

but $T_1 = 0.345$ instead of the value in Eq. (18).

The primary purpose of this note is to call attention to an approximate equation of state which fits data with considerable precision above and below the critical point. Details concerning the variations of the fit with changes in the parameters, discussion of possible modifications of this equation, and the interpretation of the parameters will be treated elsewhere² along with a presentation of our most recent data.

It is necessary to add a few words concerning this work in comparison to that of Kouvel and Rodbell⁷ who also have reanalyzed the data of Weiss and Forrer. They have given evidence for scaling laws using a procedure which is in a sense the opposite of ours. They have focused attention on the region of small $M/(T - T_c)^\beta$ by assuming that in this limit

$$H/M = \chi^{-1}(T) + D(T)M^2.$$

They then use these two parameters χ and D to normalize the isotherms and compare H/M as a function of M^2 for isotherms well above T_c . They demonstrate in this way that a scal-

ing law should hold. We have essentially ignored the region of small $M/(T - T_c)^\beta$ in obtaining our approximate equation of state and it is in this region that our equation fails, i.e., we would get from Eq. (1) that

$$H/M = \chi^{-1}(T) + D^1(T)M^{2.59}$$

in the limit of small M . Our concern is not with the proof of scaling laws for the region of $T > T_c + 2^\circ\text{C}$ as already demonstrated by Kouvel and Rodbell but rather with the behavior for region $(T_c - 2^\circ\text{C}) < T < (T_c + 2^\circ\text{C})$.

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MOTT AND WIGNER TRANSITIONS

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Wigner¹ has pointed out that the ground state of a system of interacting electrons in a uniform charge background has a completely different character in the low- and high-density limits. At high density the kinetic energy is dominant and the system is in gaslike phase, described in good approximation by a single Slater determinant of plane waves. At low density the electrostatic repulsion dominates and the electrons become localized at the points of a regular lattice.

Later, Mott² has postulated that a similar situation presumably prevails for a lattice of hydrogen atoms. If the density is high the electrons are metallic, but, at sufficiently low density, the electrons are expected to become bound to the ions, so that (at $T = 0^\circ$) the dc conductivity would be strictly zero.

The theory of these high-to-low density transitions is difficult and has received considerable attention.³ Here we outline a simple ap-

proach, based on recent work on excitonic phases,⁴ which reveals some new features. For brevity and simplicity we confine ourselves here mostly to spinless fermions. All our considerations are based on Hartree-Fock (HF) theory, with a phenomenologically screened interaction.

We begin with the Mott transition. We have a regular lattice L of N nuclei and denote the lattice parameter by d and the volume of the fundamental Brillouin zone of L by Ω_0 . For spinless fermions the appropriate number of fermions is $\frac{1}{2}N$, which, in the metallic phase, leads to a half-filled band. To have charge neutrality we take the nuclear and fermion charges as $+\frac{1}{2}e$ and $-e$, respectively.

At high density, or small d , the HF ground state has the form

$$\Psi_0 = \prod_{\vec{k} \text{ in } \Omega} a_{\vec{k}}^* \Phi_0; \quad (1)$$

here Ω is the occupied, nearly spherical, region of \vec{k} space of volume $\frac{1}{2}\Omega_0$; Φ_0 is the vacuum state; and $a_{\vec{k}}^*$ creates a fermion in the self-consistent Bloch state $\varphi_{\vec{k}}$.

On the other hand, at low density, or large d , it is evident that the lowest energy state is one in which the fermions occupy every other lattice site, thus minimizing the repulsive energy. The corresponding HF ground state has the form

$$\Psi_0' = \prod_{\vec{k} \text{ in } \Omega_0'} a_{\vec{k}}'^* \Phi; \quad (2)$$

here Ω_0' is the fundamental Brillouin zone of the new (super)lattice, L' , of volume $\frac{1}{2}\Omega_0$; and $a_{\vec{k}}'^*$ creates a fermion in a Bloch state $\varphi_{\vec{k}}'$ of the superlattice which may be decomposed into

$$\varphi_{\vec{k}}'(\vec{r}) = u_{\vec{k}} \chi_{\vec{k}}(\vec{r}) + v_{\vec{k}} \chi_{\vec{k}+\vec{w}}(\vec{r}), \quad (3)$$

where $u_{\vec{k}}$ and $v_{\vec{k}}$ are coefficients; the $\chi_{\vec{k}}$ are Bloch-like functions with the periodicity of L ; and \vec{w} is one of the new reciprocal lattice vectors of L' . This state is evidently insulating and can also be written in the form

$$\Psi_0' = \prod_{n=1}^{\frac{1}{2}N} w_n^* \Phi_0, \quad (4)$$

where the w_n^* create Wannier functions localized near each site of L' . The band gap is clearly of the order of e^2/d .

Equations (2) and (3) suggest that we look, even in the metallic phase, for a ground state of the form

$$\Psi_0 = \prod_{\vec{k} \text{ in } \Omega} (u_{\vec{k}} \alpha_{\vec{k}}^* + v_{\vec{k}} \alpha_{\vec{k}+\vec{w}}^*) \Phi_0, \quad (5)$$

where $\alpha_{\vec{k}}^*$ creates a fermion with a Bloch-like wave function of a periodicity corresponding to L .⁵ For very small d one finds $v_{\vec{k}} \equiv 0$. However, one can show that, as d is increased, there exists a critical value d_0 such that for $d > d_0$, $v_{\vec{k}} \neq 0$.⁴ We know that such a critical d_0 exists from our earlier remarks about the limit of very large d . We may also remark that the cost in kinetic energy of mixing in the wave functions with $\vec{k}+\vec{w}$ is proportional to the bandwidth, which decreases exponentially with d , while the gain in potential energy decreases only as d^{-1} . For $d = d_0 + 0$, the original symmetry of the lattice is only infinitesimally broken and thus infinitesimal gaps are introduced in-

to the original energy band at the new Brillouin zone boundaries. The system will therefore remain metallic for a finite range of lattice parameter, $d_0 < d < d_0 + \Delta d$.

Similar considerations may also be applied at finite temperatures T , which—because of the role of the entropy—disfavor the superlattice. Thus near the high-density side, d_0 will be an increasing function of T . Near the insulating limit, purely electrostatic considerations make it obvious that the critical temperature for the dissolution of the superlattice is given by

$$kT_c = \gamma(e^2/d), \quad (6)$$

where γ is a numerical constant. Thus we are led to a critical curve C whose topology is shown in Fig. 1. On dimensional grounds the maximum critical temperature has the value

$$(kT_c)_{\max} = \gamma' \text{ Ry}, \quad (7)$$

where Ry is the Rydberg and γ' is another numerical constant.

In addition, the considerations of Ref. 4 lead us to conclude that, inside C , there is an infinity of further phase boundaries, separating different “excitonic phases” in which the electronic density exhibits fluctuations characterized by additional wave vectors \vec{w}' , \vec{w}'' , etc. These phase boundaries are schematically indicated in Fig. 1 by the dashed curves. The phase transitions are all of second order.

The Wigner transition of spinless fermions is, from the present standpoint, basically similar, but somewhat more difficult. We consider a system of N fermions characterized by the Wigner-Seitz radius r_s . For high density, or small r_s , the ground state is that of a normal metal, with complete translational invariance. As r_s is increased, the first instabili-

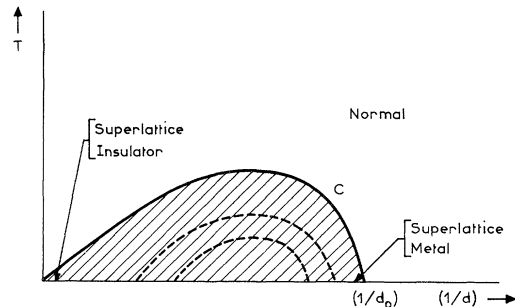


FIG. 1. Schematic phase diagram for the Mott transition. d is the lattice parameter and T the temperature.

ty, occurring at a critical value $(r_s)_0$, is a second-order transition of the Overhauser variety.⁶ The new phase has one (or more) density fluctuations characterized by some wave number \vec{w} and is again metallic. As r_s is further increased, the wave number \vec{w} will change continuously, in contrast to the Mott transition where it is locked by the reciprocal lattice of the underlying periodic lattice.

In the low-density, high- r_s limit we have an insulator⁷ in which the fermions are localized at the sites of a regular lattice⁸ (equivalence of Wannier and Bloch determinants for an insulator). The band gap is of the order e^2/r_s .

For finite temperature, we find a phase boundary separating the normal, translationally invariant phase from the phase with broken symmetry, similar to Curve C of Fig. 1. The maximum critical temperature is again of the form Eq. (8) and the behavior for large r_s is like Eq. (6) with r_s replacing d .

An interesting feature, not present in the Mott model, is the following: For fixed r_s , as T is increased from 0° , the wave number(s) characterizing the spatial order will change continuously. This is so even in the dilute (insulating) limit, where the lattice parameter of the Wigner lattice changes as "electrons and holes" are produced, so that the number of cells no longer equals the number of fermions.

Finally we expect again an infinite sequence of excitonic phases, similar to those of the Mott model.

When spin is introduced, phases with magnetic order must be also considered, in both the Wigner and Mott models. As a result the problem becomes, quantitatively, much more complicated and difficult. However, the qual-

itative character of the phenomena remains entirely similar.

How reliable are our conclusions? Within the HF approximation, we can say that the successive second-order transitions which we have discussed will certainly occur, unless some first-order electronic transitions intervene.⁹ Possibly both types of transitions may occur. We plan to carry out quantitative HF calculations of the Wigner and Mott transitions to clarify this point. As for correlation effects, they are responsible for collective modes (excitons, acoustic and optical plasmons, and spin waves) which may lead to qualitatively new effects. Especially in the Wigner model, melting associated with large amplitudes of low-lying modes may occur.

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