Normal ^{3}He: an almost localized Fermi liquid

Dieter Vollhardt

Max-Planck-Institut für Physik und Astrophysik, Werner Heisenberg-Institut für Physik, D-8000 München 40, Federal Republic of Germany

The Hubbard model is used to calculate static properties of normal-liquid ^{3}He at $T=0$. For this, Gutzwiller's variational approach to that model is employed. The work is based on an observation by Anderson and Brinkman that the results of this method, obtained by Brinkman and Rice for the metal-insulator transition in the case of one particle per site, appear to be in qualitative agreement with the experimentally measured properties of that liquid. In this sense normal ^{3}He can be understood to be close to a localization transition of the particles where their effective mass diverges. The incipient localization is found to determine the properties of that liquid. Hence ^{3}He is "almost localized" rather than "almost ferromagnetic," as often claimed by paramagnon theory. The author further investigates this motion. Discussing Gutzwiller's approach to the Hubbard model, he shows that it is well suited for a description of a liquid system like ^{3}He. The approach and its physical implications are investigated by means of the reformulation of the solution due to Ogawa *et al.* It is shown explicitly that Gutzwiller's results can be placed into the concepts of Landau-Fermi-liquid theory and that within this model the Landau parameters F_0^s and F_0^a are related. Furthermore, the author identifies two different kinds of spin-fluctuation processes inherent to the model, one of which is shown to be responsible for the largeness of F_0^s. Going beyond these qualitative aspects, the author evaluates F_0^a and F_0^s quantitatively, finding that F_0^a agrees very well with the experimentally determined values at all pressures, with $F_0^a \to -\frac{3}{4}p$ at high pressures, where p is always close to unity. Hence the system is never close to a ferromagnetic transition. By means of the forward scattering sum rule for $l<2$ an analytic expression for F_1^a is obtained. Finally, the author extends the analysis to large magnetic fields, finding that in the case of normal ^{3}He the magnetization increases very rapidly with the magnetic field. This is due to the large zero-field effective mass. There is a line of critical values for the interaction and the magnetic field where a fully magnetized state is formed via a first-order transition. Calculating the drop in melting pressure due to the magnetic field, the author finds that it essentially removes the minimum in the melting curve. Thus the melting pressure even of fully polarized ^{3}He is larger than zero, in agreement with arguments by Castaing and Nozières.

CONTENTS

I. INTRODUCTION

A. Normal ^{3}He and its description

Normal ^{3}He [for a review, see Baym and Pethick (1978)] is a liquid of high density whose spherical atoms are strongly interacting. Indeed, the interparticle distance is of the same order as the atomic diameter, and the interaction is mainly given by a strong hard-core repulsion and a weak van der Waals attraction. Owing to the small atomic mass the zero-point motion of the atoms implies that, at normal pressure, the kinetic and potential energies of the noble gas atoms are almost equal even at arbitrarily low temperatures. Therefore, ^{3}He (as well as ^{4}He) stays liquid for $T \to 0$ and solidifies only under a pressure of approximately 34 bars. As ^{3}He atoms are fermions, normal ^{3}He constitutes a Fermi liquid below the degeneracy temperature T_F. Its properties are then governed by the Fermi-Dirac quantum statistics: it is a quantum liquid.

Introducing the concept of quasiparticles, the theory of Landau (1956,1957) is highly successful in its phenomenological description of this complicated system (Pines and Nozières, 1966). It views the strongly interacting liquid as a system of quasiparticles having a distribution function that equals the one for a noninteracting system. These quasiparticles are characterized by an effective mass m^* (approximately three to six times larger than the mass of the bare ^{3}He atom) and an effective interaction. This interaction can be parametrized by means of an infinite set of "molecular fields," quantified by the Landau parameters (Leggett, 1975). The Landau theory made it possible to understand why the physical properties of liquid ^{3}He, such as the temperature dependence of the specific heat, the spin susceptibility, transport properties, etc., are qualitatively very similar to those of an interacting Fermi *gas* in spite of the strong interactions. This is essentially due to the exclusion principle, which

leads to a severe reduction of the phase-space volume in the vicinity of the Fermi energy, where most physical processes take place. For example, the specific heat c_v, the static spin susceptibility χ_s, and the compressibility κ are given by

$$c_v=\frac{m^*}{m}c_v^0\,,$$
$$\chi_s=\frac{m^*/m}{1+F_0^a}\chi_s^0\,, \tag{1}$$
$$\kappa=\frac{m^*/m}{1+F_0^s}\kappa^0\,,$$

where $m^*/m=1+F_1^s/3$. Here F_0^s, F_1^s, F_0^a are the first of the usual Landau parameters, and $c_v^0=(\pi^2/3)N(0)T$, $\chi_s^0=\mu_0^2N(0)$, $\kappa^0=N(0)/n^2$ are the respective quantities for a noninteracting system; $N(0)=mk_F/\pi^2$ is the density of states of a Fermi gas at the Fermi energy for *both* spins, μ_0 is the nuclear magnetic moment, k_F is the Fermi momentum, and n is the particle density. The units are such that $k_B,\hbar=1$.

As Landau theory is phenomenological in character, it cannot make predictions about the values of the Landau parameters—i.e., they are undetermined within that theory. It takes a microscopic theory and an explicit form of the interaction between the particles if one actually wants to make quantitative calculations of the parameters. However, due to the high density and the strong interactions in the ^{3}He liquid, such first-principle calculations are extremely hard to perform and so far have not yet yielded satisfactory quantitative results (Babu and Brown, 1973). In that respect the rather more numerical techniques of the correlated-basis-function approach (Feenberg, 1969; Krotscheck and Smith, 1983), a variational method for optimizing the wave function of the system, appear to be more promising. In view of these difficulties one would like to tackle the problem by at least investigating a particular model, hoping that it contains the dominant physical features of the actual system. However, an exact solution of even a highly simplified model mostly proves to be impossible. Therefore, one has to find an approximation. Again, it is hoped that this approximation describes most of the physics that was considered to be important when formulating the model. So, when one is trying to describe an actual physical system there are two fundamental sources of error: in the choice of the model and its subsequent approximate solution. It seems important to keep this general problem in mind when investigating an intensively studied system such as a strongly correlated Fermi liquid, e.g., normal ^{3}He or electrons in a metal. In the case of ^{3}He, for $T<T_F$, those dominant physical features appear to be

(i) the fermion character of the atom, and
(ii) the hard-core repulsion between the atoms.

These essentials can be represented by a contact interaction between two atoms that takes place only when they have opposite spin. If we neglect the actual size of the atoms, the interaction Hamiltonian is given by (Stoner model)

$$H_{\rm int}=U\int d^dr\, n_\uparrow(\mathbf{r})n_\downarrow(\mathbf{r})\,, \tag{2}$$

where U is a phenomenological interaction constant of a δ-function potential $U(\mathbf{r}-\mathbf{r}')=U\delta(\mathbf{r}-\mathbf{r}')$ and $n_\sigma=c_\sigma^\dagger c_\sigma$ are the density operators for particles of spin σ; $c_\sigma^\dagger$ (c_σ) are the usual fermion creation (destruction) operators. This model Hamiltonian for a contact interaction between fermions can be used to describe a neutral system like liquid ^{3}He,[1] or a charged system, like electrons in a metal, provided the Coulomb interaction is so strongly screened that it can be assumed to have the above δ-function form. The high density and the strong hard-core interaction between the atoms are properties shared, in fact, by both liquid ^{3}He and ^{4}He. The repulsion leads to a spatial correlation between the atoms causing them to avoid each other. Consequently the atoms in either system are rather insensitive to the full microscopic details of the bare hard core. This is one of the key points of the polarization potential theory developed by Pines and co-workers [for a recent review, see Pines (1983)], which allows for a unified description of excitations and transport in both helium liquids. In the present problem, the full model Hamiltonian has the form

$$H=\sum_{\mathbf{k},\sigma}\varepsilon(\mathbf{k})a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}+H_{\rm int}\,, \tag{3}$$

where $a_{\mathbf{k}\sigma}^\dagger$ ($a_{\mathbf{k}\sigma}$) are the creation (annihilation) operators for a fermion in a Bloch state with momentum $\mathbf{k}$, N is the total number of particles, and $\varepsilon(\mathbf{k})$ is a more or less realistic kinetic energy of the particles. As there do not exist solutions above $d=1$ dimensions, even for this highly simplified Hamiltonian, one has to resort to approximations. For example, within the generalized Hartree-Fock approximation the dynamic susceptibility is given by (Wolff, 1960; Izuyama *et al.*, 1963)

$$\chi(\mathbf{q},\omega)=\mu_0^2\frac{\Pi(\mathbf{q},\omega)}{1-U\Pi(\mathbf{q},\omega)}\,, \tag{4}$$

where $\Pi(\mathbf{q},\omega)$ is the Lindhard function. Therefore, the static susceptibility is given by

$$\chi_s\equiv\chi(0,0)=\mu_0^2\frac{2N_F}{1-UN_F}\,, \tag{5}$$

where N_F is the density of states of the *bare* particles at the Fermi energy of one spin direction. So, one finds that χ_s is by a factor $(1-\bar{I})^{-1}>1$ (the so-called Stoner

[1]Note that U does not represent the true microscopic hard-core repulsion entering, for example, in Brueckner theory (Brueckner and Gammel, 1958), which can be of the order of 10^3 K, depending on separation. The potential used above is rather softer; for ^{3}He we shall later find $U\cong 15$ K, this being about the interaction strength of two ^{3}He atoms at their average separation in the liquid. So (2) should be viewed as a renormalized interaction of (quasi)particles due to many-body effects.

enhancement factor) larger than that of a noninteracting Fermi system; here $\bar{I}=UN_F$. The enhancement can be understood to be due to the existence of strong, low-frequency spin fluctuations or "paramagnons" (for a review, see Levin and Valls, 1983). However, within the same approximation the effective mass can be calculated via the specific heat, and one finds that (Doniach and Engelsberg, 1966) $m^*/m-1\propto\ln[1/(1-\bar{I})]\propto\ln(\chi_s/\chi_s^0)$. So there is a renormalization of the mass, but it does not explicitly enter the expression for χ_s (Levin and Valls, 1979a). For $\bar{I}\to 1$ the static susceptibility diverges, indicating a transition to a ferromagnetic state. It is therefore often said that a system with a strongly enhanced Pauli susceptibility is "close to a ferromagnetic transition" or "almost ferromagnetic." For $\chi_s/\chi_s^0=1/(1-\bar{I})$ to describe the experimental data for liquid ^{3}He, $\bar{I}$ has to be as large as $\bar{I}\simeq 0.95$ and, again, ^{3}He is therefore often referred to as being almost ferromagnetic.

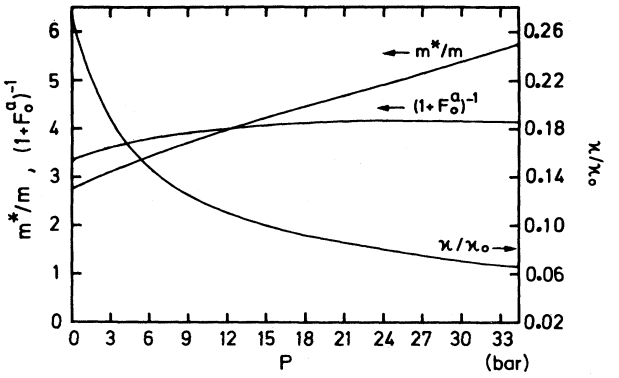

FIG. 1. Experimental values (Greywall, 1983) of the normalized effective mass m^*/m, the ratio between spin susceptibility and effective mass, $(1+F_0^a)^{-1}$, and the normalized compressibility κ/κ_0.

B. Fermi-liquid theory and the contact-interaction model

Comparing the above result for χ_s and c_v with the one of Landau theory one finds by identification

$$\frac{1}{1-\bar{I}}=\frac{(m^*/m)_L}{1+F_0^a}\ , \tag{6a}$$

$$(m^*/m)_P=(m^*/m)_L\ , \tag{6b}$$

where the subscripts P and L refer to the paramagnon results and Landau theory, respectively. So the *one* parameter $\bar{I}$ appears to combine *two* Landau parameters at the same time, the one describing the enhancement of the susceptibility due to the effective mass (arising from a spin-independent interaction, i.e., F_1^s), as well as the one due to spin-dependent interaction, i.e., F_0^a.

In Landau theory χ_s can thus be large (or even diverge), mainly for *two* different reasons, either

(1) $F_0^a\to 1$; this would correspond to $\bar{I}\to 1$ and would support the claim of the approaching ferromagnetic instability, or

(2) $m^*/m\to\infty$ (while $1+F_0^a>0$), which would indicate that the particles carrying the spin become immobile and "localize."

In Fig. 1 the experimentally determined pressure dependence of the effective mass m^*/m (from the specific heat), the ratio $(\chi_s/\chi_s^0)/(m^*/m)=(1+F_0^a)^{-1}$ of the static susceptibility and the effective mass, and the compressibility κ/κ_0 as measured by Greywall (1983) are shown. Anderson and Brinkman (1975,1978) pointed out that while m^*/m increases with pressure, the quantity $(1+F_0^a)^{-1}$ changes very little; in particular, it is essentially pressure independent at high pressures. They argued that the strong enhancement of the susceptibility was essentially due to the effective mass, rather than to the factor $(1+F_0^a)^{-1}$. In view of this, Anderson and Brinkman suggested that normal ^{3}He should *not* be considered "almost ferromagnetic" but rather "almost localized" or "solid." This notion is also supported by the fact that the compressibility (Fig. 1) is strongly reduced as pressure increases—a feature that one would attribute to a system that becomes more and more solidlike (Castaing and Nozières, 1979; Levin and Valls, 1979a). In fact, at 34.36 bars the ^{3}He liquid solidifies such that the atoms are indeed localized.

Paramagnon calculations for χ_s/m^* lead to a different behavior: there this quantity is found to diverge as $\bar{I}\to 1$. Paramagnon theory has been successful in determining various properties of liquid ^{3}He like the $T^3\ln T$ contribution to the specific heat [see the review of Baym and Pethick (1978)] and the formation of spin-triplet states in the superfluid (Layzer and Fay, 1971; Anderson and Brinkman, 1973). It has also been applied to a calculation of Landau scattering amplitudes $A_l=F_l/[1+F_l/(2l+1)]$ (Levin and Valls, 1979a,1983). If $\bar{I}$ is chosen to fit the spin susceptibility, the A_l are in reasonable agreement with the experiment. It appears essential that an interpretation of paramagnon theory within the context of Landau theory is done via the A_l parameters rather than the Landau parameters F_l. In this way Galilean invariance is maintained as $\bar{I}\to 1$ and the equality (6a) is found to apply. The conclusion that normal ^{3}He is close to a magnetic instability, such that its properties are dominated by the incipient ferromagnetic transition, is plausible only within that particular picture. However, as will be seen below, there are solutions of the Hamiltonian (3) which come to exactly the same conclusions as those reached by using Landau theory, namely, that ^{3}He is almost localized rather than ferromagnetic.

Anderson and Brinkman (1975,1978) argued that this concept is closely related to that of "localization by correlation" in the sense of Mott (1949) concerning the behavior of electrons in narrow-band systems. Such systems have been investigated by the Hubbard model, introduced by Gutzwiller (1963,1964), Hubbard (1963,1964), and Kanamori (1963) for 20 years now. In this model the electrons are considered to be on a lattice, their kinetic energy being due to hopping from one site to another, while the interaction acts only on the same site.

Obviously, the Hubbard Hamiltonian is nothing but the model Hamiltonian (3), where $\mathbf{r}$ is now discrete, describing the lattice sites. Initially, it was proposed for the investigation of the correlation-induced metal-insulator transition as well as magnetically ordered states in such a system. It is remarkable how little progress has been made in the study of this truly fundamental and seemingly simple Hamiltonian (Cyrot, 1977). Few exact results are known and all other information is based on various approximations and approaches which often lead to different results.

However, there is one treatment, due to Gutzwiller (1965), which is different from all other methods. It is a variational approach in which the wave function of the interacting system is constructed from that of the noninteracting system. Even in its simplest form it allows calculation of the ground-state energy of the system for arbitrary band filling and number of up and down spins. Using this solution (initially intended for the study of the possibility of a ferromagnetic transition), Brinkman and Rice (1970; see also Rice and Brinkman, 1971) realized that in the case of a half-filled band this solution actually describes a metal-insulator transition [a so-called "Mott transition"; see the discussion by Mott (1974)], where, at a critical value of the interaction strength, the spins become "localized," so that there is only one spin per site. They also calculated the effective mass, the static spin susceptibility, and the compressibility of this system. From these expressions they found, for example, that the enhancement of the susceptibility was essentially due to the effective mass and not due to the usual Stoner enhancement factor.

It was Anderson and Brinkman who then made an explicit connection of those results to the ones of Fermi-liquid theory and the properties of ^{3}He. Extracting the Landau parameters F_0^s, F_0^a, F_1^s, they noted that their behavior for increasing interaction qualitatively agreed with the pressure dependence found experimentally. By contrast, in paramagnon theory $\chi_s/m^* \propto (1+F_0^a)^{-1}$ is found to be pressure dependent whereas this is not the case experimentally. Gutzwiller's approach therefore yields results which are in qualitative agreement with Fermi-liquid results for ^{3}He. This gives theoretical support for the observation that it is the effective-mass behavior, i.e., the incipient localization, which dominates the physical properties of this strongly correlated Fermi system (Anderson and Brinkman, 1975, 1978; Castaing and Nozières, 1979). The importance of spin fluctuations, being the basis for paramagnon calculations, are not denied in Gutzwiller's approach (1963–1965); however, they should be understood as a consequence of the approaching localization (Anderson and Brinkman, 1975, 1978). In fact, I will explicitly show that spin-fluctuation processes are responsible for the dominant features of Gutzwiller's results. It is interesting to note that a qualitatively similar result has been obtained by Kawabata (1975,1977) by considering spin fluctuations in the Hubbard model. Kawabata aimed at a description of metals like V_2O_3 with a strongly enhanced specific-heat coefficient and spin susceptibility. Using a Green's-function approach and sum-rule arguments, he also arrived at the result that the enhancement of the specific heat and the spin susceptibility is due to the *same* factor.

I believe that the results of Gutzwiller's approach (1963–1965) to the Hubbard Hamiltonian, and the apparent connections to the properties of liquid ^{3}He call for further investigation in this direction. Therefore my intention here is

(1) to understand the physical implications of this approach and thereby try to understand the reasons for its apparent success in describing normal-liquid ^{3}He,

(2) to analyze the connections to the ideas of Landau-Fermi-liquid theory,

(3) to understand the origin of the Landau parameters by identifying the physical processes responsible,

(4) to make a *quantitative* evaluation of Fermi-liquid parameter within that approach, and finally

(5) to use this approach to go beyond the typical range of applicability for Landau theory (i.e., perturbations with energies much smaller than the Fermi energy).

As the Gutzwiller result allows for a more general analysis, I shall use it to calculate the magnetization curves for liquid ^{3}He at $T=0$ for arbitrary magnetization and interactions (i.e., pressures). So far the magnetization behavior of liquid ^{3}He at high magnetic fields is not known beyond general arguments (Castaing and Nozières, 1979) because of the very complicated nature of this highly correlated system. Its knowledge is a step towards a better understanding of this quantum liquid and is also of interest in the light of recent investigations of highly polarized liquid ^{3}He (Castaing and Nozières, 1979; Lhuillier and Laloe, 1980; Chapellier *et al.*, 1979; Godfrin *et al.*, 1980).

The paper is organized as follows. Section II discusses the Hubbard model and the result of certain approximations used to solve it; in Sec. III we turn to Gutzwiller's variational approach, in particular, examining the physical meaning and implications of this method, based on the reformulation by Ogawa *et al.* (1975). Section IV discusses the applicability of Gutzwiller's results on liquid ^{3}He and will argue why this particular approach should be especially suited for such a liquid system. The results of Gutzwiller's method are then discussed in Sec. V by making contact with the ideas of the Landau-Fermi-liquid theory. I identify the spin-fluctuation process which is the origin of the pronounced pressure dependence of the Landau parameter F_0^s. Then the Landau parameters F_0^s, F_0^a, F_1^s are determined quantitatively, and, using the forward-scattering sum rule for $l<2$, I derive an analytic expression for the parameter F_1^a. As we go beyond the limit of small magnetic fields, the magnetization for arbitrary magnetic fields at $T=0$, as well as the magnetic field dependence of the effective mass, is calculated in Sec. VI, and further comparison with the results of paramagnon theory is made. Finally, Sec. VII discusses the results and possible improvements.

II. THE HUBBARD HAMILTONIAN

As discussed in the Introduction, the Hubbard Hamiltonian (Gutzwiller, 1963, 1964; Hubbard, 1963, 1964; Kanamori, 1963) is supposed to describe the behavior of fermions on a lattice in a narrow-band system. The interaction is assumed to be extremely short ranged so that it takes place only on the same site. It is the lattice version of (3):

$$H=\sum_{ij}\sum_{\sigma}t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}+U\sum_{i}n_{i\uparrow}n_{i\downarrow}\ . \tag{7}$$

The first part is the kinetic energy due to hopping between sites i and j, which can also be expressed in momentum representation as in (3), with

$$\varepsilon(\mathbf{k})=N^{-1}\sum_{ij}t_{ij}e^{-i\mathbf{k}(\mathbf{R}_i-\mathbf{R}_j)}$$

and

$$a_{\mathbf{k}\sigma}=N^{-1/2}\sum_{i}c_{i\sigma}e^{-i\mathbf{k}\mathbf{R}_i}\ ,$$

etc. For nearest-neighbor hopping (summation index $\langle ij\rangle$) we set $t_{ij}=-t$. This term makes the model inherently quantum mechanical. The interaction part reads $U\sum_i c_{i\uparrow}^{\dagger}c_{i\uparrow}c_{i\downarrow}^{\dagger}c_{i\downarrow}$ and formally represents a four-fermion operator. As simple as this Hamiltonian is, it still represents a truly interacting system. Without interaction ($U=0$) one obtains a pure band behavior due to the small but finite overlap of the atomic wave functions. In the atomic limit ($t=0$) the particles are localized. So the Hubbard Hamiltonian describes a system which allows for both these limits; naturally, the intermediate regime $t\sim U$ is of particular interest, as in this range of parameters the competition beween band effects and localization due to correlation is most subtle. So far, only the one-dimensional case has been solved exactly (Lieb and Wu, 1968): One finds a Mott transition in the ground state for $U=0$, the ground state being antiferromagnetic (Lieb and Mattis, 1962). For higher dimensions only approximations exist besides a few exact results within perturbation theory. The approximation methods [for a review, see Cyrot (1977)] can be grouped into

(1) Green's-function methods (decoupling procedures, functional integral representation, perturbation theory, etc.),
(2) variational methods for the wave functions and spin configurations,
(3) renormalization-group calculations (Hirsch, 1980), and
(4) numerical methods using Monte Carlo (Hirsch and Scalapino, 1983, and references therein; Hirsch, 1983).

The fourth and most of the third method concentrates, however, on the $d=1,2$ case. The first method has been used most widely, and an extremely extensive literature has accumulated. The Green's-function methods first used (Hubbard, 1964) made approximations that *a priori* excluded antiferromagnetism, i.e., that explicitly considered only paramagnetic states, because they considered random distributions of the spins such that the space average $\langle n_{i\sigma}\rangle=n_\sigma$ was space independent. Therefore, only the band splitting was considered to be relevant for the transition between metal and insulator. Earlier, Anderson (1963) had shown within perturbation theory that in the half-filled band case (equal number of particles and sites) for $U\gg t$ the magnetic moments would order antiferromagnetically, the states being localized. In order to be able to obtain antiferromagnetism when calculating one-particle quantities, a trick was subsequently used: alternating lattices were introduced and the decoupling of the Green's functions was accordingly done for these different lattices (Langer *et al.*, 1969). Thereby the different lattice periodicity in the case of antiferromagnetism was built into the formalism. The decoupling was done in the simplest possible way, equivalent in spirit to a straightforward mean-field approximation. This yielded a BCS-type gap equation for the order parameter (the local magnetic moment). It turned out that the results strongly depend on the type of lattice considered: for simple cubic (sc) and body-centered-cubic (bcc) lattices the transition between the paramagnetic and the antiferromagnetic state occurs in the ground state at $U=0$ (just as in the $d=1$ case!), while in the face-centered-cubic (fcc) lattice a finite interaction strength is necessary (Cyrot, 1972). This is due to the "perfect nesting" property of sc and bcc lattices, where $\varepsilon(\mathbf{k})=-\varepsilon(\mathbf{k}+\mathbf{G})$, $\mathbf{G}$ being one-half of a reciprocal-lattice vector. So the results of these mean-field theories (Langer *et al.*, 1969; Cyrot, 1972) critically depend on the lattice in question. Of course, the applicability of a mean-field theory is yet another question. An important point is that all Green's-function techniques treat the kinetic energy part of the Hamiltonian exactly, while approximating the interaction part.

III. THE GUTZWILLER APPROACH TO THE HUBBARD MODEL

A. Calculation of the ground-state energy

In order to solve at $T=0$, the model Hamiltonian (7), Gutzwiller (1963,1964) applied a variational method. Let L, $N_\uparrow$, $N_\downarrow$, and D be the number of lattice points, up spins, down spins, and doubly occupied sites, respectively; $n_\uparrow=N_\uparrow/L$, $n_\downarrow=N_\downarrow/L$, $d=D/L$. Furthermore, let $|\psi_0\rangle$ be the state describing the spin configuration of the uncorrelated ($U=0$) system. In that case the average number of doubly occupied sites D_0 obviously is $D_0=n_\uparrow n_\downarrow L$. When the interaction is switched on, the number of doubly occupied sites must decrease, because the interaction energy is given just by UD, so $D<D_0$ to reduce this energy. In order to obtain the state $|\psi\rangle$ of the correlated state, Gutzwiller's idea was to construct a trial wave function by starting from the uncorrelated state $|\psi_0\rangle$ and then to reduce the number of doubly occupied sites. This is the central aspect of his approach. The correlated state is thus written as (Gutzwiller, 1963—1965)

$$|\psi\rangle = \prod_i [1-(1-g)n_{i\uparrow}n_{i\downarrow}]\,|\psi_0\rangle \tag{8}$$

$$= g^D |\psi_0\rangle \ , \tag{9}$$

i.e., to obtain the correlated state the amplitude of the uncorrelated state is systematically reduced. Here g is a variational parameter that has to be determined so as to minimize the ground-state energy given by

$$E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \tag{10}$$

$$= \left[\left\langle\psi\left|\sum_{ij}\sum_{\sigma} t_{ij}c^{\dagger}_{i\sigma}c_{j\sigma}\right|\psi\right\rangle + \left\langle\psi\left|U\sum_i n_{i\uparrow}n_{i\downarrow}\right|\psi\right\rangle\right] \Big/ \langle\psi|\psi\rangle \ . \tag{11}$$

In the thermodynamic limit, $|\psi\rangle$ is an eigenstate of the number operator $\sum_i n_{i\uparrow}n_{i\downarrow}$, and therefore the interaction term in the expression for E_g is simply give by UD.

The choice $g=1$ obviously corresponds to the uncorrelated state ($U=0$), while $g=0$ yields $|\psi\rangle\neq 0$ only if $D=0$, i.e., when there are no doubly occupied sites. As, per construction, the interaction term is treated exactly in this approach (in contrast to the Green's-function methods) the problem now reduces to the evaluation of the norm $\langle\psi|\psi\rangle$ and, above all, an approximation for the matrix elements of the kinetic energy $\langle\psi|H_{\rm kin}|\psi\rangle$. This leads to determinants for which Gutzwiller made certain assumptions concerning the amplitudes of general nth-order density functions, and phase relations between different spin configurations (Gutzwiller, 1965). He claimed that the motion of the up-spin electrons was essentially independent of the behavior of the down-spin particles (and vice versa) and that therefore the down-spin electrons could just as well be assumed to be infintely heavy, i.e., that they acted only as an obstruction for the up-spin particles. Although this treatment was far from transparent, it turned out that under these assumptions the problem reduced to one of mere combinatorics. Indeed, after minimalization with respect to the variational parameter g, Gutzwiller (1965) obtained an extremely simple result for the ground-state energy, namely

$$E_g/L = q_{\uparrow}(d,n_{\uparrow},n_{\downarrow})\bar{\varepsilon}_{\uparrow} + q_{\downarrow}(d,n_{\uparrow},n_{\downarrow})\bar{\varepsilon}_{\downarrow} + Ud \ , \tag{12}$$

which still has to be minimized with respect to d. Here q_σ are the discontinuities in the single-particle occupation number $\langle a^{\dagger}_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}\rangle$ at the Fermi surface. They are given by

$$q_\sigma = \frac{\{[(n_\sigma - d)(1-n_\sigma-n_{-\sigma}+d)]^{1/2} + [(n_{-\sigma}-d)d]^{1/2}\}^2}{n_\sigma(1-n_\sigma)} \ . \tag{13}$$

Furthermore,

$$\bar{\varepsilon}_\sigma = L^{-1}\left\langle\psi_0\left|\sum_{ij} t_{ij}c^{\dagger}_{i\sigma}c_{j\sigma}\right|\psi_0\right\rangle = \sum_{|\mathbf{k}|<k_{F\sigma}} \varepsilon(\mathbf{k}) < 0$$

is the average energy of the σ spins in the *uncorrelated* state; here $k_{F\sigma}$ is the respective Fermi momentum (only if $n_\uparrow = n_\downarrow$ one has $k_{F\uparrow}=k_{F\downarrow}$). One can easily see that always $q\leq 1$ ($q=1$ only if $U=0$) as one should expect for a noninteracting system. So, while treating the interaction term exactly, the Gutzwiller approach concentrates on an approximation of the kinetic energy term, calculating its reduction due to the decrease of doubly occupied sites (and therefore also of empty sites), which makes hopping energetically unfavorable.

B. Properties of the solution

Using (12) Gutzwiller (1965) discussed the possibility of ferromagnetism in this model, concluding that in three dimensions the ground state was never ferromagnetic. Arguing from a different point of view, Brinkman and Rice (1970) realized that Gutzwiller's result, in fact, predicted a metal-insulator transition. For a half-filled band ($n=1$) and $n_\uparrow = n_\downarrow$ they found that ($q_\uparrow = q_\downarrow \equiv q$, $\bar{\varepsilon}_\uparrow = \bar{\varepsilon}_\downarrow \equiv \bar{\varepsilon}_0/2$)

$$q = 8d(1-2d) \ ; \tag{14}$$

and, minimizing the ground-state energy, they obtained

$$d = \frac{1}{4}\left[1-\frac{U}{U_c}\right] , \tag{15a}$$

$$q = 1-\left[\frac{U}{U_c}\right]^2 , \tag{15b}$$

$$E_g/L = -|\bar{\varepsilon}_0|\left[1-\frac{U}{U_c}\right]^2 , \tag{15c}$$

where $U_c = 8|\bar{\varepsilon}_0|$. This implies that at a finite, critical interaction U_c the number of doubly occupied sites vanishes, such that every lattice point is singly occupied, i.e., that the particles are localized. At this point $q=0$ (reduction of the kinetic energy to zero); and, as $d=0$, the ground-state energy E_g vanishes, indicating the metal-insulator transition. Clearly, very close to the transition, (15c) cannot be correct (Brinkman and Rice, 1972). It is well known from perturbation theory (Anderson, 1963) that for $U/|\bar{\varepsilon}_0|$ or $U/t \gg 1$, when the spins are localized and antiferromagnetically ordered, the ground-state energy is proportional to t^2/U. In contrast, the above result implies the formation of a paramagnetic, localized ground

state. It has recently been shown that in $d=1$ Gutzwiller's ansatz (8) in fact does yield a ground-state energy $E_g=-\alpha t^2/U$ when no approximations in the calculation of the matrix elements are made (Kaplan, Horsch, and Fulde, 1982). However, α is shown to be too small compared with the exact result (Bonner and Fisher, 1964). The reason for this is found to be too weak a binding of empty and doubly occupied sites. This deficiency has been almost completely removed by the introduction of a second variational parameter (Kaplan *et al.*, 1982). To allow for the possibility of antiferromagnetism Ogawa *et al.* (1975) and Takano and Uchinami (1975) extended Gutzwiller's analysis. Introducing alternating lattices, they found that before localization sets in ($d=0$), a transition to an antiferromagnetic state was indeed energetically favorable. The results slightly differ, because different approximations were used, but the overall feature is that for $U/U_c<0.41$ (Takano and Uchinami, 1975) [or $U/U_c<0.35$ (Ogawa *et al.*, 1975)] the system is paramagnetic, being described by Gutzwiller's earlier results, while for an interaction strength larger than these critical values antiferromagnetism appears. A state with a vanishing number of doubly occupied sites is thus never reached at finite U, in agreement with the Green's-function results (Langer *et al.*, 1969; Cyrot, 1972). The validity of these results has been questioned by Florencio and Chao (1976), who find a first-order paramagnetic to antiferromagnetic transition at $U/U_c=0.71$, also using an extended Gutzwiller approach.

As a by-product, however, the work of Ogawa *et al.* (1975) clarified the physics contained in Gutzwiller's approximation. While starting from Gutzwiller's idea of constructing a trial wave function, they applied a much more transparent formalism to the problem. Especially, they showed that it was *one* particular approximation in their formulation which exactly yielded Gutzwiller's results. This approximation concerns the dependence of the energy expectation values on the spin configurations of the wave function. While spin configurations with the same number of doubly occupied sites all have the same expectation value for the interaction term, their expectation value for the kinetic energy will generally be different (in some configurations the hopping is more advantageous than in others). Ogawa *et al.* (1975) showed that *neglecting* the configuration dependence of the expectation values was equivalent to all assumptions made by Gutzwiller (1965) and leads to an identical result. So, while the interaction term is treated exactly, the kinetic energy is approximated in a way which includes all possible hopping processes but neglects the environment where this hopping takes place. Recently it was shown (Razafimandimby, 1982) that Gutzwiller's result for the ground-state energy of a nonmagnetic, half-filled band system can be reproduced by a very simple factorization approximation essentially equivalent to a one-site cluster expansion. Furthermore, a two-site cluster expansion reduces to Gutzwiller's results in the limit of the space dimension going to infinity, and already in three dimensions gives only very small corrections.

C. Comparison with Hartree-Fock approximations

In this context it is interesting to compare his results with those of Green's-function methods using Hartree-Fock decoupling approximations. As shown by Dichtel *et al.* (1971,1972), the latter results are indeed identical to those obtained by applying a canonical transformation on the Hubbard Hamiltonian (7) and then using the method developed by Bardeen, Cooper, and Schrieffer (1957) in the problem of superconductivity. In the present problem the order parameter is the local magnetic moment in the antiferromagnetic phase. In both approaches the double occupancy of a space point by a spin-up and a spin-down particle is therefore of major importance. The results, however, significantly differ: the Green's-function method (Langer *et al.*, 1969; Cyrot, 1972) predicts a transition to an antiferromagnetic state for $U=0$ in the ground state for sc and bcc lattices, while in the Gutzwiller approach a finite correlation is necessary (Ogawa *et al.*, 1975; Takano and Uchinami, 1975; Florencio and Chao, 1976). The ground-state energies in the two approximations for very small correlation are given by

$$E_g/L\,|_{\rm Gutz}=-|\bar{\varepsilon}_0|+\frac{U}{4}-\frac{U^2}{64\,|\bar{\varepsilon}_0|}\,, \tag{16a}$$

$$E_g/L\,|_{\rm HF}=-|\bar{\varepsilon}_0|+\frac{U}{4}-O(e^{-|\bar{\varepsilon}_0|/U})\,, \tag{16b}$$

i.e., the Gutzwiller solution has a much lower energy. Also, the single-particle occupation numbers differ significantly: in the Gutzwiller case the momentum distribution $\langle n_{\rm k}\rangle$ has a discontinuity $q<1$ for $U>0$ at the Fermi energy. This is characteristic for an interacting Fermi system (Migdal, 1957) for which a perturbation expansion in terms of the interaction can be used (Luttinger, 1960). In the other case, however, the distribution is hardly affected at all as is typical for a BCS condensate where all relevant phenomena take place only in the very vicinity of the Fermi surface. This also has consequences for the effective mass (see below). It appears to be connected to the fact that in Gutzwiller's approach the momentum distribution is constructed by systematically building up states such that the Fermi surface always encloses the correct volume. The latter method concentrates only on the antiferromagnetic phase and hence only on the anomalous Hartree-Fock averages of the interaction term, exactly as in the BCS case. Thereby spin fluctuations, which are important in the Hubbard model, do not seem to be included sufficiently.

However, the Hartree-Fock ground state, rather than the one of the noninteracting system, can actually serve as a starting point in (8) for a considerable refinement of Gutzwiller's approach, as shown by Stollhoff and Fulde (1977). Their variational wave function even takes into account density—density-like correlations and has been successfully applied to molecules (Stollhoff and Fulde, 1977,1978,1980). The consequences for magnetic ordering in the Hubbard model have also been investigated (Oles, 1982).

D. The physical meaning of Gutzwiller's approximation

Let us finally discuss how in the rederivation of Gutzwiller's results by Ogawa *et al.* (1975) the discontinuities $q_\uparrow$ and $q_\downarrow$ are obtained.[2] This will later prove to be very useful in the understanding and identification of physical processes responsible for the structure and size of the Landau parameters. Calculating the energy expectation value of the kinetic energy in (11) due to the hopping of an ↑ particle from site j to site i, we must consider four different configurations of spins on sites i and j as shown in Fig. 2 (similarly for the hopping of ↓ particles). Note, in particular, that in the first two cases [Fig. 2(a)] the hopping process does not change the total number of doubly occupied sites D, while in the last two cases [Fig. 2(b)] this number is changed by one. Only in the latter case, therefore, does the total interaction energy UD change. These four processes can also be understood in more physical terms: the ones shown in Fig. 2(a) correspond to the motion of an empty site to the left and of a doubly occupied site to the right, respectively; therefore they represent the propagation of such objects. In Fig. 2(b), on the other hand, a doubly occupied and an empty site annihilate each other or are created, respectively; therefore these processes represent the polarization of a medium of singly occupied sites in terms of doubly occupied sites ("particles") and empty sites ("holes"). When the spin-configuration dependence of the norm $\langle\psi\,|\,\psi\rangle$ and of the energy expectation values is neglected, as in the work of Ogawa *et al.* (1975), the calculations are greatly simplified and, in fact, reduce to a mere combinatorial problem. If we classify the spin configurations by D, the number of doubly occupied sites, this then involves only N_D, the number of different spin configurations for given $L,N_\uparrow,N_\downarrow$

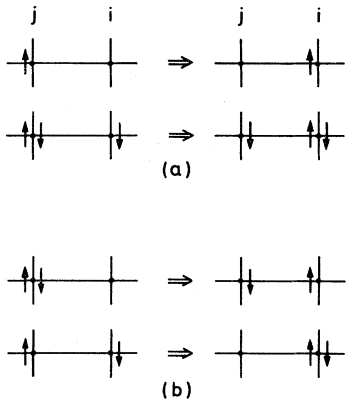

FIG. 2. The four possible hopping processes for an up-spin particle in the Hubbard model; (a) leaving the number of doubly occupied sites unchanged, (b) changing the number by one.

$$N_D(L,N_\uparrow,N_\downarrow)=\frac{L!}{(N_\uparrow-D)!(N_\downarrow-D)!D!(L-N_\uparrow-N_\downarrow+D)!}\,, \tag{17}$$

and $P(L,N_\sigma)$, the probability for a configuration of σ spins to occur (which are all equal and independent because spatial correlations are neglected):

$$P(L,N_\sigma)=n_\sigma^{N_\sigma}(1-n_\sigma)^{L-N_\sigma}\,. \tag{18}$$

Using this notation, we can cast the expectation values into the simple form

$$\langle\psi\,|\,\psi\rangle=\sum_D g^{2D}N_D(L,N_\uparrow,N_\downarrow)P(L,N_\uparrow)P(L,N_\downarrow)\,, \tag{19a}$$

$$\left\langle\psi\left|\sum_{ij}t_{ij}c_{i\uparrow}^\dagger c_{j\uparrow}\right|\psi\right\rangle=\sum_D g^{2D}[N_D(L-2,N_\uparrow-1,N_\downarrow)+g^2N_D(L-2,N_\uparrow-1,N_\downarrow-2)$$
$$+2gN_D(L-2,N_\uparrow-1,N_\downarrow-1)]P(L-2,N_\uparrow-1)P(L,N_\downarrow)\bar{\varepsilon}_\uparrow\,, \tag{19b}$$

$$\left\langle\psi\left|\sum_i n_{i\uparrow}n_{i\downarrow}\right|\psi\right\rangle=L\sum_D g^{2D+2}N_D(L-1,N_\uparrow-1,N_\downarrow-1)P(L,N_\uparrow)P(L,N_\downarrow)\,. \tag{19c}$$

The expression for the ↓ particles in (19b) is obtained by replacing ↑ and ↓.

The results are indeed plausible within the approximation scheme of neglecting spatial correlations. Take, for example, the result for the kinetic energy as given in (19b). The four contributions, corresponding to the four hopping processes shown in Fig. 2, can be obtained as follows. We take a lattice of L sites and single out the two sites between which the hopping on an ↑ spin is supposed to take place, such that there are D doubly occupied sites in the remaining lattice. The number N_D of spin configurations in this environment of the two lattice sites depends on the number of spins on these two sites. In the first process in Fig. 2(a) there is only one ↑ spin involved, so the number is $N_D(L-2,N_\uparrow-1,N_\downarrow)$, because we have taken out two lattice sites and one ↑ spin. In the second process in Fig. 2(a) there are one ↑ spin and two ↓ spins

[2]Note that in their approach q enters as a "loss factor" of the hopping energy. Only in Gutzwiller's original work does it become clear that q is the discontinuity of the momentum distribution at the Fermi energy.

missing in the surrounding environment, so the number of spin configurations is $N_D(L-2,N_\uparrow-1,N_\downarrow-2)$; and, similarly, in the processes shown in Fig. 2(b) it is $N_D(L-2,N_\uparrow-1,N_\downarrow-1)$. Furthermore, in the first case the number of doubly occupied sites of the total configuration is D in the initial and the final states, leading to a factor $g^D g^D = g^{2D}$ in the matrix elements. In the second case it is $D+1$ both initially and finally, giving a factor of $g^{D+1}g^{D+1}=g^{2D+2}$. In the last two cases the initial (final) state has $D+1$ (D) such sites and vice versa, leading to a factor of $g^{D+1}g^D = g^D g^{D+1} = g^{2D+1}$. Finally, the actual probability for finding any $\uparrow$-spin configuration in the environment of the two sites is $P(L-2,N_\uparrow-1)$. However, the probability for the $\downarrow$-spin configuration is $P(L,N_\downarrow)$, because we left this configuration untouched, letting only the $\uparrow$ spin move. As spatial correlations were neglected, the total probability is the product of both in every case. In this way one arrives at the expression shown in (19b) multiplied by the average energy $\bar{\varepsilon}_\uparrow$ of the noninteracting case. The first term corresponds to the first process in Fig. 2(a), the second to the second one in Fig. 2(a), and the third to the two (factor of 2) in Fig. 2(b).

In the thermodynamic limit ($L,N_\uparrow,N_\downarrow \to \infty$) the sums in (19) can be approximated by their largest terms, yielding a relation between g and D (Gutzwiller, 1965; Ogawa *et al.*, 1975)

$$g^2 = \frac{d(1-n_\uparrow-n_\downarrow+d)}{(n_\uparrow-d)(n_\downarrow-d)} ;$$

it is symmetric in σ.[3] Inserting (19) into (11) leads to the ground-state energy of the form shown in (12), with the discontinuities now given by

$$q_\sigma = \frac{n_\sigma-d}{n_\sigma(1-n_\sigma)}\left[(1-n_\sigma-n_{-\sigma}+d)+g^2\frac{(n_{-\sigma}-d)^2}{1-n_\sigma-n_{-\sigma}+d} + 2g(n_{-\sigma}-d)\right] \tag{20a}$$

$$= \{[(1-n_\sigma-n_{-\sigma}+d)(n_\sigma-d)\,|_0 + d(n_{-\sigma}-d)\,|_{\uparrow\downarrow}]_{\text{prop}} + [2[d(1-n_\sigma-n_{-\sigma}+d)(n_\sigma-d)(n_{-\sigma}-d)]^{1/2}]_{\text{pol}}\} \times [n_\sigma(1-n_\sigma)]^{-1} , \tag{20b}$$

where (20b) has been obtained by eliminating g.[4] The square brackets in (20b) with subscripts *prop* and *pol* refer to the contributions to q_σ from the processes shown in Fig. 2(a) [propagation of an empty site (subscript 0) and of a doubly occupied site (subscript $\uparrow\downarrow$), respectively] and Fig. 2(b) (polarization process). This way of writing permits us to keep track of the different contributions of processes contributing to the kinetic energy.

IV. THE APPLICABILITY OF GUTZWILLER'S RESULTS TO NORMAL ^{3}He

Brinkman and Rice not only realized that Gutzwiller's results predicted a transition to a localized state, they also calculated the effective mass and the static spin susceptibility (Brinkman and Rice, 1970) as well as the screening constant in the strongly correlated phase (Rice and Brinkman, 1971). Now, in the electron-phonon and paramagnon problem the discontinuity $Z_{\mathbf{k}}$ of the momentum distribution at the Fermi surface determines the mass renormalization [see, for example, Brown (1972)], i.e.,

$$Z_{k_F} = n_{k_F-} - n_{k_F+} = \left[1-\frac{\partial\Sigma}{\partial\omega}\bigg|_{E_F}\right]^{-1} , \tag{21}$$

where $\partial\Sigma/\partial\omega$ is the frequency change of the self-energy. Applying this result to the present problem, Brinkman and Rice (1970) identified Z_{k_F} and the discontinuity q and obtained

$$\frac{m^*}{m} = q^{-1} = \left[1-\left[\frac{U}{U_c}\right]^2\right]^{-1} . \tag{22}$$

Therefore, as U approaches U_c, the effective mass diverges. The spin susceptibility (see Sec. V) they obtained as (Brinkman and Rice, 1970)

$$\chi_s = \mu_0^2 N(0)\left\{\left[1-\left[\frac{U}{U_c}\right]^2\right] \times \left[1-\tfrac{1}{2}N(0)U\frac{1+U/(2U_c)}{[1+U/U_c]^2}\right]\right\}^{-1} \propto m^*/m . \tag{23}$$

So they found that the susceptibility is proportional to the renormalized mass m^*/m and therefore is enhanced

[3] As noted by Gutzwiller (1965), this expression shows that g is equivalent to the Boltzmann factor in the law of mass action, which can be obtained by the "quasichemical approximation" [see also Chao (1974)] in the theory of mixtures. In fact, this is also a first approximation for the Ising problem, showing that at least at that stage both this and the present problem are somewhat similar [Ogawa and Kanda (1978)].

[4] In fact, as d has already been determined as a function of the variational parameter g,d, rather than g, should actually be eliminated; however, as the relation between d and g is one to one, and as d can be directly interpreted, it is more sensible to use d as a variational parameter from now on.

mainly because of the effective mass m^*/m and not because of the second factor in (23). In particular, the ratio $\chi_s/(m^*/m)$ tends towards a constant at $U=U_c$, in contrast to paramagnon calculations, where this ratio diverges, because m^*/m is proportional only to the logarithm of χ_s. The divergence of the susceptibility hence is seen to be a result of the ever-increasing localization of particles carrying the spin. Investigating the static dielectric constant, Rice and Brinkman (1971) calculated the screening constant $q_s^2=(4\pi e^2/V)(dN/d\mu)$, where e, N, and μ are the electronic charge, the number of particles, and the chemical potential, respectively. Their result shows that for $U\to U_c$ $q_s^2\propto 1-U/U_c\propto(m^*/m)^{-1}$—i.e., the screening constant vanishes at $U=U_c$, and the screening length $\propto q_s^{-1}$ diverges. In terms of Landau-Fermi-liquid theory one has $(q_s/q_s^0)^2=(m^*/m)/[1+F_0^s]$, so that the Landau parameter $F_0^s\propto(m^*/m)^2$ diverges at $U=U_c$.

Anderson and Brinkman (1975,1978) suggested a connection of these results for a metal-insulator transition with the properties of normal ^{3}He. Identifying (22),(23) for m^*/m and χ_s and the respective ones in Landau theory (1), they obtained expressions for the Landau parameters F_0^a and F_1^s (note that the minus sign is missing in their equation for F_0^a):

$$1+\frac{F_1^s}{3}=\left[1-\left[\frac{U}{U_c}\right]^2\right]^{-1}, \tag{24}$$

$$F_0^a=-\tfrac{1}{4}N(0)U\frac{2+U/U_c}{(1+U/U_c)^2}\,. \tag{25}$$

They observed that these results qualitatively agreed with the experimentally determined properties of normal ^{3}He, as discussed in the Introduction.

The Hubbard model to which the Gutzwiller approach is applied treats fermions on a lattice. Normal ^{3}He, on the other hand, is a liquid, and therefore *a priori* it is not evident why this model should give even a reasonable description of liquid ^{3}He. Indeed, all other methods show that the lattice is of crucial importance to the results for the Hubbard model. Depending on the particular *type* of lattice, one obtains, at $T=0$, an antiferromagnetic state at arbitrarily small interaction (sc and bcc lattice) or above a critical value U_c (fcc lattice) (Cyrot, 1972). Those results therefore also strongly depend on the dispersion relation $\varepsilon(\mathbf{k})$, which is determined by

(i) the lattice structure, and
(ii) the character of hopping (next-neighbor or larger-range hopping).

This in turn determines the density of states. In the ^{3}He liquid there is no lattice, however. At 34.36 bars a first-order transition occurs, and the liquid solidifies, immediately forming an antiferromagnetic state in a bcc structure. Presumably, the antiferromagnetic state would have formed already at lower pressure (i.e., interaction U) but was obstructed from doing so because of the lack of lattice structure. Note, that this antiferromagnetic state is *not* due to the normal two-particle nearest-neighbor exchange mechanism as in electronic magnetic materials. Rather it appears to be of the up-up-down-down type (Osheroff, Cross, and Fisher, 1980), which can so far only be explained by three- or four-spin ring exchanges (for a review, see Roger *et al.*, 1983). Furthermore, an incipient antiferromagnetic instability of the normal ^{3}He liquid as proposed by Dyugaev (1976) has been rejected by Levin and Valls (1979b) and Aldrich and Pines (1980).

Of course, in a liquid the term "localization of particles" (where sites are only singly occupied) changes its meaning. It must rather be understood as a state where the particles want to have a maximum separation to avoid interaction. This makes a reduced compressibility as in liquid ^{3}He intuitively plausible.

The Gutzwiller variational approach is independent of all these details. As seen from Eq. (12), the only quantity appearing in the ground-state energy which does depend on the particular features of the system is $\bar{\varepsilon}_\sigma$, the average energy of the σ-spin particles in the uncorrelated state. Clearly,

$$\bar{\varepsilon}_\sigma=\tfrac{1}{2}\int_{-\infty}^{\mu_\sigma} dE\,EN(E)\,, \tag{26}$$

where μ_σ is the chemical potential of the σ-spin particles (with fixed number n_σ) and $N(E)$ is the density of states of the noninteracting system for both spins. Only in the average quantity $\bar{\varepsilon}_\sigma$ does the information enter whether the system has a lattice structure or is a liquid and how $\varepsilon(\mathbf{k})$ actually looks [see the discussion of the density of states in liquid metals by Ballentine (1975)]. Also the range of hopping of the fermions which determines $\varepsilon(\mathbf{k})$ and $N(E)$ is therefore not explicitly needed at all; it comes in via $\bar{\varepsilon}_\sigma$ and only sets the scale $U_c=8\,|\,\bar{\varepsilon}_0\,|$ for the coupling parameter U. It becomes clear that Gutzwiller's approach is therefore well suited for the study of a system without a fixed lattice structure like liquid ^{3}He (on a short scale a liquid resembles a solid in many aspects, anyway). *This method treats not only the Hubbard Hamiltonian (7) but, more generally, the Hamiltonian (3) for a contact interaction between fermions which also is assumed to be a valid model for ^{3}He.*

V. THE GUTZWILLER APPROACH AND FERMI-LIQUID THEORY

A. Changes in the ground-state energy; Landau parameters

I now want to show that Gutzwiller's result for the ground-state energy of the Hubbard model is closely connected to the concepts of Landau-Fermi-liquid theory. Therefore, the possibility of extracting Landau parameters from those results appears quite natural. The ground-state energy per particle $\tilde{E}_g\equiv E_g/L$ is given by (12). Let us assume that, without external disturbances, the equilibrium of the system was given by $n_\uparrow=n_\downarrow=\frac{1}{2}$, although this is irrelevant for the arguments to follow. If,

due to such a disturbance, the system is forced to find a new equilibrium, the ground-state energy changes by

$$\delta\tilde{E}_g=\sum_\sigma (q_\sigma\delta\bar{\varepsilon}_\sigma+\delta q_\sigma\bar{\varepsilon}_\sigma)+U\delta d \ . \tag{27}$$

On the other hand, minimization of $\tilde{E}_g$ with respect to d yields

$$\sum_\sigma \frac{\partial q_\sigma}{\partial d}\bar{\varepsilon}_\sigma+U=0 \ . \tag{28}$$

Therefore, (27) can be written as

$$\delta\tilde{E}_g=\sum_\sigma (q_\sigma\delta\bar{\varepsilon}_\sigma+\bar{\varepsilon}_\sigma\delta q_\sigma)\,|_d \ , \tag{29}$$

where $\delta\bar{\varepsilon}_\sigma,\delta q_\sigma$ imply a variation at fixed d. So the change of the particle energy is due to two separate effects:

(i) $q_\sigma\delta\bar{\varepsilon}_\sigma$, an explicit change of the particle energy, and
(ii) $\bar{\varepsilon}_\sigma\delta q_\sigma$, a change of the distribution function, characterized by a change of the discontinuity at the Fermi surface.

In this respect there is a close analogy to the concepts of Landau-Fermi-liquid theory (Baym and Pethick, 1978). There the quasiparticle energy $\varepsilon_{p\sigma}$ is given by

$$\varepsilon_{p\sigma}=\varepsilon^0_{p\sigma}+\frac{1}{V}\sum_{p',\sigma'} f_{p\sigma,p'\sigma'}\delta n_{p'\sigma'} \ , \tag{30}$$

where $\varepsilon^0_{p\sigma}$ is the quasiparticle energy in the ground state and the second term is due to the interaction of the quasiparticles reflecting the corresponding change of the quasiparticle distribution $n_{p\sigma}$. Therefore, the change of the equilibrium by some external effect leads to a change of the particle energy for the noninteracting case plus a change of the quasiparticle distribution:

$$\delta\varepsilon_{p\sigma}=\delta\varepsilon^0_{p\sigma}+\frac{1}{V}\sum_{p'\sigma'} f_{p\sigma,p'\sigma'}\delta n_{p'\sigma'} \ . \tag{31}$$

The change of the ground-state energy is then

$$\delta\tilde{E}_g=\frac{1}{V}\sum_{p\sigma}\varepsilon^0_{p\sigma}\delta n_{p\sigma}+\frac{1}{2}\frac{1}{V^2}\sum_{p\sigma}\sum_{p'\sigma'} f_{p\sigma,p'\sigma'}\delta n_{p\sigma}\delta n_{p'\sigma'} \ , \tag{32}$$

where $f_{pp'}=f^s_{pp'}+f^a_{pp'}\tau\cdot\tau'$ are spin-independent and spin-dependent parts of f_{pp}, respectively, and τ is the Pauli spin matrix. Using the usual decomposition of $f_{pp'}$ by means of Landau parameters and neglecting higher parameters than F^a_0,F^s_0, one finds

$$\delta\tilde{E}_g-\frac{1}{V}\sum_{p\sigma}\varepsilon^0_{p\sigma}\delta n_{p\sigma}=\frac{1}{2N^*(0)}[F^s_0(\delta n_\uparrow+\delta n_\downarrow)^2+F^a_0(\delta n_\uparrow-\delta n_\downarrow)^2] \ , \tag{33}$$

where $N^*(0)=(m^*/m)N(0)$ and $\delta n_\uparrow,\delta n_\downarrow$ are the variations of $n_\uparrow,n_\downarrow$ due to the change in equilibrium. The right-hand side expresses the change of the distribution in terms of "molecular fields" F^a_0,F^s_0, which parametrize the quasiparticle interaction (Leggett, 1975). The similarities between Gutzwiller's approach and Landau theory also serve as a different way of identifying q as the inverse effective mass. In Landau theory the quasiparticle energy $\varepsilon^0_{p\sigma}$ in the ground state is given by

$$\varepsilon^0_{p\sigma}=p^2/(2m^*)=(m^*/m)^{-1}\varepsilon^0_{p\sigma}\,|_{\text{bare}} \ ,$$

where the renormalized mass m^* appears. A comparison of (29) and (32) naturally lead to the identification $q=(m^*/m)^{-1}$ via the comparison of the (quasi)particle energies in the ground state. [This is similar in spirit to the discussion of Mott (1974) concerning the effective mass of current carriers in the Gutzwiller approach.] In the interacting Fermi system the discontinuity $q\le 1$ characterizes the quasiparticle contribution to the spectrum, while in Landau theory *only* quasiparticles are involved ($q=1$). It appears as if Gutzwiller's approach yields a quasiparticle description of the system where the character of those quasiparticles, however, is not yet clear.

We now want to obtain an explicit expression for $\delta\tilde{E}_g$ within the present formulation. Note that in (33) the first term of the right-hand side corresponds to a change in particle number and the second to a change in the magnetization. We define

$$\begin{aligned}\delta&\equiv\delta n_\uparrow+\delta n_\downarrow \ ,\\ m&\equiv\delta n_\uparrow-\delta n_\downarrow \ .\end{aligned} \tag{34}$$

Let us then rewrite the expression for q_σ (23) by introducing

$$\begin{aligned}n&=n_\uparrow+n_\downarrow \ ,\\ m&=n_\uparrow-n_\downarrow=\delta n_\uparrow-\delta n_\downarrow \ ,\end{aligned} \tag{35}$$

where $M=\mu_0 mL$ is the magnetization of the system. We take the half-filled band case ($n=1$) as equilibrium, i.e., $\delta=1-n$ and $0\le m\le 1$. We can then rewrite (20) as

$$q_\sigma=qf_\sigma \ , \tag{36}$$

where $q=8d(1-2d)$ and

$$f_\uparrow(\delta,m)=\frac{1}{4}\left\{\left[\left[\left(1+\frac{\delta}{d}\right)\left(1+\frac{m-\delta}{1-2d}\right)+\left(1-\frac{m+\delta}{1-2d}\right)\right]\right]_{\text{prop}}+2\left[\left(1+\frac{\delta}{d}\right)\left[\left(1-\frac{\delta}{1-2d}\right)^2-\left(\frac{m}{1-2d}\right)^2\right]\right]^{1/2}_{\text{pol}}\right\}[1-(m-\delta)^2]^{-1} \ , \tag{37}$$

and $f_\downarrow(\delta,m)=f_\uparrow(\delta,-m)$. Obviously, $f_\uparrow=f_\downarrow=1$ for $\delta=m=0$; furthermore,

$$n_\sigma=\tfrac{1}{2}\int_{-\infty}^{\mu_\sigma} dE\, N(E)\ . \tag{38}$$

For a symmetric density of states $N(E)$ the chemical potential for a half-filled band is zero and therefore $\mu_\uparrow=-\mu_\downarrow$. The ground-state energy is then given by

$$\tilde{E}_g=q\sum_\sigma f_\sigma \bar{\varepsilon}_\sigma+dU\ . \tag{39}$$

To obtain $\delta\tilde{E}_g$ we expand q and f_σ in (39) in a Taylor series up to second order in $d-d_0$, where $d_0=d(m=0,\delta=0)$. One finds

$$\tilde{E}_g=q_0\sum_\sigma f_{\sigma,0}\bar{\varepsilon}_\sigma+16(d-d_0)^2\bar{\varepsilon}_0+d_0U\ , \tag{40}$$

where q_0 and $f_{\sigma,0}$ are the respective quantities at $d=d_0$, and $\bar{\varepsilon}=\bar{\varepsilon}_\uparrow+\bar{\varepsilon}_\downarrow$, $\bar{\varepsilon}_0=\bar{\varepsilon}(m=\delta=0)$. The change of the ground-state energy is then found to be

$$\delta\tilde{E}_g=q_0\sum_\sigma(\delta f_{\sigma,0}\bar{\varepsilon}_\sigma+f_{\sigma,0}\delta\bar{\varepsilon}_\sigma)+16(d-d_0)^2\bar{\varepsilon}_0 \tag{41}$$

$$\simeq q_0\delta\bar{\varepsilon}+\tfrac{1}{2}q_0(\delta f_{\uparrow,0}+\delta f_{\downarrow,0})\bar{\varepsilon}_0+16(d-d_0)^2\bar{\varepsilon}_0\ , \tag{42}$$

where

$$\delta\bar{\varepsilon}=\frac{1}{2N(0)}(m^2+\delta^2)\ . \tag{43}$$

The first term in (42) is due to the change of the particle energy and the second one due to the change of the momentum distribution. It is clear from the symmetry of the problem that for $\delta=0$ one has $d-d_0\propto m^2$, and therefore as $f_{\uparrow,0}=f_{\downarrow,0}\equiv f_0$, $\tilde{E}_g=q_0f_0\bar{\varepsilon}+d_0U$. Let us investigate this case first.

1. $\delta=0$. Then (37) reduces to

$$f_{\uparrow,0}=f_{\downarrow,0}\equiv f_0$$

$$=\frac{1}{2}\left\{1+\left[1-\left[\frac{m}{1-2d}\right]^2\right]^{1/2}\right\}\Big/(1-m^2) \tag{44}$$

$$\simeq 1+\left[1-\frac{1}{4(1-2d_0)^2}\right]m^2\ . \tag{45}$$

Because of $d_0=(1-I)/4$, where $I\equiv U/U_c$, $\delta\tilde{E}_g$ is given by

$$\delta\tilde{E}_g=q_0\delta\bar{\varepsilon}-\frac{q_0}{2N(0)}p\left[1-\frac{1}{(1+I)^2}\right]m^2 \tag{46}$$

$$=\frac{q_0}{2N(0)}\left[1-p\left[1-\frac{1}{(1+I)^2}\right]\right]m^2\ , \tag{47}$$

with $p=2\,|\,\bar{\varepsilon}_0\,|\,N(0)$, where the first term in parentheses is due to $\delta\bar{\varepsilon}$ and the second one due to the change of the distribution function. It can therefore also be written as

$$\delta\tilde{E}_g=\frac{q_0}{2N(0)}\left[1-p\frac{\partial f_0}{\partial m^2}\bigg|_{m=0}\right]m^2\ . \tag{48}$$

The spin susceptibility is then obtained by $\delta\tilde{E}_g=M^2/(2\chi_s)$, as

$$\chi_s=\mu_0^2N(0)\frac{q_0^{-1}}{1-p\dfrac{\partial f_0}{\partial m^2}\Big|_{m=0}}\ . \tag{49}$$

This result allows for a natural comparison with the corresponding Landau expression which has an identical form and gives (Rice and Brinkman, 1971; Anderson and Brinkman, 1975)

$$F_0^a=-p\frac{\partial f_0}{\partial m^2}\bigg|_{m=0}=-p\left[1-\frac{1}{(1+I)^2}\right]\ . \tag{50}$$

Naturally, the same expression for F_0^a results by explicitly comparing (46) with the corresponding expression (33) in Landau theory. As $0\le I\le 1$, F_0^a takes the values $-\frac{3}{4}p\le F_0^a\le 0$, i.e., is always *negative.*

2. $m=0$. In this case one finds from (28) that $d-d_0=-\frac{1}{2}\delta+O(\delta^2)$, and

$$\tfrac{1}{2}q_0(\delta f_{\uparrow,0}+\delta f_{\downarrow,0})\simeq\left[4(1-4d_0)\delta-2\delta^2-\frac{1+2d_0}{2d_0}\delta^2\right](1+\delta^2)+q_0\delta^2\ , \tag{51}$$

so that

$$\delta\tilde{E}_g+\frac{U}{2}\delta=q_0\delta\bar{\varepsilon}+\frac{q_0}{2N(0)}p\left[\frac{1}{(1+I)^2}-1\right]\delta^2 \tag{52}$$

$$=\frac{q_0}{2N(0)}\left[1+p\left[\frac{1}{(1-I)^2}-1\right]\right]\delta^2\ . \tag{53}$$

We observe that $\partial\tilde{E}_g/\partial\delta=-\mu$ yields $\mu=U/2$, the exact result for the half-filled band case (Methfessel and Mattis, 1968) [this term should have actually been subtracted already in the original Hamiltonian (7)]. Using $\partial^2\tilde{E}_g/\partial\delta^2=1/\kappa$ for the compressibility or comparing (52) directly with Landau theory (33) provides us with a result for the Landau parameter F_0^s:

$$F_0^s=p\left[\frac{1}{(1-I)^2}-1\right]\ . \tag{54}$$

Note that this result is *exact* within the present approach and is therefore slightly different from the one obtained by Rice and Brinkman (1971), who only calculated to leading order in $(1-I)^{-1}$. The main qualitative feature, however, is the same: As $U\to U_c(I\to 1)$, F_0^s becomes very large and, at $I=1$, where localization occurs, diverges as the square of the effective mass.

Nevertheless, the exact result for F_0^s is of interest when F_0^a and F_0^s are compared; then one finds

$$F_0^a(U)=F_0^s(-U)\ , \tag{55}$$

i.e., the Landau parameters associated with density fluctuations (F_0^s) and spin fluctuations (F_0^a) are closely *related* and, in fact, change role when the sign of the interac-

tion is reversed. At first sight this relation is surprising, because F_0^a and F_0^s are so different in size and even sign. But it can be understood by analyzing the physical processes responsible for these molecular fields. The on-site interaction at site i in (7) can be written as (Mühlschlegel, 1965)

$$Un_{i\uparrow}n_{i\downarrow}=\frac{U}{4}[(n_{i\uparrow}+n_{i\downarrow})^2-(n_{i\uparrow}-n_{i\downarrow})^2] \ . \tag{56}$$

The first term in (56) represents density fluctuations and the second one spin fluctuations. For repulsive interaction ($U>0$) the number of doubly occupied sites is reduced for increasing U, while the opposite is true for attractive interaction. While in the first case spin fluctuations can be expected to lead to the dominant physical effects, in the second case it will be the density fluctuation. In fact, Gutzwiller's approach can be applied to both the attractive and the repulsive cases. From (15c) one finds that the ground-state energies in these two cases are related by $E_g(U)=E_g(-U)+U/2$. This is actually a rigorous result for the Hubbard model in the case of a half-filled band.[5]

B. Comparison with paramagnon results

It is interesting to note that in the limit of weak interaction, $U\to 0$, we find $F_0^s=UN_F$, $F_0^a=-UN_F$—i.e., one has $F_0^a(U)=F_0^s(-U)$ as a trivial consequence. At the same time the effective mass m^*/m, (22), has only a quadratic correction in U and therefore does not enter the expression for the susceptibility in that limit. So our results reduce to those of paramagnon theory in *lowest* (i.e., linear) order in the interaction U, leading to $\chi_s=(1-\bar{I})^{-1}$.

I now want to show that this result, correct to linear order in U, is a *general* property of a contact interaction of the sort used in (2) or (7). For this we start from the expectation value of the interaction term, written in the form of (56). In linear order one has $U\langle n_{i\uparrow}n_{i\downarrow}\rangle \simeq U\langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle = Un_\uparrow n_\downarrow$. Using the notation of (35), with $n=1-\delta$, one finds

$$U\langle n_{i\uparrow}n_{i\downarrow}\rangle \simeq \frac{U}{4}[(1-\delta)^2-m^2] \tag{57}$$

$$=\frac{U}{4}-\frac{U}{2}\delta+\frac{U}{4}(\delta^2-m^2) \ . \tag{58}$$

This expression yields the exact result for the chemical potential, $\mu=-\partial E/\partial\delta=U/2$ (Methfessel and Mattis, 1968). Comparison with (33) then leads to $F_0^s=-F_0^a=2N(0)(U/4)=UN_F$, as mentioned above.

It is important to point out that in the opposite limit, $U\to U_c$, the divergence of the spin susceptibility does not occur at $UN_F=1$, as in paramagnon theory (corresponding to a magnetic instability). Rather, the divergence of χ_s occurs at $U=U_c=2p/N_F$, where the effective mass diverges, i.e., at $UN_F=2p\simeq 2$ (because $p\simeq 1$ as will be shown in V.D).

C. The physical origin of the Landau parameters F_0^a, F_0^s

One can now show explicitly how, and due to what physical processes, the Landau parameters arise in the present formulation. At a small but finite magnetization m, the ground-state energy $\tilde{E}_g$ (40) is given by

$$\tilde{E}_g=\frac{1}{4}\left\{\left[\left[\bar{\varepsilon}_\uparrow+\bar{\varepsilon}_\downarrow+\frac{m}{1-2d_0}(\bar{\varepsilon}_\uparrow-\bar{\varepsilon}_\downarrow)\right]_0+\left[\bar{\varepsilon}_\uparrow+\bar{\varepsilon}_\downarrow-\frac{m}{1-2d_0}(\bar{\varepsilon}_\uparrow-\bar{\varepsilon}_\downarrow)\right]_{\uparrow\downarrow}\right]_{\text{prop}}\right.$$
$$\left.+2\left[1-\left[\frac{m}{1-2d_0}\right]^2\right]^{1/2}(\bar{\varepsilon}_\uparrow+\bar{\varepsilon}_\downarrow)\Big|_{\text{pol}}\right\}(1-m^2)^{-1}+d_0U \ . \tag{59}$$

First of all, we observe that in the general case of an unsymmetric density of states one has $\bar{\varepsilon}_\uparrow\neq\bar{\varepsilon}_\downarrow$, and therefore the propagation of an empty site ($[\ ]_0$) has a different kinetic energy from that of a doubly occupied site ($[\ ]_{\uparrow\downarrow}$). However, the sum of the energies is independent of this fact. In the case of a symmetric density of states, the Landau parameter F_0^a (50) is then given by

$$F_0^a=-\frac{p}{2}\frac{\partial}{\partial m^2}\left.\left(\frac{[1]_{\text{prop}}+\left[1-\left[\frac{m}{1-2d_0}\right]^2\right]^{1/2}\Big|_{\text{pol}}}{1-m^2}\right)\right|_{m=0} \tag{60}$$

$$=p\left([-\tfrac{1}{2}]_{\text{prop}}+\left[-\frac{1}{2}+\frac{1}{4(1-2d_0)^2}\right]_{\text{pol}}\right) \ . \tag{61}$$

[5] I am grateful to U. Wolff for pointing this out to me.

We observe that the propagation and polarization processes contribute quite differently to the kinetic energy and therefore to F_0^a. The propagation of empty and doubly occupied sites altogether always lead to a negative, i.e., ferromagnetic, contribution to F_0^a. [It should be noted that the results for the Hubbard model obtained by Nagaoka (1966) concerning the possibility of a ferromagnetic ground state for $U=\infty$ and $N=L\pm1$ in several finite lattices are not conclusive in the present case.] In contrast to this, the polarization effects lead to a positive, i.e., antiferromagnetic, contribution of $\frac{1}{2}p$ at small interactions ($d_0\simeq\frac{1}{4}$) and to a ferromagnetic one of $-\frac{1}{4}p$ close to the localization transition, when $d_0=0$. Qualitatively, this can be easily understood; at small interactions a polarization process costs no interaction energy and is favorable for the kinetic energy in a state of antiferromagnetic ordering. When the interaction becomes strong, however, this process becomes unfavorable and can be suppressed in a more ferromagnetic environment. As ^{3}He is always close to the localization transition, its value of F_0^a is approaching $-\frac{3}{4}p>-1$; we therefore find that the enhancement of the spin susceptibility is partly due to a ferromagnetic contribution ($F_0^a<0$), but that one is always far away from a ferromagnetic *transition*. This finding is supported by recent results of Ainsworth, Bedell, Brown, and Quader (1983) obtained from a refined version of the induced interaction model (Babu and Brown, 1973). These authors find that within the simplest model for the direct interaction of the quasiparticles, given by a zero range interaction (2), the value of F_0^a is bounded from below ($F_0^a>-0.63$) regardless of the interaction strength U. They also find that small changes of F_0^a are accompanied by large changes in F_0^s. Although they cannot obtain a value for F_0^a from this simple model which is consistent with the experimental result (in contrast to our findings) their results qualitatively agree with ours. Using the experimental values for F_0^s, F_0^a, and F_1^s the model developed by Ainsworth *et al.* (1983) allows one to calculate higher-order F_l parameters. The authors explicitly note that F_0^a is never close to -1; if it were, many of the F_l would turn out too large, in contrast to the experimental values (Greywall, 1983). Their results appear to be consistent with the notion of ^{3}He as an almost-localized system—a notion which is also implicitly contained in the most recent model approach to the quasiparticle interaction by Bedell and Ainsworth (1983).

Our formulation explicitly allows us to distinguish between a transition to a localized or to a ferromagnetic state. We find that normal ^{3}He is almost localized rather than almost ferromagnetic.

The contributions to F_0^a can be analyzed in a similar way. One finds

$$F_0^s=-p\frac{\partial}{\partial\delta^2}\left\{\left(\left[\frac{1}{2}-\frac{2\delta^2}{q_0}\right]_{\text{prop}}+\left[\frac{1}{2}-\frac{1+2d_0}{2d_0q_0}\delta^2\right]_{\text{pol}}\right)(1-\delta^2)^{-1}+\frac{4}{q_0}\delta^2\right\}\Bigg|_{\delta=0} \tag{62}$$

$$=p\left(\left[\frac{2}{q_0}-\frac{1}{2}\right]_{\text{prop}}+\left[\frac{1+2d_0}{2d_0q_0}-\frac{1}{2}\right]_{\text{pol}}-\frac{4}{q_0}\right). \tag{63}$$

For $U\to U_c$ both d_0, the number of doubly occupied sites, and q_0, the discontinuity, vanish. Equation (63) expresses the fact that the dominant divergent term contributing to F_0^s is given by $(1+2d_0)/(2d_0q_0)$, arising from the spin fluctuation process shown in Fig. 2(b), i.e., a polarization process. As $U\to U_c$, such processes are of dominant importance, because they become more and more disadvantageous. In a charged system, this explains the vanishing of the screening constant q_s in this limit (Rice and Brinkman, 1971); the screening length diverges—there is no screening any more because polarization of the medium is too costly in energy. In the present case, the polarization processes give rise to the term $1/(1-I)^2$ in F_0^s, which measures the sensitivity of the system's energy to density fluctuations, and which leads to a strongly decreased compressibility.

D. Quantitative results

In order to get a quantitative estimate of the results for F_0^a and F_0^s we proceed as follows: First of all, we calculate $p=2\,|\,\bar{\varepsilon}_0\,|\,N(0)$ within some reasonable model for the density of states $N(E)$ of the uncorrelated system. For a tight-binding band, $N(E)$ can be approximated by Hubbard's half-ellipse (Hubbard, 1963, 1964) for most purposes:

$$N(E)=\frac{8}{\pi\Delta}\left[1-\left[\frac{E}{\Delta/2}\right]^2\right]^{1/2}, \tag{64}$$

where Δ is the total width of the band. Using this expression, we find $N(0)=8/\pi\Delta$, $|\,\bar{\varepsilon}_0\,|=2\Delta/3\pi$ and therefore

$$p=\frac{32}{3\pi^2}\simeq1.08\,. \tag{65}$$

With the exact density of states for nearest-neighbor hopping on a simple cubic lattice one obtains about the same value, while for a square-shaped form [$N(E)=2/\Delta$, for $|\,E\,|\le\Delta/2$] $p=1$ exactly. It is not hard to see that for any form of $N(E)$ which is symmetric and somehow resembles (64), p is always approximately given by $p\simeq1$. This has a very interesting consequence for F_0^a, because for $U\to U_c$ one finds

$$\lim_{U\to U_c}F_0^a=-\tfrac{3}{4}p\,. \tag{66}$$

So F_0^a not only stays constant for $U\to U_c$ (as found in the

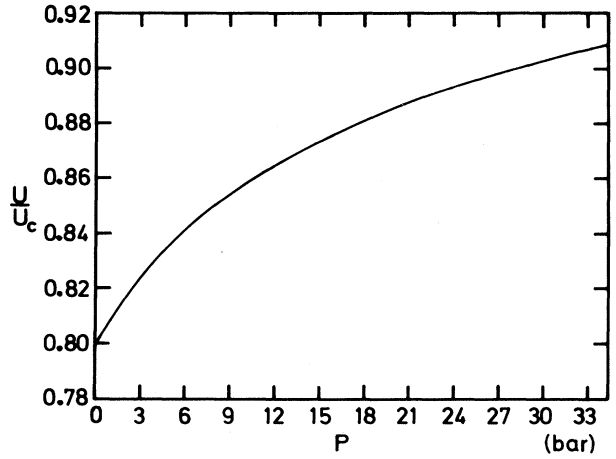

FIG. 3. The pressure dependence of the scaled interaction parameter U/U_c for normal ^{3}He.

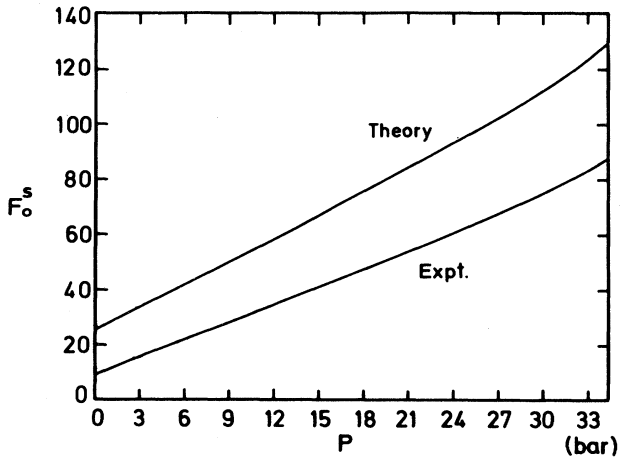

FIG. 5. The Landau parameter F_0^s for normal ^{3}He as calculated, in comparison with the experimentally obtained values (Greywall, 1983).

experiment) but, in fact, approaches a value within a few percent of the one experimentally measured. Using the relation

$$\frac{m^*}{m}=1+F_1^s/3=\frac{1}{1-I^2}\ , \tag{67}$$

we find

$$I\equiv\frac{U}{U_c}=(1+3/F_1^s)^{-1/2}\ . \tag{68}$$

As the Landau parameter F_1^s is experimentally known as a function of pressure, we thereby find the actual pressure dependence of the interaction parameter $I(P)$, which is shown in Fig. 3. We see that at $P=0$, $I\simeq 0.8$ and at melting pressure ($P=34.36$ bars) $I\simeq 0.9$—i.e., the interaction parameter varies like $0.8\lesssim I\lesssim 0.9$ as pressure is changed. This means that at all pressures one is rather close to the transition $I=1$. Note that the solidification of liquid ^{3}He occurs at an interaction strength $U<U_c$, where the number of doubly occupied sites is very small ($d=0.025$–0.05) but still finite. Localization and solidification are hence not identical. This is not surprising, because even in a solid there are interstitials and vacancies—particularly so in a quantum solid such as solid ^{3}He (Andreev and Lifshitz, 1969). Furthermore, the "localization" of particles in a liquid implies that they want to keep apart as much as possible: this is then a first step towards solidification into a crystalline structure (Kirzhnits and Nepomnyashchii, 1971), which in the case of ^{3}He sets in by a first-order transition.

The pressure dependence of U/U_c now permits us to plot the pressure dependence of F_0^a, F_0^s according to expressions (50) and (54); using p given in (65), they are shown in Figs. 4 and 5 in comparison with the actually

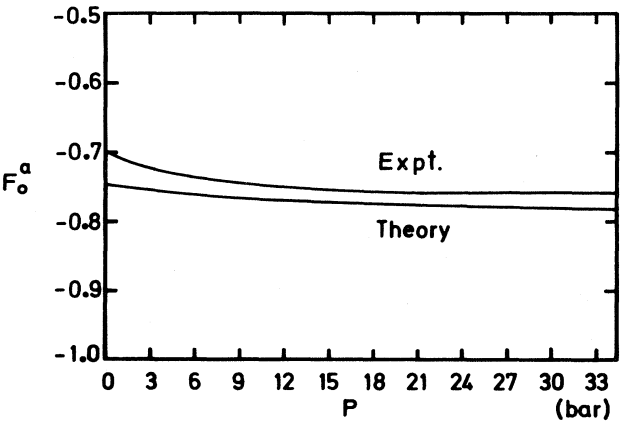

FIG. 4. The Landau parameter F_0^a for normal ^{3}He as calculated, in comparison with the experimental values (Greywall, 1983).

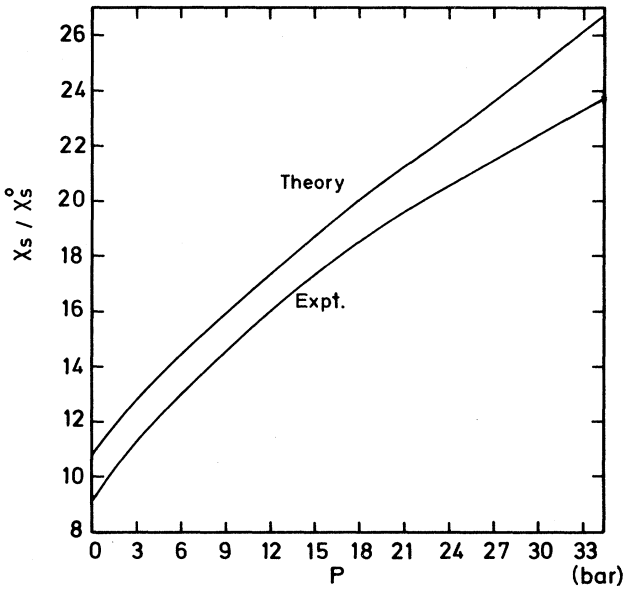

FIG. 6. The normalized spin susceptibility of normal ^{3}He as calculated, compared with the experimental values (Greywall, 1983).

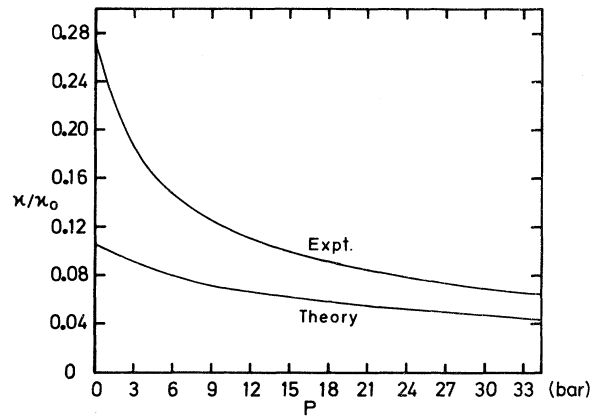

FIG. 7. The normalized compressibility of normal ^{3}He as calculated, in comparison with the experimentally obtained values (Greywall, 1983).

measured values (Greywall, 1983). While for F_0^s there is only a qualitative agreement (the shapes of the curves are very similar, and F_0^s is large and positive), the pressure dependence of F_0^a agrees with the experimental one at all pressures within a few percent. Using the results for F_0^a and F_0^s, we can calculate the spin susceptibility χ_s/χ_s^0 and the compressibility κ/κ^0 as given by (1). The results are shown in Figs. 6 and 7. Only the effective mass expression has been fitted to obtain the pressure dependence of I; besides that, essentially no other parameter has to be adjusted. In view of this fact, the agreement with the experimental points is indeed remarkable.

The fact that F_0^a approaches the value $-\frac{3}{4}p$, $p\simeq 1$, finds an interesting analog in the results of Castaing (1980). He showed that *if* (for any unknown reason) normal ^{3}He could be described by a set of two-level systems, such that ↑ spins and ↓ spins had different energies, then F_0^a should tend towards a limiting value $F_0^a=-\frac{3}{4}$ as pressure is increased, i.e., as the solid is approached. Just as in Gutzwiller's approach spin correlations are neglected in his model.

E. Landau parameter F_1^a

The remarkable quantitative agreement between theory and experiment concerning F_0^a leads to a possible extension of the results: the calculation of one more Landau parameter, namely, F_1^a, involved in spin currents. Little is known about F_1^a, because there is no exact relation of it to a measurable quantity, as in the case of F_0^a, F_0^s, and F_1^s, and therefore even its measurement is rather indirect (Greywall, 1983). To obtain an expression for F_1^a we use the forward-scattering sum rule for Landau parameters

$$\sum_{l=0}^{\infty}(A_l^s+A_l^a)=0\ . \tag{69}$$

Keeping only Landau parameters with $l<2$ [which is equivalent to the s-p approximation (Dy and Pethick, 1969) and which is known to be in good agreement with experimental data at least at low pressures (Baym and Pethick, 1978)], allows us to obtain an analytic result for F_1^a. In this approximation we have

$$F_1^a=-\left\{\left[\left[\left(\frac{1}{F_0^s}+1\right)^{-1}+\left(\frac{1}{F_0^a}+1\right)^{-1}+\left[\frac{1}{F_1^s}+\frac{1}{3}\right]^{-1}\right]^{-1}+\frac{1}{3}\right\}^{-1}. \tag{70}$$

We observe two points:

(i) the merely qualitative agreement between the result for F_0^s and the experiment is quite unimportant here, because F_0^s is large and positive and therefore $1/F_0^s$ is small in any case, and

(ii) the above expression for F_1^a can depend only on I^2, because $F_0^a(I)=F_0^s(-I)$ and $F_1^s=3I^2/(1-I^2)$.

We find

$$F_1^a=-3I^2\frac{B+\frac{2}{3}pA}{B(1+I^2)+\frac{2}{3}pA}\ , \tag{71}$$

where $A=-1+(4-I^2)(1-p)$, $B=[1+I^2(1-p)]^2-4I^2(1-p)^2$. It is interesting to note that the case $p=2\,|\,\bar{\varepsilon}_0\,|\,N(0)=1$ proves to be a special one. In this case $A=-1$, $B=1$, and one obtains

$$F_1^a\,|_{p=1}=-\frac{3I^2}{3+I^2}\ , \tag{72}$$

while

$$F_0^a\,|_{p=1}=-\frac{I(2+I)}{(1+I)^2}\ .$$

In both cases these Landau parameters have the limiting value $-\frac{3}{4}$ as $U\to U_c$. In general, however, $p\neq 1$ although, as argued above, it is always close to one. Setting $1-p=\varepsilon$, we expand to first order in ε and obtain

$$F_1^a=-\frac{3I^2}{3+I^2}\left[1+\frac{6(5+I^2)}{3+I^2}\varepsilon\right]+O(\varepsilon^2)\ . \tag{73}$$

The prefactor of the first-order correction term is always between 9 and 10, i.e., is large. This has the consequence that the pressure dependence of F_1^a depends extremely sensitively on the size and sign of ε, particularly at higher pressures (where the s-p approximation is not very good, anyway). To obtain a quantitative result for F_1^a using (71) we have to make a particular choice for p. We find that only the case $\varepsilon=1-p\leq 0$ is able to reproduce the experimentally determined behavior (Greywall, 1983) $F_1^a<0$, $\partial F_1^a/\partial p<0$ ($\varepsilon=0$ is already sufficient for that). In that case we find $F_1^a=-0.53$ at $P=0$ decreasing to $F_1^a=-0.65$ at melting pressure. However, as a small change of ε from, say, 0.01 to -0.01, already produces a large change in the pressure dependence of F_1^a, (71) and (72) should not be used beyond the qualitative result that for $U\to U_c$ F_1^a approaches a constant value, as does F_0^a.

VI. BEHAVIOR AT HIGH MAGNETIC FIELDS

A. Magnetization curves

The calculation of the static spin susceptibility by means of the Gutzwiller approach to the Hubbard model and the correspondence between these results and Landau theory as analyzed above involve only small deviations from the paramagnetic, half-filled band case ($m=0$, $n=1$). Initiated by the observation of Anderson and Brinkman (1975, 1978) concerning the qualitative agreement between the results of this approach and the properties of normal ^{3}He, we have seen that in the case of χ_s, involving the magnetization of the liquid, there is even quantitative agreement. In any case, Gutzwiller's result for the ground-state energy appears to allow for a description of ^{3}He in qualitative agreement with the basic experimental facts. Furthermore, these results are not *a priori* limited to small fields and magnetizations, but are, in fact, applicable to arbitrary magnetization. Therefore, they open the possibility to study the high-field magnetization behavior of the Hubbard model and thereby of liquid ^{3}He, going beyond the linear regime where $M=\chi_s H$. No other simple, theoretical method exists so far which is able to reproduce the low-field results for normal ^{3}He and which, in addition, allows for a straightforward extension to higher fields. It is therefore our aim to calculate the magnetization curves $m(H,U)$ for arbitrary magnetic fields H and interaction strengths U. From the success of the low-field results, we expect them to describe normal, liquid ^{3}He.

For this we proceed as follows: We start from Gutzwiller's expression for the ground-state energy (39), which can be written as ($n=1$)

$$\tilde{E}_g = qf\bar{\varepsilon} + dU \,, \tag{74}$$

where $q=8d(1-2d)$ and f is given by (44). Using the density of states (64) and (35), we find the magnetization m and average energy $\bar{\varepsilon}$ to be given by

$$m=\frac{2}{\pi}[\bar{\mu}(1-\bar{\mu}^2)^{1/2}+\sin^{-1}\bar{\mu}] \,, \tag{75}$$

$$\bar{\varepsilon}=\bar{\varepsilon}_0(1-\bar{\mu}^2)^{3/2} \,, \tag{76}$$

where $\bar{\mu}=2\mu/\Delta$ and μ is the shift in chemical potential due to the magnetic field ($\mu_\uparrow=-\mu_\downarrow\equiv\mu$, because the equilibrium chemical potential is zero). Eliminating $\bar{\mu}$, we obtain $\bar{\varepsilon}$ as a function of m.

The expression for the ground-state energy can then be written as

$$\tilde{E}_g/|\bar{\varepsilon}_0| = -4d(1-2d)(1+W)F+8dI \,, \tag{77}$$

where

$$W=\left[1-\left[\frac{m}{1-2d}\right]^2\right]^{1/2} \,, \qquad F=\frac{(1-\bar{\mu}^2)^{3/2}}{1-m^2} \,. \tag{78}$$

Minimizing this equation with respect to d yields an

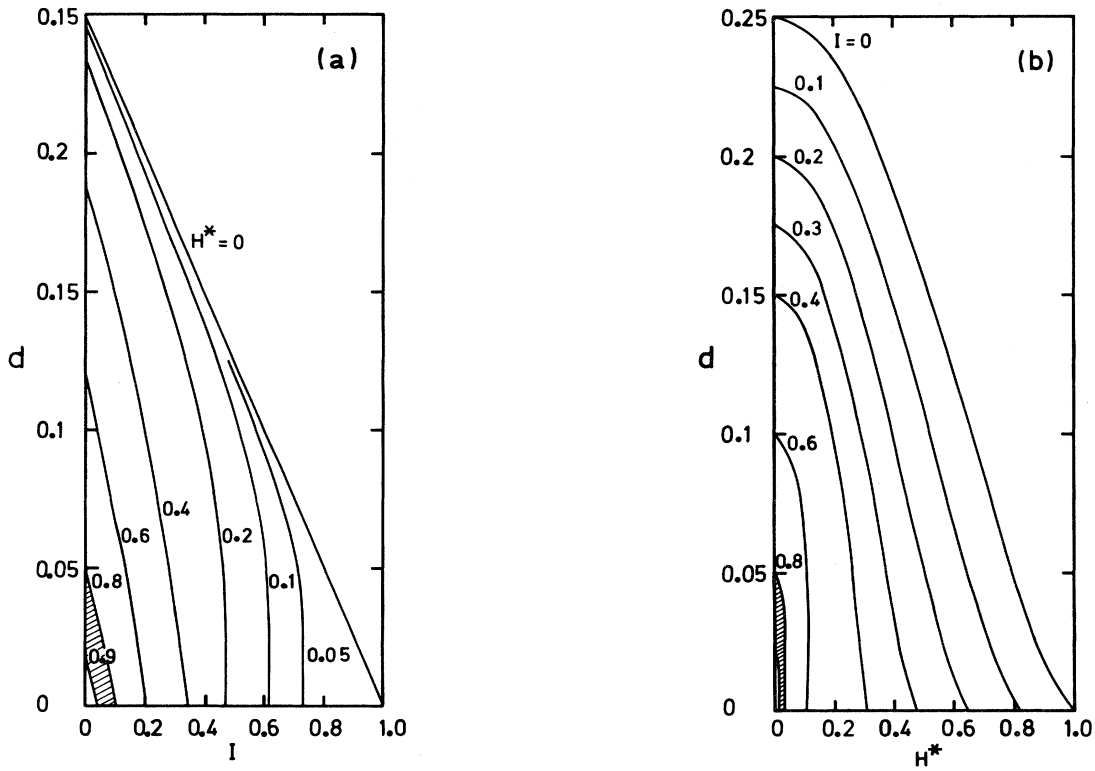

FIG. 8. (a) The number of doubly occupied sites, d, as a function of the interaction I for constant values of the magnetic field H^*; (b) d, as function of H^* for constant I. (The shaded areas apply to normal ^{3}He.)

equation for d:

$$I=\tfrac{1}{2}F\left[(1-4d)(1+W)-\frac{m^2}{1-2d}\right]\Big/W\,. \tag{79}$$

The magnetic field H leading to a magnetization $M=\mu_0 Lm$ is obtained from the ground-state energy by

$$\frac{\partial E_g}{\partial M}=H\,, \tag{80}$$

which leads to

$$H^*=\frac{4d(1-2d)}{1-m^2}\left[\bar{\mu}(1+W)-\frac{8}{3\pi}mF\left[1+W-\frac{1}{2}\frac{1-m^2}{(1-2d)^2W}\right]\right], \tag{81}$$

where $H^*=2\mu_0 H/\Delta$. Fixing $I=U/U_c$, we choose a value for $0\le m\le 1$, calculate $\bar{\mu}$ via (75) and then solve (79) for d. This value is inserted into (81) to obtain $H^*=H^*(m,I)$. By inversion we find $d=d(H^*,I)$, the number of doubly occupied sites as shown in Figs. 8(a) and 8(b) [as well as the magnetization curves $m=m(H^*,I)$ shown in Figs. 10–12].

We see that the magnetic field H^* and the on-site repulsion I have similar effects on the system: both reduce the number of doubly occupied sites and thereby drive it towards a localized state where the particles maintain the maximally possible separation between each other. The magnetic field turns the spins around so that due to the Pauli principle fewer and fewer sites will be doubly occupied. In the limit $m=1$ spins of only one species exist, and therefore one finds $d=0$, as is evident from the relation $d\le n_\uparrow n_\downarrow=\frac{1}{4}(1-m^2)$. Note that in the uncorrelated case ($U=0$), q, the discontinuity of the distribution function at the Fermi energy, is always given by $q=1$, irrespective of the field. In this case the localization, characterized by $d=0$, is not due to a divergence of the effective mass, but because the average energy $\bar{\varepsilon}=\bar{\varepsilon}_0(1-\bar{\mu}^2)^{3/2}$ goes to zero (because $\bar{\mu}\to 1$). Only at *finite* interaction strength does a magnetic field have an effect on q, i.e., on the effective mass m^*/m, as will be discussed in the end of this section. As H^* and I aid each other in suppressing d, the critical interaction strength for which $d=0$—i.e., where the system localizes—depends on H^* and vice versa, as shown in Fig. 9. As liquid ^{3}He is strongly correlated ($0.8<I<0.9$), relatively small values of H^* are necessary for that, because the number of doubly occupied sites is small already and therefore the effective mass is large. This becomes even more evident from the magnetization curves $m(H^*,I)$ in Fig. 10, where m is shown as a function of H^* for fixed I. For $I<0.44$ the magnetization continuously increases with increasing magnetic field; for $I>0.44$, however, there is a critical field at which the system magnetizes completely via a transition of first order. At this point d and m discontinuously go to their limiting values $d=0$, $m=1$. As mentioned earlier $P=0$ corresponds to $I=0.80$ and $P=34.36$ to $I=0.91$; in the first case the critical field is $H^*=0.03$, while in the second case $H^*=0.008$. For reasons of clarity I show this portion of Fig. 10, which is relevant for liquid ^{3}He, on a larger scale in Fig. 11. The magnetization starts linearly ($M=\chi_s H$) and then its slope increases dramatically. Finally, in Fig. 12 m is shown as a function of the interaction, i.e., the pressure, at constant magnetic field. Increasing the pressure also increases the magnetization and can even induce a first-order transition to a fully magnetized and hence localized state. Note that any kind of antiferromagnetic state (which is energetically unfavorable anyway because of the lack of lattice periodicity in liquid ^{3}He) will be suppressed by the external magnetic fields. In terms of actual magnetic fields, H^* corre-

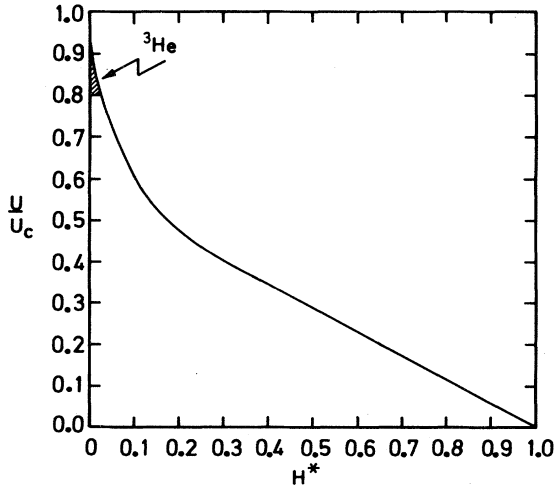

FIG. 9. The critical line U/U_c vs H^* where d vanishes. The shaded area applies to normal ^{3}He.

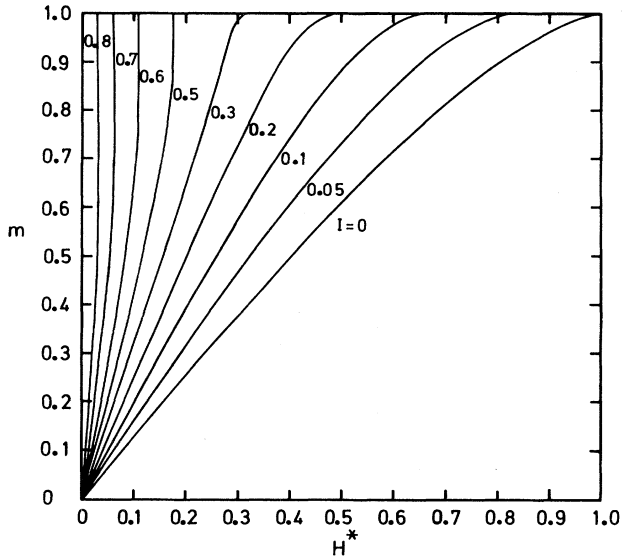

FIG. 10. The magnetization curves m as a function of the magnetic field H^* for constant interaction I.

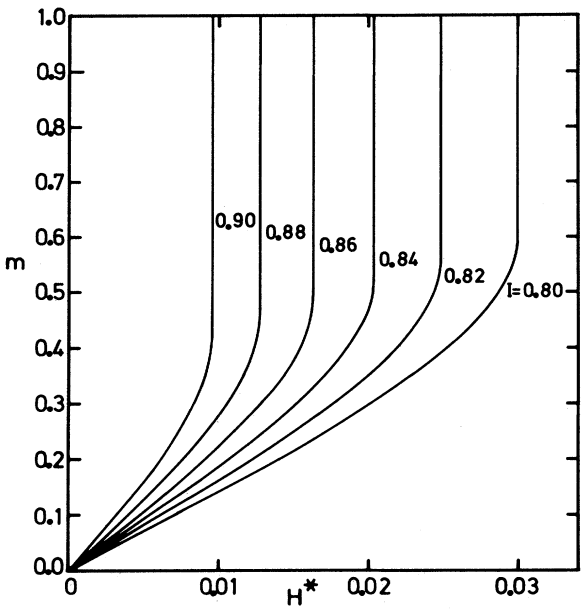

FIG. 11. Enlarged portion of Fig. 10 relevant for normal ^{3}He.

sponds to

$$H=\frac{\Delta/2}{\mu_0}H^*\simeq\frac{E_F^0}{\mu_0}H^* , \tag{82}$$

where E_F^0 is the Fermi energy of the uncorrelated system. The prefactor is approximately given by $E_F^0/\mu_0\simeq 9.88\times 10^{-16}/a^2$ (T), where $a=(N/V)^{1/3}$ is the interparticle distance in Å (Wheatley, 1975). Therefore, $E_F^0/\mu_0\simeq 6.37\times 10^3$ T at $P=0$ and 8.11×10^3 T at melting pressure. For $I=0.9$ ($P\simeq 27$ bars) we find that a field of 2.3 T leads to a magnetization of 1%, while at 7.3 T it is 3%. These results for the magnetic field dependence of liquid ^{3}He, obtained from an absolute scale for the magnetic field and where only the effective mass has been taken from experiment, agree with those measured by Chapellier *et al.* (1979) and and Thoulouze *et al.* (1980).

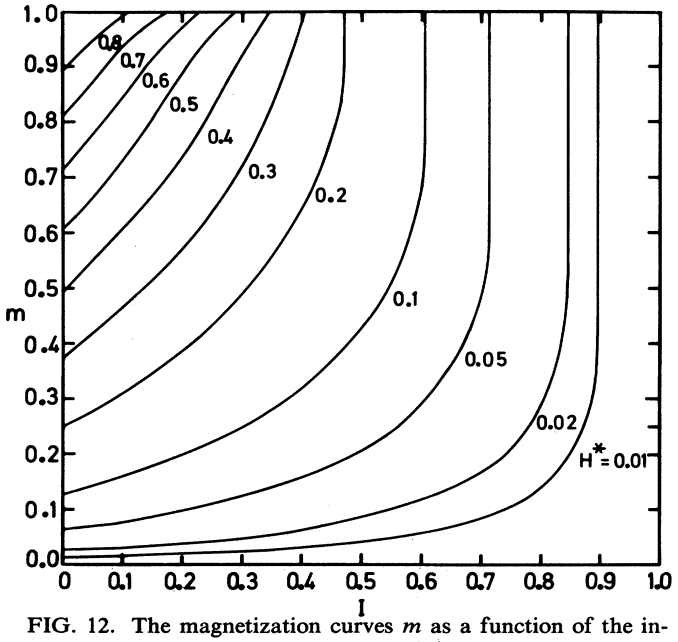

FIG. 12. The magnetization curves m as a function of the interaction I for constant magnetic field H^*.

B. The nonlinear susceptibility

The linear relation between M and H is valid only for $H^*\ll 1$. Let us now calculate the deviations from linearity as H^* increases, i.e., higher-order corrections in H^* to the spin susceptibility $\chi_s(H^*,I)$. For this we write

$$\chi_s(H^*,I)\simeq\chi_s+c(I)H^{*2} , \tag{83}$$

where $\chi_s=\chi_s(0,I)$. The calculation of $c(I)$ is straightforward but tedious, and the result will not be reproduced here. One finds ($\gamma\equiv m^*/m_{\rm bare}$)

$$c(I)\propto\gamma\chi_s^3 , \tag{84}$$

i.e., a very large prefactor for the lowest-order correction to χ_s, essentially proportional to the fourth power of the already large zero-field effective mass. This explains why the magnetization curves become even steeper rather than flatter beyond the linear regime and why the transitions to a fully magnetized state occur at such small H^*. Indeed, this fact can be expressed by a scaling relation, valid close to the transition:

$$\chi_s(H^*,I)\propto\left[\frac{H^*}{H_c}\right]^2 , \quad H_c=(1-I^2)^2 . \tag{85}$$

This is in contrast to paramagnon theory (Béal-Monod, 1982), where one finds $c(I)\propto(1-\bar{I})^{-4}\propto\chi_s^4$—i.e., there $c(I)$ is proportional to the fourth power of the zero-field susceptibility (the Stoner enhancement factor). As already discussed in detail, we find that it is the effective mass which leads to the strong enhancement of the susceptibility rather than the vicinity of a ferromagnetic state.

C. Influence on the melting curve

The magnetization curves now allow us to estimate the change in melting pressure due to a magnetic field [see the detailed discussion of this point by Castaing and Nozières (1979)] by the thermodynamic relation

$$\left.\frac{\partial P}{\partial H}\right|_T=\frac{M_L-M_s}{v_L-v_s} , \tag{86}$$

where $M_{L,S}$ and $v_{L,S}$ are the magnetization and molar volume of the liquid and the solid, respectively. At high fields ($H\gtrsim 20$ T) the solid will be almost fully polarized, $M_s\simeq\mu_0 N$,[6] so that the change in melting pressure is given

[6]Already at $H=7$ T the magnetization of the solid has reached almost 80% (Roger *et al.*, 1983).

by the differential equation

$$\Delta v \frac{dP}{dH} = -\mu_0 N[1-m(H,P)] \ . \tag{87}$$

Here $\Delta v \simeq 1.2$ cm^3 is the change in molar volume (we neglect the small effect of magnetostriction) and $N=6\times 10^{23}$ atoms/mole. In dimensionless units (87) reads

$$\frac{dP}{dH^*} = -\frac{N}{\Delta v} E_F^0(P)[1-m(H^*,P)] \ . \tag{88}$$

To estimate its solution this equation has been solved numerically by using approximate analytic functions for $m(H^*,P)$ and $E_F^0(P)$, assuming that the relation between U and P, as shown in Fig. 3, roughly holds even at finite magnetic fields. The maximum change in melting pressure is then found to be

$$\Delta P_{\max} = -3.4 \text{ bars} \ .$$

Therefore, the melting pressure at $T=0$ is lowered from $P_{\text{melt}}^{H=0}=34.4$ bars to $P_{\text{melt}}^{H}=31$ bars. However, the resulting curve in zero field has a minimum of $P_{\min}\simeq 29.4$ bars at $T=0.32$ K [see, for example, Greywall (1983)], because at very low temperatures ($T \ll T_F$) the entropy of the liquid, S_L, decreases linearly with temperature, becoming smaller than that of the solid, $S_s = N \ln 2$ (Pomeranchuk, 1950). We then find that this minimum almost vanishes, as was anticipated (Castaing and Nozières, 1979; Lhuillier and Laloe, 1980). In fact, the minimum must disappear completely at very high fields, because the spin entropy of the polarized solid is zero (Castaing and Nozières, 1979). This is not the case here, indicating that the calculated magnetization curves $m(H^*,I)$, Fig. 11, as a function of P are slightly too steep close to H_c, where the liquid becomes totally polarized. It can be understood as being due to the approximation used, in which the kinetic energy of the particles in the totally polarized system is strictly zero. On the other hand, improvements in this point do not lead to drastic changes of the results. To show this, I have, for comparison, calculated the drop in melting pressure if the magnetization curve kept on going up *linearly* with magnetic field until full magnetization is realized. In this case one finds $\Delta P_{\max} = -12.6$ bars. So the melting pressure of the totally polarized liquid is at any rate larger than zero. The above finding is in essential agreement with the result of Castaing and Nozières (1979), who obtain $\Delta P_{\max}\simeq -7$ bars *assuming* liquid ^{3}He to be "solidlike" and those suggested by the refined induced interaction model due to Bedell and Quader (1983).

D. The effective mass

Finally, we can calculate the change of the effective mass $q^{-1}=\gamma$ due to a magnetic field, i.e., $\gamma(H^*,I)-\gamma(0,I)$. For electronic systems with an enhanced Pauli spin susceptibility such a calculation has been performed by Hertel, Appel, and Fay (1980), who considered the magnetic field dependence of the electron-paramagnon interaction within a two-parameter paramagnon model [see also the review of Béal-Monod (1982)].

For magnetizations $m \ll 1$ q can be written as

$$q=(1-I^2)[1-Q(I)m^2] \ , \tag{89}$$

and therefore

$$\gamma(H^*,I)-\gamma(0,I)=\gamma(0,I)Q(I)m^2 = \gamma(0,I)Q(I)\chi_s^2 H^{*2} \ , \tag{90}$$

where $\gamma(0,I)=(1-I^2)^{-1}$. For $Q(I)$ one obtains

$$Q(I)=-\frac{2I^2}{1-I^2}\left[\frac{1}{2}-\frac{1}{p}+\frac{1}{(1+I)^2}\right] , \tag{91}$$

and so the change in effective mass is given by

$$\gamma(H^*,I)-\gamma(0,I) \propto [\gamma(0,I)\chi_s]^2 H^{*2} \ , \tag{92}$$

i.e., it is essentially proportional to the fourth power of the zero-field effective mass. This is again different from paramagnon theory (Béal-Monod, 1982), which calculates this quantity via the temperature dependence of the spin susceptibility and finds that $\gamma(H^*,I)-\gamma(0,I) \propto \chi_s^3 H^2$, the prefactor being proportional to a third power of the Stoner enhancement factor. Although this magnetic field dependence, in absolute terms, is still rather weak, we find that the effective mass is affected much more strongly by a magnetic field than previously assumed. At $I=0.9$ ($P\simeq 27$ bars) we find that $\gamma(H^*,I)/\gamma(0,I)$ is enhanced by about 0.75% at 17.6 T and by 1.4% at 23.2 T.

It should be remarked that $Q(I)$ in (90) has a peculiar dependence on I: For $I \lesssim 0.5$ one finds $Q<0$—i.e., the effective mass decreases for increasing magnetic field and only for $I>0.5$ (as is the case for ^{3}He) $Q>0$, indicating an increase of the effective mass. The sign of the change in effective mass is hence seen to depend on the strength of correlation I. This might explain why in some substances like Pd or $LuCo_2$, whose susceptibility enhancement is not as large as that of normal ^{3}He (where I is therefore smaller), this change is, in fact, negative (Béal-Monod, 1982). Such a lowering of the electronic effective mass in a strong magnetic field has also been found in the work of Hertel *et al.* (1980) who apply their results to UAl_2.

Very interesting predictions for the effective mass of fully polarized ^{3}He have recently been made by Bedell and Quader (1983) and Bedell (1983). Based on the induced interaction model (Babu and Brown, 1973; Ainsworth *et al.*, 1983) these authors calculated the effective mass and transport properties of a fully polarized system, in which spin fluctuations and singlet scattering are frozen out. They find a strong depression of m^*/m to about 0.8.

VII. DISCUSSION

We have seen that Gutzwiller's variational approach (Gutzwiller, 1963–1965) to the Hubbard model goes beyond the lattice aspects of this model. More generally, it treats a Hamiltonian for a contact interaction between fermions, which is assumed to be a valid model for normal ^{3}He. Its results are in good qualitative and—in the

case of the spin susceptibility—even quantitative agreement with the static properties of normal ^{3}He. For this agreement only the pressure dependence of the interaction strength U/U_c has to be determined; in principle, no other adjustable parameter is necessary to describe the spin susceptibility and the compressibility. The present formulation allows one to distinguish between a localization transition, where m^* diverges, and a magnetic instability, where $F_0^a \to -1$. We find that while m^* does diverge at a critical interaction U_c, the Landau parameter F_0^a approaches a constant value $-\frac{3}{4}p$—i.e., the ferromagnetic transition is never close. Furthermore, we have found that spin fluctuations are important but that they are only a secondary effect, the primary effect being the localization of the particles at $U=U_c$. It has been shown that, at all pressures, ^{3}He is always close to this localization transition: $0.8 \lesssim U/U_c \lesssim 0.9$. A truly localized state is never reached, however. Solidification takes place before that, at $U \simeq 0.91 U_c$. In view of these facts, normal ^{3}He should be considered almost localized.

This property becomes particularly evident in the case of high magnetic fields. The magnetization depends very strongly on the field, bending upward beyond the linear regime. This is due to the large zero-field effective mass. We found the melting pressure at $T=0$ to be only weakly reduced. Therefore, the fully polarized liquid still has a finite melting pressure.

Finally, it is interesting to note that the half-filled band case ($n=1$) is a very special one. Only for $n=1$ (equal number of particles and sites) does the transition to a localized state (with $d=0$) occur at *finite* $U=U_c$. In all other cases an infinite U is necessary for that (Gutzwiller, 1965); in fact, for large $I=U/U_c$ and $\delta=1-n \ll 1$ one finds $d \propto \delta/I^2$. This can easily be verified by means of (37) and (39), which then contains terms of the kind $\delta/\sqrt{d}$. Taken by itself, this fact is unimportant for our intentions because it would only rescale U. More importantly, however, in this case the discontinuity q never vanishes, so that the effective mass $m^*/m = q^{-1}$ approaches a constant for $d=0$, namely, $m^*/m = (1+\delta)/2\delta$. This implies a very sensitive dependence of the possible values that m^*/m can assume on δ, the deviation from $n=1$. (For m^*/m to reach a value of 6, δ may not be larger than $\delta=\frac{1}{12}$.) This is interesting, because changing n can be interpreted as a change of the particle density, i.e., the interparticle separation (smaller n means fewer particles per lattice constant). In this sense one realizes that the maximum value of m^*/m is very sensitive to a change in the filling factor n, i.e., density, of the system: for $n=0.8$ this maximum value is $m^*/m=3$ and for $n=0.5$ only $m^*/m=1.5$. There is a certain arbitrariness in choosing $n=1$ to describe liquid ^{3}He: as there is no lattice, this choice appears natural but might not be imperative. In particular, in the case $n=1$ the kinetic energy of the particles is reduced to zero in the fully magnetized state $m=1$. This is too strong a limitation on the energy and the particle motion and can be avoided by working with $n<1$.

In the Hubbard model the particles are considered to be pointlike, so that any finite-size effects (obstruction of the movement of particles other than for reasons of spin) are neglected. On the other hand, in a system as dense as liquid ^{3}He these effects (leading to back flow, etc.) will be as important for dynamical properties as they are in solid ^{3}He (Roger *et al.*, 1983). Apart from the repulsive contact interaction there is also an attractive van der Waals interaction. This could be treated by means of the extended Hubbard model (Beni and Pincus, 1974) containing an attractive next-neighbor interaction. These points and their consequences for the Landau parameters and the magnetization behavior are presently under investigation.

ACKNOWLEDGMENTS

I wish to thank Peter Wölfle for many fruitful and stimulating discussions; also, I gratefully acknowledge useful discussion—at various stages of the work—with M. C. Cross, D. Fay, P. Fulde, W. Gasser, W. Götze, R. J. Jelitto, H. A. Razafimandimby, T. M. Rice, and U. Wolff (who also introduced me to our computer). The final draft of this paper was written during a stay at Bell Laboratories. I wish to thank everybody for the kind hospitality extended to me on that occasion.

REFERENCES

Ainsworth, T. L., K. S. Bedell, G. E. Brown, and K. F. Quader, 1983, J. Low Temp. Phys. **50**, 319.
Anderson, P. W., 1963, Solid State Phys. **14**, 99.
Anderson, P. W., and W. F. Brinkman, 1973, Phys. Rev. Lett. **30**, 1108.
Anderson, P. W., and W. F. Brinkman, 1975, "Theory of anisotropic superfluidity in He," in *The Helium Liquids,* edited by J. G. M. Armitage and I. E. Farqhar (Academic, New York), p. 315.
Anderson, P. W., and W. F. Brinkman, 1978, in *The Physics of Liquid and Solid Helium, Part II,* edited by K. H. Bennemann and J. B. Ketterson (Wiley, New York).
Andreev, A. F., and I. F. Lifshitz, 1969, Zh. Eksp. Teor. Fiz. **56**, 2057 [Sov. Phys.—JETP **29**, 1107 (1969)].
Babu, S., and G. E. Brown, 1973, Ann. Phys. **78**, 1.
Ballentine, L. E., 1975 in *Non-Simple Liquids 31,* edited by I. Prigogine and S. A. Rice (Wiley, New York), p. 263.
Bardeen, J., L. N. Cooper, and J. R. Schrieffer, 1957, Phys. Rev. **108**, 1175.
Baym, G., and C. Pethick, 1978, in *The Physics of Liquid and Solid Helium, Part II,* edited by K. H. Bennemann and J. B. Ketterson (Wiley, New York).
Béal-Monod, M. T., 1982, Physica **109** & **110B** 1837.
Bedell, K. S., 1983 (unpublished).
Bedell, K. S., and T. L. Ainsworth, 1982 (unpublished).
Bedell, K. S., and D. Pines, 1980, Phys. Rev. Lett. 45, 39.
Bedell, K. S., and K. F. Quader, 1983, Phys. Lett. **96A**, 91.
Beni, G., and P. Pincus, 1974, Phys. Rev. B **9**, 2963.
Bonner, J., and M. E. Fisher, 1964, Phys. Rev. **135**, A640.
Brinkman, W. F., and T. M. Rice, 1970, Phys. Rev. B **2**, 4302.
Brown, G. E., 1972, *Many Body Problems* (North-Holland, Amsterdam).
Brueckner, K. A., and J. L. Gammel, 1958, Phys. Rev. **109**, 1040.
Castaing, B., 1980, J. Phys. (Paris) Lett. **41**, 335.
Castaing, B., and P. Nozières, 1979, J. Phys. (Paris) **40**, 257.

Chao, K. A., 1974, Solid State Commun. **14**, 525.
Chapellier, M., G. Frossati, and F. B. Rasmussen, 1979, Phys. Rev. Lett. **42**, 907.
Cyrot, M., 1972, J. Phys. (Paris) **33**, 125.
Cyrot, M., 1977, Physica **91B**, 141.
Dichtel, R., J. Jelitto, and H. Koppe, 1971, Z. Phys. **246**, 248.
Dichtel, R., J. Jelitto, and H. Koppe, 1972, Z. Phys. **251**, 173.
Doniach, S., and S. Engelsberg, 1966, Phys. Rev. Lett. **17**, 750.
Dy, K. S., and C. J. Pethick, 1969, Phys. Rev. **185**, 373.
Dyugaev, A. M., 1976, Zh. Eksp. Teor. Fiz. **70**, 2390 [Sov. Phys.—JETP **43**, 1247 (1976)].
Feenberg, E., *Theory of Quantum Fluids* (Academic, New York).
Florencio, J., and K. A. Chao, 1976, Phys. Rev. B **14**, 3121.
Godfrin, G., G. Frossati, A. S. Greenberg, B. Hebral, and D. Thoulouze, J. Phys. (Paris), Colloq. C **7**, 125.
Greywall, D. S., 1983, Phys. Rev. B **27**, 2747.
Gutzwiller, M. C., 1963, Phys. Rev. Lett. **10**, 159.
Gutzwiller, M. C., 1964, Phys. Rev. **134**, A923.
Gutzwiller, M. C., 1965, Phys. Rev. **137**, A1726.
Hertel, P., J. Appel, and D. Fay, 1980, Phys. Rev. B **22**, 534.
Hirsch, J. E., 1980, Phys. Rev. B **22**, 5259.
Hirsch, J., 1983, Phys. Rev. Lett. **51**, 1900.
Hirsch, J. E., and D. J. Scalapino, 1983, Phys. Rev. Lett. **50**, 1168.
Hubbard, J., 1963, Proc. R. Soc. London, Ser. A **276**, 238.
Hubbard, J., 1964, Proc. R. Soc. London, Ser. A **281**, 401.
Izuyama, T., D.-J. Kim, and R. Kubo, 1963, J. Phys. Soc. Jpn.**18**, 1025.
Kanamori, J., 1963, Prog. Theor. Phys. **30**, 275.
Kaplan, T. A., P. Horsch, and P. Fulde, 1982, Phys. Rev. Lett. **49**, 889.
Kawabata, A., 1975 Prog. Theor. Phys. **54**, 45.
Kawabata, A., 1977, Physica **86—88B**, 387.
Kirzhnits, D. A., and Yu. A. Nepomnyashchii, 1970, Zh. Eksp. Teor. Fiz. **59**, 2203 [Sov. Phys.—JETP **32**, 1191 (1971)].
Krotscheck, E., and R. A. Smith, 1983, Phys. Rev. B **27**, 4222.
Landau, L. D., 1956, Zh. Eksp. Teor. Fiz **30**, 1058 [Sov. Phys.—JETP **3**, 920 (1957)].
Landau, L. D., 1957, Zh. Eksp. Teor. Fiz. **32**, 59 [Sov. Phys.—JETP **5**, 101 (1957)].
Langer, W., M. Plischke, and D. Mattis, 1969, Phys. Rev. Lett. 23, 1448.
Layzer, A., and D. Fay, 1971, Int. J. Magn. **1**, 135.
Leggett, A. J., 1975, Rev. Mod. Phys. **47**, 331.
Levin, K., and O. T. Valls, 1979a, Phys. Rev. B **20**, 105.
Levin, K., and O. T. Valls, 1979b, Phys. Rev. B **20**, 120.
Levin, K., and O. T. Valls, 1983, Phys. Rep. **98**, 1.
Lhuillier, C., and F. Laloe, 1980, J. Phys. (Paris), Colloq. C **7**, 51.
Lieb, E. H., and D. C. Mattis, 1962, Phys. Rev. **125**, 164.
Lieb, E. H., and F. Y. Wu, 1968, Phys. Rev. Lett. **20**, 1445.
Luttinger, J. M., 1960, Phys. Rev. **119**, 1153.
Mahan, G. D., 1981, *Many-Particle Physics* (Plenum, New York).
Methfessel, S., and D. C. Mattis, 1968, "Magnetic Superconductors," in *Handbuch der Physik,* edited by S. Flügge (Springer, Berlin), Vol. 18, Part I, p. 389.
Midgal, A. B., 1957, Zh. Eksp. Teor. Fiz. **32**, 399 [Sov. Phys.—JETP **5**, 333 (1957)].
Mott, N. F., 1949, Proc. Phys. Soc., London **62**, 416.
Mott, N. F., 1974, *Metal-Insulator Transitions* (Taylor and Francis, London).
Mühlschlegel, B., 1965, unpublished lecture notes, University of Pennsylvania.
Nagaoka, Y., 1966, Phys. Rev. **147**, 392.
Ogawa, T., and K. Kanda, 1978, Z. Phys. B **30**, 355.
Ogawa, T., K. Kanda, and T. Matsubara, 1975, Prog. Theor. Phys. **53**, 614.
Olés, A. M., 1982, J. Phys. C **15**, L1065.
Osheroff, D. D., M. C. Cross, and D. S. Fisher, 1980, Phys. Rev. Lett. **44**, 792.
Pines, D., 1983, Proceedings of the International School of Physics, "Enrico Fermi," Varenna, Italy (North-Holland, Amsterdam, in press).
Pines, D., and P. Nozières, 1966, *The Theory of Quantum Liquids* (Benjamin, New York), Vol. I.
Pomeranchuk, I., 1950, Zh. Eksp. Teor. Fiz. **20**, 919.
Razafimandimby, H. A., 1982, Z. Phys. B **49**, 33.
Rice, T. M., and W. F. Brinkman, 1971, "Some aspects of the theory of the Mott transition," in *Alloys, Magnets, and Superconductors,* edited by R. E. Mills, E. Ascher, and R. Jaffee (McGraw-Hill, New York), p. 593.
Roger, M., J. H. Hetherington, and J. M. Delrieu, 1983, Rev. Mod. Phys. **55**, 1.
Stollhoff, G., and P. Fulde, 1977, Z. Phys. B **26**, 257.
Stollhoff, G., and P. Fulde, 1978, Z. Phys. B **29**, 231.
Stollhoff, G., and P. Fulde, 1980, J. Chem. Phys. **73**, 4548.
Takano, F., and M. Uchinami, 1975, Prog. Theor. Phys. **53**, 1267.
Thoulouze, D., G. Bonfait, and Y. Chabre, 1980, J. Phys. (Paris) **7**, C-11.
Wheatley, J. C., 1975, Rev. Mod. Phys. **47**, 415.
Wolff, P. A., 1960, Phys. Rev. **120**, 814.