators H is written as[3]

$$H = -2t\sum_i (S_i^xS_{i+1}^x + S_i^yS_{i+1}^y + T_i^xT_{i+1}^x + T_i^yT_{i+1}^y)$$
$$+ U\sum_i S_i^zT_i^z + \tfrac{1}{2}U\sum_i (S_i^z + T_i^z) + \tfrac{1}{4}NU\ . \qquad (4)$$

The Hubbard model is now in the form of the sum of two spin-$\frac{1}{2}$ XY models; each is in a transverse uniform magnetic field and the z components of the two spin systems are coupled by an intrasite exchange. The equivalence of (a class of models of) an interacting, one-dimensional electron gas to a spin model was discussed by Lieb and Mattis.[4]

Although the equivalence allows one to regard the Hubbard model from a different point of view, the transformation to the spin variables does not lead to an apparent simplification of the problem (but its usefulness is illustrated in Ref. 4). In this paper, we use the spin equivalence to generalize the Hubbard model to arbitrary spin. In particular, we study the classical-spin limit of Eq. (4). The connection with the original spin-$\frac{1}{2}$ problem is now remote and in fact we expect the two systems to have qualitative differences. The classical Hubbard model can be thought of as a system of interacting multidegenerate bands in the limit of an infinite number of bands. The band model thus obtained [by working back to a set of fermion operators from the classical-spin generalization of Eq. (4)] is not completely realistic since it does not sort out Hund's-rule effects, allows intersite, interband hopping of electrons and includes interaction terms beyond the usual short-ranged variety.

We introduce two sets of spherical coordinates such that

$$S_i^z=\tfrac{1}{2}\cos\theta_i,\qquad T_i^z=\tfrac{1}{2}\cos\alpha_i\ ,$$
$$S_i^x=\tfrac{1}{2}\sin\theta_i\cos\phi_i,\qquad T_i^x=\tfrac{1}{2}\sin\alpha_i\cos\beta_i\ , \tag{5}$$
$$S_i^y=\tfrac{1}{2}\sin\theta_i\sin\phi_i,\qquad T_i^y=\tfrac{1}{2}\sin\alpha_i\sin\beta_i\ .$$

H is now expressed as

$$H=-\tfrac{1}{2}t\sum_i[\sin\theta_i\sin\theta_{i+1}\cos(\phi_i-\phi_{i+1})+\sin\alpha_i\sin\alpha_{i+1}\cos(\beta_i-\beta_{i+1})]+\tfrac{1}{4}U\sum_i\cos\theta_i\cos\alpha_i+\tfrac{1}{4}U\sum_i(\cos\theta_i+\cos\alpha_i)+\tfrac{1}{4}NU\ . \tag{6}$$

The total number of particles is given by

$$N_e=\sum_i(n_{i\uparrow}+n_{i\downarrow})=N+\tfrac{1}{2}\sum_i(\cos\theta_i+\cos\alpha_i);$$

N_e can vary continuously for $0\le N_e\le 2N$.

We first consider the case $N_e=N$ (the half-filled band). This implies that $\sum_i(\cos\theta_i+\cos\alpha_i)=0$ or, by translational invariance, $\cos\theta_i+\cos\alpha_i=0$. The last condition implies that the polar angles satisfy the condition $\theta_i+\alpha_i=\pi$. Thus Eq. (6) can be simplified to

$$H=-\tfrac{1}{2}t\sum_i\sin\theta_i\sin\theta_{i+1}[\cos(\phi_i-\phi_{i+1})+\cos(\beta_i-\beta_{i+1})]-\tfrac{1}{4}U\sum_i\cos^2\theta_i+\tfrac{1}{4}NU\ . \tag{7}$$

We wish to find the ground state of Eq. (7). We observe that since $0\le\theta_i\le\pi$, $\sin\theta_i\sin\theta_{i+1}\ge 0$. With $t>0$, we must maximize the quantity in brackets in Eq. (7) (since the azimuthal angles do not occur elsewhere in H). We get $\phi_i-\phi_{i+1}=0$ (or 2π) and $\beta_i-\beta_{i+1}=0$ (or 2π). If we had taken $t<0$, then we would get $\phi_i-\phi_{i+1}=\pm\pi$ and $\beta_i-\beta_{i+1}=\pm\pi$. In either case Eq. (7) becomes

$$H=-|t|\sum_i\sin\theta_i\sin\theta_{i+1}+\tfrac{1}{4}U\sum_i\sin^2\theta_i\ . \tag{8}$$

Here we have used the identity $\cos^2\theta_i=1-\sin^2\theta_i$. We introduce new variables f_k, according to the Fourier transform

$$f_k\equiv\frac{1}{\sqrt{N}}\sum_n e^{-ikna}\sin\theta_n\,; \tag{9}$$

here a is the lattice spacing. In terms of the new variables, Eq. (8) is written as

$$H=\sum_k(-|t|\cos ka+\tfrac{1}{4}U)|f_k|^2\ . \tag{10}$$

We study Eq. (10) for two cases.

Case I: $4|t|<U$

This implies that $\omega_k\equiv-|t|\cos ka+\frac{1}{4}U>0$ for all k. Equation (10) takes its minimum value for $|f_k|^2=0$ for all k. This implies that $\sin\theta_n=0$ for all n, or $\theta_n=0$ or π for each n.

Case II: $4|t|>U$

In this case the minimum of ω_k occurs for $\omega_0=-|t|+\frac{1}{4}U$. The ground-state energy is minimized by taking $|f_k|^2=N\delta_{k,0}$, where $\delta_{k,0}$ is the Kronecker δ. This implies that $\sin\theta_n=1$ for all n or $\theta_n=\frac{1}{2}\pi$ for all n. Thus $4|t|=U$ is a phase-transition point of the ground state.[5] The phase change is characterized by the abrupt change in the polar angle of the spin vector. From Eq. (5) we see that for $4|t|>U$, $S_i^x=\frac{1}{2}\cos\phi_i$, $S_i^y=\frac{1}{2}\sin\phi_i$, $S_i^z=0$, $T_i^x=\frac{1}{2}\cos\beta_i$, $T_i^y=\frac{1}{2}\sin\beta_i$, $T_i^z=0$. For $4|t|<U$, we see that $S_i^x=S_i^y=0$, $S_i^z=\frac{1}{2}$ (or $-\frac{1}{2}$), $T_i^x=T_i^y=0$, $T_i^z=-\frac{1}{2}$ (or $\frac{1}{2}$). Since the transverse degrees of freedom are associated with the hopping motion of the original Hamiltonian, Eq. (1), the abrupt disappearance of $S_i^x, S_i^y, T_i^x, T_i^y$ at $4|t|=U$ suggests that the transition is a metal-to-insulator transition. This will be shown to be the case in the calculation of the electrical conductivity.

We can define a magnetic moment per site as $m_i\equiv n_{i\uparrow}-n_{i\downarrow}=\frac{1}{2}(\cos\theta_i-\cos\alpha_i)$. Since $\theta_i+\alpha_i=\pi$, we have $m_i=\cos\theta_i$. In the metallic state, $\theta_i=\frac{1}{2}\pi$, so that $m_i=0$. In the insulator $\theta_i=0$ (or π), so that $m_i=1$ (or -1). There are no moments in the metal, but at the transition point a moment appears. We note that the moment is fully saturated but that since there is a complete degeneracy between $\theta_i=0$ and $\theta_i=\pi$, the moments are not ordered. In the spin-$\frac{1}{2}$ Hubbard model, antiferromagnetism occurs for small $|t|/U$ because of (quantum-mechanical) mixing in of virtual polar states[6] in the ground state. In the classical case, the ground-state *configuration* is either that of the simple metal ($U=0$) for $4|t|>U$ or that of the simple insulator ($t=0$) for $4|t|<U$. Of course, the ground-state energy varies continuously between these limits; $H=(-|t|+\frac{1}{4}U)\Theta(|t|-\frac{1}{4}U)$; here $\Theta(x)$ is the familiar unit step function.

We confirm the suggestion of the ground-state calculation that the phase transition is a metal-insulator transition by calculating the dc conductivity in linear response. The current operator (with e denoting electric charge) is given by

$$J=ieat\sum_{i,\sigma}(C^\dagger_{i\sigma}C_{i+1\,\sigma}-C^\dagger_{i+1\,\sigma}C_{i\sigma})\ ,$$

which, in terms of classical spin variables is written as

$$J=\tfrac{1}{2}eat\sum_i[\sin\theta_i\sin\theta_{i+1}\sin(\phi_i-\phi_{i+1})+\sin\alpha_i\sin\alpha_{i+1}\sin(\beta_i-\beta_{i+1})].$$

From the conditions found on the azimuthal angles, we immediately deduce that the ground state does not carry current. In order to calculate the current induced by an electric field, E, we introduce the Hamiltonian

$$H_{ext} = eE \sum_{i,\sigma} R_i n_{i\sigma} ,$$

which describes the presence of a uniform time-independent electric field. In terms of the classical-spin variables,

$$H_{ext} = eE \sum_i R_i (S_i^z + T_i^z) .$$

In obtaining J in linear response, we note that since the azimuthal angles lead to zero current in equilibrium, we need only consider the change in the azimuthal angles to first order in E. The polar angles are evaluated at their equilibrium values. The change in the aximuthal angles can be found by studying the time (τ) evolution of $S_i^+(\tau)$. It is readily found from the equation of motion for $S_i^+(\tau)$ that

$$S_i^+(\tau) = \hat{S}_i^+(\tau)\, e^{ieER_i\tau} ;$$

here $\hat{S}_i^+(\tau)$ denotes the value of $\hat{S}_i^+(\tau)$ in the absence of E. When we express $S_i^+(\tau)$ in terms of classical spin variables we find that $\phi_i(\tau) = \hat{\phi}_i(\tau) + eER_i\tau$. Since $\hat{\phi}_i(\tau) = \hat{\phi}_{i+1}(\tau)$ (mod 2π), we get (we have $t > 0$; if $t < 0$, the equilibrium phase difference is $\pm\pi$, but the sign of t will not affect the current)

$$\phi_{i+1}(\tau) - \phi_i(\tau) = eEa\tau . \qquad (11)$$

From Eq. (11) we note the Josephson-type relation[7] $d(\Delta\phi)/d\tau = eEa$. $\Delta\phi \equiv \phi_{i+1} - \phi_i$ is the relative azimuthal angle between sites $i+1$ and i and eEa is the potential across these sites. The same relation holds for $\Delta\beta = \beta_{i+1} - \beta_i$. To lowest order in E we have

$$J = e^2 a^2 |t| \tau E \sum_i \sin\theta_i \sin\theta_{i+1} ;$$

we use the equilibrium ground-state results found for the polar angles to rewrite J as

$$J = Ne^2 a^2 |t| \tau E \Theta(|t| - \tfrac{1}{4}U) . \qquad (12)$$

We see that the current falls abruptly to zero at $4|t| = U$; this proves that the transition at $4|t| = U$ is indeed a metal-insulator transition. For $4|t| > U$, Eq. (12) shows free acceleration behavior, consistent with Newton's Law for a free particle, i.e., the current for N free point particles with velocity v is $J = Nev$ and the equation of motion is $m\dot{v} = eE$. This implies that $J = Ne^2\tau E/m$. This is identical to Eq. (12) for $4|t| > U$ if one identifies the effective mass of the discrete system as $a^2|t| \to 1/m$.

The analysis of the ground state for arbitrary density is completely straightforward and similar to the above. We briefly outline this calculation and give the results. The particle number density $n_e \equiv N_e/N$ imposes the condition $\cos\theta_i + \cos\alpha_i = 2(n_e - 1)$ on the polar angles. We use this condition, the identity

$$2\cos\theta_i \cos\alpha_i = (\cos\theta_i + \cos\alpha_i)^2 - 2 + \sin^2\theta_i + \sin^2\alpha_i ,$$

and the condition on the azimuthal angles (as before) to rewrite Eq. (6) as

$$H = \tfrac{1}{2}\sum_k \omega_k (|f_k|^2 + |g_k|^2) + \tfrac{1}{2}NU(n_e^2 - n_e) . \qquad (13)$$

Here we have introduced g_k, the Fourier transform of $\sin\alpha_i$. The energy is minimized by choosing $|f_k|^2$ and $|g_k|^2$ to have weight only at $k=0$. This implies that $\sin\theta_i$ and $\sin\alpha_i$ are independent of i. With the help of the particle number condition, Eq. (13) can be expressed as

$$H/N = (-|t| + \tfrac{1}{4}U)[\sin^2\theta + 2(n_e - 1)\cos\theta] + 2|t|(n_e - 1)^2 + \tfrac{1}{2}U(n_e - 1) .$$

After maximizing or minimizing[8] the factor containing θ for $4|t| > U$ or $4|t| < U$, respectively, we find that

(1) for $4|t| > U$, the ground state is paramagnetic and has a finite conductivity;

(2) for $4|t| < U$, the ground state is ferromagnetic[9] with maximum magnetization for all $|n_e - 1| > 0$. Although there is a finite conductivity, it is smaller (at a given n_e) than in the case $4|t| > U$. There is a discontinuous jump in the conductivity at $U = 4|t|$ for all n_e.

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