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Nonexistence of Magnetic Ordering in the One- and Two-Dimensional Hubbard Model

Dipan K. Ghosh*
International Centre for Theoretical Physics, Miramare, 34100 Trieste, Italy
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It is shown that for nonzero temperature, Hubbard's narrow-energy-band model is neither ferromagnetic nor antiferromagnetic in one and two dimensions.

The Hubbard model[1] for the description of electron correlation in a narrow energy band has been of great theoretical interest for the last few years. The model retains only that part of the electron-electron interactions which arises as a result of the repulsion between two electrons of opposite spins located at the same site. In spite of this simplifying assumption, the model remains essentially a many-body problem and an exact solution cannot be found in the general three-dimensional situations. The one-dimensional problem with nearest-neighbor electron transfer has been solved exactly by Lieb and Wu,[2] who obtained the ground-state energy, the wave function, and the chemical potential for the system. In three dimensions Nagaoka[3] considered the case of nearest-neighbor hopping and has discussed the ferromagnetism of various lattices for a nearly half-filled band. Apart from these, not many exact results are known for the model.

In this work we demonstrate explicitly the impossibility of the existence of spontaneous ferromagnetic or antiferromagnetic ordering for this model in one and in two dimensions at an arbitrary nonzero

temperature. In showing this we use an inequality due to Bogoliubov,[4] which has been exploited by Mermin and Wagner[5] to establish similar results for the Heisenberg model, and also by Hohenberg[6] to exclude superfluidity in one and two dimensions.

The Hamiltonian for this model for a system of electrons in a narrow energy band is written as

$$\mathcal{H}=\sum_{i,j}\sum_{\sigma}T(\vec{R}_i-\vec{R}_j)C_{i\sigma}{}^{\dagger}C_{j\sigma}+I\sum_i n_{i\sigma}n_{i-\sigma}-\tfrac{1}{2}H\sum_i(n_{i\uparrow}-n_{i\downarrow})\exp(-i\vec{q}\cdot\vec{R}_i), \tag{1}$$

where the last term represents the extra energy of the electrons in the presence of a space-dependent static magnetic field $H\exp(-i\vec{q}\cdot\vec{R}_i)$. For notational simplicity we have dropped the Bohr-magneton factor in the last term. The sums over i and j in (1) go over all the N ($=L^d$, d = dimensionality) lattice sites. Because of the Pauli principle, the total number of electrons $n\leq 2N$.

We define the local spin-density operators S_i by the following relations:

$$S_{i+}=C_{i\uparrow}{}^{\dagger}C_{i\downarrow},\quad S_{i-}=C_{i\downarrow}{}^{\dagger}C_{i\uparrow},\quad S_{iz}=\tfrac{1}{2}(n_{i\uparrow}-n_{i\downarrow}). \tag{2}$$

These operators obey the usual spin commutation rules. The Fourier transforms of the operators, defined through

$$\vec{S}(\vec{k})=\sum_i\exp(i\vec{k}\cdot\vec{R}_i)\vec{S}_i,\quad \vec{S}_i=N^{-1}\sum_{\vec{k}}\exp(-i\vec{k}\cdot\vec{R}_i)\vec{S}(\vec{k}), \tag{3}$$

satisfy

$$[S_{\pm}(\vec{k}),S_z(\vec{k}')]=\mp S_{\pm}(\vec{k}+\vec{k}'),\quad [S_+(\vec{k}),S_-(\vec{k}')]=2S_z(\vec{k}+\vec{k}'). \tag{4}$$

Using the relations $(S_{i+})^{\dagger}=S_{i-}$, one has for their Fourier components $[S_+(\vec{k})]^{\dagger}=S_-(-\vec{k})$. Using these operators we can re-express the Hamiltonian (1) as

$$\begin{aligned}\mathcal{H}&=\sum_{i,j}\sum_{\sigma}T(\vec{R}_i-\vec{R}_j)C_{i\sigma}{}^{\dagger}C_{j\sigma}-\tfrac{2}{3}I\sum_i\vec{S}_i\cdot\vec{S}_i+\tfrac{1}{2}In-H\sum_i S_{iz}\exp(-i\vec{q}\cdot\vec{R}_i)\\&=\sum_{\vec{k}}\sum_{\sigma}\epsilon_{\vec{k}}n_{\vec{k}\sigma}-\tfrac{2}{3}I\sum_{\vec{k}}\vec{S}(\vec{k})\cdot\vec{S}(-\vec{k})+\tfrac{1}{2}In-HS_z(-\vec{q}),\end{aligned} \tag{5}$$

where the one-electron energies $\epsilon_{\vec{k}}$ are given by

$$\epsilon_{\vec{k}}=\sum_{\vec{R}_i}T(\vec{R}_i)\exp(i\vec{k}\cdot\vec{R}_i),\quad T(\vec{R}_i)=N^{-1}\sum_{\vec{k}}\exp(-i\vec{k}\cdot\vec{R}_i)\epsilon_{\vec{k}}, \tag{6}$$

and $n_{\vec{k}\sigma}=C_{\vec{k}\sigma}{}^{\dagger}C_{\vec{k}\sigma}$, where the $C_{\vec{k}\sigma}$'s are defined by

$$C_{i\sigma}=\sum_{\vec{k}}\exp(-i\vec{k}\cdot\vec{R}_i)C_{\vec{k}\sigma},\quad C_{\vec{k}\sigma}=N^{-1/2}\sum_i\exp(i\vec{k}\cdot\vec{R}_i)C_{i\sigma}. \tag{6a}$$

Without any loss of generality, it can be assumed[2] that

$$S_z=\tfrac{1}{2}\sum_i\sum_{\sigma}\sigma n_{i\sigma}=\tfrac{1}{2}\sum_k\sum_{\sigma}\sigma n_{\vec{k}\sigma}\geq 0.$$

We shall now use Bogoliubov's inequality[4]:

$$\tfrac{1}{2}\langle\{A,A^{\dagger}\}\rangle|\langle[[B,\mathcal{H}],B^{\dagger}]\rangle|\geq k_BT|\langle[B,A]\rangle|^2, \tag{7}$$

where

$$\langle A\rangle=\mathrm{Tr}(e^{-\beta\mathcal{H}}A)/\mathrm{Tr}e^{-\beta\mathcal{H}};\quad \beta=1/k_BT.$$

We choose $A=S_-(-\vec{p}-\vec{q})$ and $B=S_+(\vec{p})$. Then

$$\langle[[B,\mathcal{H}],B^{\dagger}]\rangle=\sum_{\vec{k}}(\epsilon_{\vec{k}-\vec{p}}-\epsilon_{\vec{k}})\langle n_{\vec{k}\uparrow}-n_{\vec{k}\downarrow}\rangle+2H\langle S_z(-\vec{q})\rangle. \tag{8}$$

Now

$$|\langle[[B,\mathcal{H}],B^{\dagger}]\rangle|=|\textstyle\sum_{\vec{R}_i}T(\vec{R}_i)[1-\exp(i\vec{p}\cdot\vec{R}_i)]\sum_{\vec{k}}\exp(-i\vec{k}\cdot\vec{R}_i)\langle(n_{\vec{k}\uparrow}-n_{\vec{k}\downarrow})\rangle+2H\langle S_z(-\vec{q})\rangle|.$$

Since $T(\vec{R}_i)=T(-\vec{R}_i)$, we can see that

$$\begin{aligned}\sum_{\vec{R}_i}T(\vec{R}_i)[1-\exp(i\vec{p}\cdot\vec{R}_i)]&=\sum_{\vec{R}_i>0}T(\vec{R}_i)[1-\exp(i\vec{p}\cdot\vec{R}_i)]+\sum_{\vec{R}_i<0}T(\vec{R}_i)[1-\exp(i\vec{p}\cdot\vec{R}_i)]\\&=2\sum_{\vec{R}_i>0}T(\vec{R}_i)(1-\cos\vec{p}\cdot\vec{R}_i)\\&=\sum_{\vec{R}_i}T(\vec{R}_i)(1-\cos\vec{p}\cdot\vec{R}_i),\end{aligned}$$

where we have chosen the zero of energy at $\sum_{\vec{k}} \epsilon_{\vec{k}} = 0$, so that $T(0) = 0$. Thus, using the triangle inequality we can write

$$|\langle[[B,\mathcal{H}],B^\dagger]\rangle| \leq \sum_{\vec{R}_i} |T(\vec{R}_i)|\,|(1-\cos\vec{p}\cdot\vec{R}_i)|\,|\sum_{\vec{k}}\langle(n_{\vec{k}\uparrow}-n_{\vec{k}\downarrow})\rangle| + 2H|\langle S_z(-\vec{q})\rangle|$$

$$\leq \sum_{\vec{R}_i} |T(\vec{R}_i)|\,\frac{R_i^2 p^2}{2}\,2N + 2HN|S_{0z}(-\vec{q})|, \tag{9}$$

where $S_{0z}(-\vec{q}) = N^{-1}\langle S_z(-\vec{q})\rangle$. In writing down the last expression, we have used the fact that $|(1-\cos x)| < x^2/2$, and have also replaced $|\langle\sum_{\vec{k}}(n_{\vec{k}\uparrow}-n_{\vec{k}\downarrow})\rangle|$ by its extreme upper bound[7] $2N$.

The $T(\vec{R}_i)$'s are the matrix elements of the one-electron operators between Wannier functions which fall off fast with distance for the narrow bands considered here and hence $\sum_{\vec{R}_i} R_i^2|T(\vec{R})|$ is well defined. Denoting this by Q,

$$|\langle[[B,\mathcal{H}],B^\dagger]\rangle| \leq N[Qp^2 + 2H|S_{0z}(-\vec{q})|]. \tag{10}$$

Using (10) in (7), we get

$$\tfrac{1}{2}\langle\{S_-(-\vec{p}-\vec{q}), S_+(\vec{p}+\vec{q})\}\rangle \geq \frac{Nk_BT|S_{0z}(-\vec{q})|^2}{Qp^2 + 2H|S_{0z}(-\vec{q})|}. \tag{11}$$

On summing both sides of (11) over $\vec{p}$, the left-hand side gives $(N/2)\sum_i\langle\{S_{i+}, S_{i-}\}\rangle$. Recalling the definitions (2), we find that its maximum value is $\frac{1}{2}N^2$. Thus we have

$$|S_{0z}(-\vec{q})|^2 \leq \frac{N}{2k_BT}\left[\sum_{\vec{p}}\frac{1}{Qp^2 + 2H|S_{0z}(-\vec{q})|}\right]^{-1}. \tag{12}$$

We now replace the sum over $\vec{p}$ by an integral. If p_0 be the distance of the nearest Bragg reflection plane from the origin in $\vec{p}$ space, we get in one dimension

$$|S_{0z}(-\vec{q})|^2 \leq \frac{N\pi}{Lk_BT}[2HQ|S_{0z}(-\vec{q})|]^{1/2}\left\{\tan^{-1}\left[\left(\frac{Q}{2H|S_{0z}(-\vec{q})|}\right)^{1/2}p_0\right]\right\}^{-1}. \tag{13a}$$

We shall now go over to the thermodynamic limit, so that both the volume ($=L$ in one dimension) and the number N are infinitely large but the density $L/N = \rho = \text{const}$. This gives

$$|S_{0z}(-\vec{q})|^2 \leq \frac{\pi}{\rho k_BT}[2HQ|S_{0z}(-\vec{q})|]^{1/2}\left\{\tan^{-1}\left[\left(\frac{Q}{2H|S_{0z}(-\vec{q})|}\right)^{1/2}p_0\right]\right\}^{-1}.$$

Since for large x, $\tan^{-1}x < x$, we obtain from above in the limit of small H,

$$|S_{0z}(-\vec{q})| \leq \frac{\text{const}}{T}|H|. \tag{13b}$$

In two dimensions one has

$$|S_{0z}(-\vec{q})|^2 \leq \frac{\text{const}}{T}\left[\ln\left(1 + \frac{Qp_0^2}{2H|S_{0z}(-\vec{q})|}\right)\right]^{-1}, \tag{14a}$$

and for small fields this gives

$$|S_{0z}(-\vec{q})| \leq \frac{\text{const}}{T^{1/2}}\frac{1}{|\ln|H||^{1/2}}. \tag{14b}$$

Both in one and two dimensions, from (13b) and (14b) it follows that $|S_{0z}(-\vec{q})| \to 0$ as $H \to 0$. Thus a class of magnetic ordering is excluded. In particular, setting $\vec{q} = 0$, we obtain the result that for nonzero temperature the Hubbard model is not ferromagnetic. Similarly, if we choose q such that $\exp(i\vec{q}\cdot\vec{R}) = 1, -1$ when $\vec{R}$ connects sites in the same sublattice and different sublattices, respectively, then we conclude that is is not antiferromagnetic either. However, it must be added that the above argument does not rule out the possibility of other kinds of phase transitions. For instance, a second-order phase change, where $S_z \to 0$ but $\partial S_z/\partial H|_{H\to 0}$ diverges has not been excluded automatically. Another important point that we would like to emphasize is that the proof above rules out only the occurrence of spontaneous magnetic ordering.

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*Present address: H. H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1Tl, England.

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Mean Lifetime and Magnetic Moment of the 2.95-MeV (6^+) State of ^{54}Fe†

R. Hensler, J. W. Tape, and N. Benczer-Koller
Rutgers, The State University, New Brunswick, New Jersey 08903

and

Jack R. MacDonald*
Bell Telephone Laboratories, Murray Hill, New Jersey 07974
(Received 13 September 1971)

The mean lifetime and g factor of the 2.95-MeV 6^+ state of ^{54}Fe were measured to be $\tau=1.76\pm0.03$ nsec and $|g|=1.37\pm0.03$, respectively. These results are in agreement with the shell-model assignment $(f_{7/2}^{-2})_\pi$ plus a small amount of configuration mixing which accounts for the quenching of the magnetic moment from the Schmidt limit and the enhanced $E2$ rate $B(E2;6^+\rightarrow 4^+)=3.2$ Weisskopf units.

Within the framework of the shell model, the $^{54}_{26}Fe_{28}$ ground state (0^+) and excited states at 1.409 MeV (2^+), 2.540 MeV (4^+), and 2.948 MeV (6^+) can be described in terms of configurations of two proton holes in the $f_{7/2}$ shell. The 28 neutrons close the $f_{7/2}$ neutron shell. $E2$ transition rates between these states are sensitive to impurities admixed to the pure $(f_{7/2}^{-2})_\pi$ wave function such as would be caused by particle-hole excitations involving the $2s$-$1d$ shell, mixtures of $1f$-$2p$ configurations, or collective effects leading to vibrations and deformations. Cochavi *et al.*[1] and Nomura *et al.*[2] have measured lifetimes of some of the 6^+ states of the $(f_{7/2}^{\pm2})$ configurations in ^{42}Ca, ^{50}Ti, and ^{54}Fe. Their results are similar to those reported by Hensler *et al.*[3] in the case of ^{54}Fe. These authors have interpreted their results in terms of shell-model wave functions and have concluded that at least ^{50}Ti and ^{54}Fe exhibit a fairly pure $f_{7/2}^{\pm2}$ structure based on the rather inert cores of ^{48}Ca and ^{56}Ni.

A further test of the purity of the $f_{7/2}^{-2}$ configuration of the 6^+ state of ^{54}Fe can be obtained from the measurement of its magnetic moment μ or of the g factor $g=\mu/I$, I being the total angular momentum. The shell model, in its simplest form, predicts that the g factor for a state (j^n) should be independent of I and of n, the number of nucleons in the j shell. In particular, for particles or holes in the $f_{7/2}$ shell, g should be equal to the Schmidt value, $g=1.65$. However, the experimental g values for the $f_{7/2}^{-n}$ ground states of $^{55}_{27}Co_{28}$, $^{53}_{25}Mn_{28}$, and $^{51}_{23}V_{28}$ are smaller than the Schmidt value.[4,5]

Experimental techniques.—A preliminary measurement[3] of the 2.948-MeV (6^+) state mean lifetime gave an approximate value $\tau_m=1.7$ nsec. As the 6^+ state is so long lived, its magnetic moment is amenable to measurement by the time-differential perturbed angular-correlation technique. A 2.28-mg/cm^2 self-supporting ^{54}Fe target was placed within the pole pieces of a 3 kG permanent magnet whose field was perpendicular to the reaction plane. This field is sufficient to