COMMENTS AND ADDENDA

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Free-Spin Magnetic Behavior of the One-Dimensional Near-Neighbor Hubbard-Model Electron System

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Using the solution of the near-neighbor hopping Hubbard model in one dimension by Leib and Wu, it is shown that in the limit of interaction energy much greater than hopping energy, this system has the temperature dependence of magnetization of a free-spin system even for temperatures much less than the bandwidth, for nearly all occupancies of the band.

Lieb and Wu[1] have solved the one-dimensional near-neighbor hopping Hubbard-Hamiltonian model with periodic boundary conditions. Let us find the magnetization for their solution in the limit $\tau/U \to 0$ [τ and U are the hopping and interaction parameters of Eq. (1) in Ref. 1] for a mean number of electrons per site $n<1$. The magnetic susceptibility for the case of $n>1$ will be the same by electron-hole equivalence. It can easily be shown that in this limit for $n<1$, an electron cannot hop onto a site containing a second electron because that part of the hopping term causing such hops can be removed by a canonical transformation.[2] Throughout this discussion, when we say that a site is occupied by a hole, we mean that the Wannier function on that site is not occupied by an electron of either spin. The energies of the one-dimensional system described by the Hamiltonian

$$H=\tau\textstyle\sum_{ij\sigma} C_{i\sigma}^{\dagger} C_{j\sigma}+U\sum_i n_{i\uparrow}n_{i\downarrow} \quad , \tag{1}$$

where $j=i\pm1$, were found in Ref. 1 to be given by

$$E=-2\tau\sum_{j=1}^{N}\cos k_j \quad , \tag{2}$$

where $\{k_j\}$ is a set of unequal real numbers $<2\pi$. In the limit $\tau/U\to 0$, Eqs. (9) and (10) in Ref. 1 reduce to

$$N_a k_j=2\pi I_j-\sum_{\beta=1}^{M}\theta(2\lambda_\beta) \quad , \tag{3a}$$

$$N\theta(2\lambda_\alpha)=2\pi J_\alpha-\sum_{\beta=1}^{M}\theta(\lambda_\alpha-\lambda_\beta) \quad , \tag{3b}$$

where $\theta(p)=-2\arctan(2p/U)$, N_a is the number of atoms, N the total number of electrons, and M the number of spin-up electrons. I_j is an integer (half-odd integer) for M even (odd), and J_α is an integer (half-odd integer) for N-M odd (even). Combining (3a) and (3b) to eliminate the λ_α's, we find

$$k_j=2\pi L_j/N_a+2\pi m/N_aN \quad , \tag{4}$$

where L_j and m are integers.

There are

$$N_a!/N!\,(N_a-N)! \tag{5}$$

sets $\{L_j\}$ of N integers less than N_a. Then looking at Eq. (4), since there are N values of M which give a new set of k_j's for each set $\{L_j\}$, there are a total of

$$N_a!/(N-1)!\,(N_a-N)! \tag{6}$$

sets of $\{k_j\}$. The total number of eigenstates is equal to the total number of basis functions in which they are expanded, which is equal to the number of ways of placing the N electrons, M of

which have spin up, on a ring having N_a lattice sites, which is

$$N_a!/(N_a-N)!\,(N-M)!\,M!\ . \tag{7}$$

Once the electron spins are placed on the ring, for the case $\tau/U \to 0$, the Hamiltonian [Eq. (1)] will not change their spin ordering around the ring. Consequently, the secular determinant which determines the eigenvalues of Eq. (1) will break up into blocks, not connected by the Hamiltonian, one block for each spin ordering. The number of such blocks in the secular determinant is equal to the number of ordering of the spins around the ring. There are

$$N!/M!\,(N-M)! \tag{8}$$

permutations of the spins on the ring for fixed hole positions. To find the number of orderings, we must divide by the number of cyclic permutations of the spins. Included among the various spin orderings will be those orderings such that when the spins are cyclically permuted $1/n$th of the way around the ring (keeping the holes on fixed sites), where n is an integer, the ring will not be changed. The number of such "high-symmetry" spin orderings is simply the number of ways of placing M/n up spins and $(N-M)/n$ down spins on N/n sites, and thus the total number of high-symmetry spin orderings is given by

$$\sum_{n=2}^{N}{}' \frac{(N/n)!}{(M/n)!\,(N-M)/n!}\ , \tag{9}$$

where the summation is only taken over those values of n for which N/n and M/n are integers. It will now be shown that for large N such orderings are a very small fraction of the total number of orderings. Since the number of such states will clearly be maximum when $M \approx \frac{1}{2}N$, let us consider this case. Then, Eq. (9) becomes for large N, using Sterling's approximation,

$$\sum_{n=2}^{N}{}' \frac{(N/n)!}{(M/n)!\,(N-M)/n!} \approx \sum_{n=2}^{N}{}' 2^{N/n}\ .$$

Using Sterling's approximation on Eq. (8), we find that the ratio of the number of these orderings to the total number of ways of placing spins on the rings is less than or equal to

$$\sum_{n=2}^{N}{}' (\tfrac{1}{2})^{N(1-1/n)}\ , \tag{10a}$$

which is less than

$$N(\tfrac{1}{2})^{N/2}\ . \tag{10b}$$

This is $\ll 1$ for large N. Neglecting these high-symmetry orderings compared to all the other orderings, the number of cyclic permutations of the spins is $\approx N$, and hence, the total number of spin orderings is

$$(N-1)!/M!\,(N-M)!\ . \tag{11}$$

From Eqs. (6), (7), and (11), we see that for each ordering of the spins, we get all of the eigenvalues given by Eq. (2) (i.e., all allowed sets $\{k_j\}$). Then, in the presence of a weak magnetic field,

$$Z = \frac{1}{N}\sum_{M} \frac{(N)!}{M!\,(N-M)!}\, e^{\beta\mu H(2M-N)} \sum_{\{k_j\}} \exp\Big(2\tau\beta \sum_j \cos k_j\Big),$$

$$Z = \frac{1}{N}\, e^{-\beta\mu NH}(1+e^{2\beta\mu H})^N \sum_{\{k_j\}} \exp 2\beta\tau \sum_j \cos k_j\ , \tag{12}$$

neglecting high-symmetry spin orderings. Then, the magnetization is given by

$$\langle 2M-N\rangle = \frac{\partial \ln Z}{\partial(\beta\mu H)} = N\tanh\beta\mu H\ , \tag{13}$$

which is just the magnetization of N free spins in a magnetic field. The high-symmetry spin orderings which we have neglected have eigenvalues given by Eq. (2) but have fewer sets $\{k_j\}$, since for these orderings the integer m in Eq. (4) is restricted to be a multiple of n. Since there are low-symmetry orderings which have states with the same energies as the states of the high-symmetry orderings, there is no danger of any high-symmetry states dominating at some temperature. Hence, it is safe to include only the more numerous low-symmetry spin orderings in the calculation of Z for $N \gg 1$.

Thus it has been shown in this paper that an electronic system can exhibit both metallic electrical conduction (because the band is partially filled and the electrons in the band are free to hop) and at the same time magnetic properties characteristic of a localized spin system, for KT much smaller than the bandwidth. This is just the behavior observed by Jarrett *et al.*[3] The proof in one dimension is dependent on the fact that in one dimension, in the limit $U/\tau \to \infty$, no reordering of electron spins can occur by near-neighbor hopping. The three-dimensional Hubbard model, which may be applicable to the experimental systems reported by Jarrett *et al.*,[3] will be the subject of a future publication.

I would like to thank F. Y. Wu for useful discussions of his work during the course of the work reported here.

[1]E. H. Lieb and F. Y. Wu, Phys. Rev. Letters 20, 1445 (1968). Although there is some question of the completeness of the eigenfunctions of this paper, this solution does appear to give all of the finite-energy eigensolutions of Eq. (1) in the infinite U limit.

[2]A. B. Harris and R. V. Lange, Phys. Rev. 157, 292 (1967).

[3]H. S. Jarrett, W. H. Cloud, R. J. Bouchard, S. R. Butler, C. G. Frederick, and J. L. Gillson, Phys. Rev. Letters 21, 617 (1968); J. Appl. Phys. 40, 1258 (1969).

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Alpha-Particle Stopping Cross Section in Solids from 400 keV to 2 MeV, W. K. Chu and D. Powers [Phys. Rev. 187, 478 (1969)]. The authors are grateful to W. D. Mackintosh for kindly pointing out an error in the empirical formula given on p. 490, left column, second line from the bottom. The formula should read

$$\epsilon_\alpha = \epsilon_\alpha(E, Z_2) = 1.66(A'/E)\ln(B'E),$$

instead of the constant 1.66 being omitted. The correct form was used in the calculation for generating the curves appearing in Figs. 4–7.

Linear Chain Antiferromagnetism in $CsMnCl_3 \cdot 2H_2O$. T. Smith and S. A. Friedberg [Phys. Rev. 176, 660 (1968)]. The labels of the a and b axes have been inadvertently interchanged in Figs. 2, 3, and 4 of this paper and, consequently, also in the discussion of the results (Sec. IV) and in the abstract. This was kindly pointed out to us by Professor J. A. Cowen and verified independently in this laboratory by Dr. H. Kobayashi. As a result, the anisotropy axis above ~9 °K (taken as the z axis in the calculation on p. 663) is the a axis. The preferred axis of antiferromagnetic spin alignment in the three-dimensionally ordered phase ($T < 4.8$ °K) should be the b axis. Dr. Kobayashi's measurements also establish the anomalous susceptibility near 1 °K to be an impurity effect.

Equation (9) should read

$$\chi_n = \frac{Ng^2\mu_B^2 S(S+1)}{(n+1)3kT}\left\{(n+1)\frac{1+u}{1-u} - 2u\frac{1-u^{n+1}}{(1-u)^2}\right\}.$$

Magnetic Susceptibility of $FeCl_2 \cdot 4H_2O$ from 0.35 to 4.2 °K. J. T. Schriempf and S. A. Friedberg [Phys. Rev. 136, A518 (1964)]. To be consistent with the sign convention for D and E employed in Eq. (1) and elsewhere in this paper, Eqs. (14a)–(14c) should read $g_{x'} = g - (2D/3\lambda) + (2E/\lambda)$, $g_{y'} = g - (2D/3\lambda) - (2E/\lambda)$, $g_{z'} = g + (4D/3\lambda)$, respectively. The splitting factors given on p. A524 should thus read $g_{x'} = 2.18$, $g_{y'} = 2.17$, $g_{z'} = 2.22$.