Phase separation instability in the Hubbard model*

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The simple cubic Hubbard model is examined at zero temperature, for the case of strong interactions and average densities near but not at the half-filled band. It is shown that the ferromagnetic state which is usually assumed to be the ground state is unstable against phase separation. A new phase diagram is proposed, featuring a two-phase region in which the equilibrium state is separated into macroscopic antiferromagnetic and ferromagnetic phases (of differing density).

High-temperature numerical results reported in the preceding paper[1] (referred to below as I) suggest a condensation may take place at low temperature in the simple cubic non-half-filled-band Hubbard model. In the present paper we examine the situation at zero temperature, starting from some exact results of Nagaoka.[2] We find that some of the inferences made by Nagaoka from these results must be modified. In particular, we find a region of parameter space in which we believe the zero-temperature state exhibits phase separation, confirming the prediction of Paper I.

The Hubbard Hamiltonian (given in Paper I) is determined by the ratio t/I of the hopping parameter to the intra-atomic repulsion energy. We will discuss deviations from the half-filled band in terms of the introduction of a number of holes (unoccupied sites) in a lattice originally having exactly one electron on each site (for small t/I, there are very few doubly occupied sites). Nagaoka proves rigorously[2] that if $I=\infty$ and there is exactly one hole, the ground state is a saturated ferromagnet. The ground state is most easily described in terms of the tight-binding bands; the band of one spin is empty and the other is completely full except for one hole, in a state of energy $6t$ at the top of the band. It is then plausible that for n holes (where $n \ll N$, the number of sites) the ground state again has one band empty, with the other having a pocket of n holes at the top of the band. The total energy of the ferromagnet is thus

$$E_F \approx -6tn \ . \tag{1}$$

Nagaoka next allows t/I to become nonzero, and tries to determine at what critical value of t/I the system with n holes ceases to be ferromagnetic. He does this by looking for spin-wave instabilities, finding an instability (hence a transition to an antiferromagnetic state) when

$$t/I > 0.246\ (n/N) \ . \tag{2}$$

As he points out, this does not prove the state is ferromagnetic for smaller t/I; a different instability can destroy the ferromagnetic state before Eq. (2) is satisfied. We have found such an instability, which always precedes (and therefore invalidates) Nagaoka's spin-wave instability at low hole densities. It involves the condensation of a region of half-filled-band antiferromagnet; all the holes remain in the ferromagnetic region.

It is assumed in most work on the Hubbard model (including Nagaoka's and the present work) that for the half-filled band and $t/I \ll 1$, the ground state is antiferromagnetic. This assumption is based on an analogy with the Heisenberg model [Eq. (18) of paper I]. The ground-state energy is not known; the analogy suggests that (counting one J per nearest-neighbor pair)

$$E_{AF} \approx -6(t^2/I)N_{AF} \ , \tag{3}$$

where N_{AF} is the number of sites within the antiferromagnetic region. [Our qualitative result does not depend on the exact value of the binding energy; we use Eq. (3) only for definiteness.]

We can now see qualitatively why the ferromagnetic state is unstable against condensation of antiferromagnet. The binding of the ferromagnetic state is due to the holes (so its binding energy is proportional to the number of holes) whereas the binding energy of the antiferromagnetic state is simply proportional to its volume. Thus by forming an antiferromagnetic region, we gain an energy proportional to its volume, and lose no ferromagnet energy (because the number of holes is unchanged).

This simple argument is strictly valid only as $n/N \to 0$ for fixed t/I; it does not tell us the critical density at which condensation begins. To get this, we must account for the work done in compressing the holes, i.e., correct Eq. (1). From the tight-binding density of states (letting $h=n/N$ be the density of holes) it can be shown that

$$E_F = -6tn(1-\zeta h^{2/3}) \ , \tag{4}$$

(plus terms of order $tnh^{4/3}$) where

$$\zeta = \tfrac{1}{15}(2\pi)^3(\tfrac{4}{3}\pi)^{-5/3} \approx 1.52. \tag{5}$$

We obtain directly from Eqs. (3) and (4) the in-

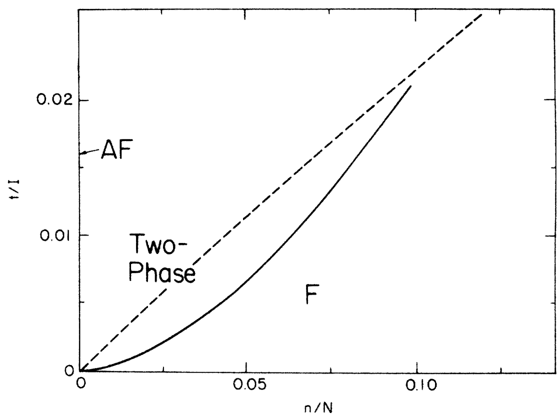

FIG. 1. Phase diagram for the simple cubic Hubbard model at zero temperature, for small t/I and hole concentration n/N. Nagaoka's phase boundary [roughly Eq. (2)] is the dashed line. The system is antiferromagnetic (AF) only on the line $n/N=0$; the solid line [Eq. (7)] separates the pure ferromagnetic region (F) from the two-phase equilibrium region.

stability condition

$$0 > \frac{d(E_F + E_{AF})}{dN_{AF}} = -6\left(\frac{t^2}{I}\right) + 4t\zeta h^{5/3} . \qquad (6)$$

Thus if

$$t/I > (\tfrac{2}{3}\zeta)(n/N)^{5/3} , \qquad (7)$$

the ferromagnet is unstable against condensation of a region of half-filled-band antiferromagnet. This condition supercedes (2) at low hole densities; Eqs. (2) and (7) are shown as dashed and solid curves in Fig. 1.

It is clear that Nagaoka's[2] phase diagram (predicting ferromagnetism below the dashed curve in Fig. 1) must be modified; Nagaoka's state cannot be the ground state between the two curves. If one knew the energies of all possible homogeneous states, one could work out the entire phase diagram by minimizing the total energy of a several-phase system (for each point of the diagram) with respect to the proportions of the homogeneous phases. I shall attempt here to come as close as possible to this ideal, by including the homogeneous states known to be important and using the best available estimates of their energies. The calculation will be confined to small t/I and low hole concentration h. In this region[3] the relevant states are antiferromagnetic (the ground state for $h=0$) and ferromagnetic (the ground state for $t/I=0$). The energy of Nagaoka's ferromagnetic state is known for all h; for small h it is given by Eq. (4). It is not obvious, however, what happens to the antiferromagnetic state for nonzero h. This question was studied by Brinkman and Rice,[4] who found that the energy of an antiferromagnet with a hole is lowered by the formation of a microscopic ferromagnetic cloud ("spin polaron") around the hole. So in principle one should include a Brinkman-Rice n polaron antiferromagnetic state as a possible homogeneous state of hole density $h=n/N$. However, it can be shown that such a state is always unstable against coalescence of the polarons into a separate ferromagnetic phase.[5] Thus for any state containing an antiferromagnetic phase with $h>0$, there is a state of lower energy having only ferromagnetic and $h=0$ antiferromagnetic phases.

So in calculating the phase diagram, I consider only Nagaoka's ferromagnetic phase and the half-filled-band ($h=0$) antiferromagnetic phase. Finding the absolute minimum of the energy with respect to the proportions of each is straightforward [using Eqs. (3) and (4)]. The result, for each choice of t/I and h, is indicated in Fig. 1. It is perhaps easier to think of the condensation phenomenon in terms of electrons rather than holes. The pure ferromagnetic phase on the right in Fig. 1 is a Fermi gas of electrons. If we fix t/I and add more electrons (move to the left on Fig. 1) the density of the gas increases. When it reaches a critical density [given by Eq. (7)] an antiferromagnetic phase of fixed density (i.e., a solid) begins to condense out. As we add still more electrons, the gas remains at its critical density and we form more solid, until we have one electron per atom (half-filled band) and there is no gas left.

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[1]P. B. Visscher, preceding paper, Phys. Rev. B 10, 932 (1974).

[2]Y. Nagaoka, Phys. Rev. 147, 392 (1966).

[3]The reason for the small-h restriction is that for $h \approx 1$ (low electron density) paramagnetic states become important. See J. Kanamori, Prog. Theor. Phys. 30, 275 (1963); J. Callaway and D. M. Edwards, Phys. Rev. 136, A1333 (1964).

[4]W. F. Brinkman and T. M. Rice, Phys. Rev. B 2, 1324 (1970).

[5]To compute the optimal size of the polaron and its binding energy, Brinkman and Rice used a simple model with a cubical polaron; the hole wave function was required to vanish at the cube faces. Within this model, instability against coalescence can be shown either by direct comparison of energies or by the following argument: If we stack the polarons together, the wave function of the Brinkman-Rice n-polaron state (a single determinant of n functions each confined to a small cube) is an allowed wave function for the n holes in the large cavity formed

by the coalesced polarons, but clearly not the one of lowest energy. Thus the ground state of the coalesced polarons has lower energy than that of the separated polarons. Brinkman and Rice's cubical polaron model does not treat the polaron boundary exactly, but it seems likely that a proper treatment of the surface energy would just further unbind the polaron state.