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Random one-body approximation to the Hubbard model. I. Formalism

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An approximation scheme is presented for treating the Hubbard Hamiltonian through an effective self-consistent random potential. The random variables determining the effective potential are statistically correlated to simulate many-body correlations. The formalism is developed in detail for the half-filled Hubbard model; it is shown that the proposed scheme reproduces exactly the metallic and atomic limits and interpolates between the two.

I. INTRODUCTION

Many of the properties of diverse substances can be adequately understood in the context of models neglecting many-body effects. However, these effects are of crucial importance in understanding for example, magnetism, metal-insulator (Mott) transitions,[1] and the appearance of charge-density waves.[2] Coulomb electron-electron interactions and to a lesser degree electron-phonon interactions play the fundamental role in explaining these phenomena and the resultant many-body problem has proven extremely difficult to treat in any quantitative fashion. This is true in spite of the powerful and sophisticated many body techniques that have been developed in the last 20 years[3] and usually results are obtained after making over simplified assumptions or for a limited range of values of the relevant parameters. Furthermore, the conceptual difficulties associated with interpreting the standard many-body formulas in terms of simple physical pictures make it hard to develop reasonable approximations when following these traditional lines.

A possible way to overcome some of these problems while retaining the basic physical features of the many-body system is to replace the nonlinear many-body Hamiltonian by a random one-body one. That is, the many-body system is replaced by a system of independent quasiparticles moving in a properly determined random potential. Such a replacement naturally includes fluctuations which is one of the two important aspects of many-body effects. In addition, correlations, the other important aspect of many-body effects, can be incorporated into this approach by making the variables characterizing the random one-body potential statistically dependent. Finally, due to the dynamic nature of the system, this random potential should be time dependent.

Although this way of treating the problem does not help in obtaining exact solutions, it can be very useful in finding reasonable approximate solutions. This follows, since, in contrast to the traditional many-body methods, this approach allows immediate and direct introduction into the formalism of the fluctuations and correlations believed to be important. Thus, one of the chief merits of this method is its direct connection with physical intuition which, as it turns out, allows for the development of reasonable approximations with simple physical interpretations. Such a replacement also has the advantage of permitting a quantitative study of the problem over a much wider range of values of the physical parameters, and, in addition, it can be generalized to treat more complicated systems such as those exhibiting both electron-electron correlations and structural disorder, etc.

On the other hand, the method relies heavily on physical intuition in deciding which are the more important correlations and fluctuations and is not always as accurate as some of the more sophisticated many-body techniques. Also it is rather complicated from the computational point of view, and as a matter of fact, one finds it necessary, at least as a first approximation, to omit altogether the explicit time dependence of the random potential in order to make headway in solving the problem. This omission is called the static approximation and its consequences as well as possible ways to remedy some of its more undesirable features will be discussed later.

Even within the context of the static approximation one is faced with extracting whatever quantities are of interest from a random one-body Hamiltonian. Fortunately in the last several years considerable progress has been made in this area[4] and in particular, one can greatly facilitate the computational effort involved by employing the techniques that have been developed in the study of disordered systems. The most important such technique is the so-called coherent-potential approximation[4] which allows an accurate determination of $\langle \hat{G} \rangle$ and a rather reasonable determination of $\langle \hat{G}\hat{G} \rangle$, where $\hat{G}$ is the Green's function of a particle moving in the given random potential and the symbol $\langle\ \rangle$ denotes averaging over the random variables characterizing this potential.

To make the above ideas more specific one can employ either of the following two approaches: (i) A properly determined self-consistent random potential is introduced for which the quantities $\langle \hat{G}\rangle$ and $\langle \hat{G}\hat{G}\rangle$ are calculated. (The self-consistent determination of the random potential will be discussed in detail later.) $\langle \hat{G}\rangle$ and $\langle \hat{G}\hat{G}\rangle$ are then taken as good approximations for the many-body Green's function $\hat{\mathcal{G}}$ and $\hat{\mathcal{G}}_2$, respectively, and in this way any physical quantity, such as the thermodynamic or response functions, which is expressable in terms of $\hat{\mathcal{G}}$ or $\hat{\mathcal{G}}_2$ can be found. This is admittedly an *ad hoc* procedure that is physically motivated as outlined in the preceding discussion and which can be ultimately justified by its ability to reproduce the established results in various cases. Furthermore, at least in some instances, it can be deductively rationalized by following the second approach described below. (ii) Using Stratonovitch's[5,6] identity one can on occasion express the partition function of the system as a functional integral over "time"-dependent random Gaussian fields.[7] This formally proves the intuitively reasonable statement that the many-body problem can be recast as a one-body system moving in a time-dependent random field. If one makes the approximation of omitting the time dependence of the random fields, the functional integral is then reduced to the usual integral over random variables and the whole formulation becomes essentially equivalent to approach (i) above.

Hubbard[8] employed the above ideas in replacing a many-body term by a random field in his original treatment of the so-called Hubbard model. Most of the subsequent work along these lines has been done within the framework of this model; however, it should be stressed that the basic concepts, at least as expressed in approach (i) above, are applicable (but not necessarily conveniently so) to other many-body systems. For example, Chen *et al.*[9] have treated the role of electron-phonon interactions in electrical conductivity using a simplified version of this approach.

In the present work we shall restrict ourselves to the study of the Hubbard model, because this is a relatively simple, well-studied system where our methods are easily applicable and our results can be checked against a host of well-established data. The Hubbard model is also a prototype of many-body effects in solids in the same way that the tight-binding model (TBM) serves as a prototype of band-structure properties. The Hamiltonian used in this model is given by

$$\hat{H}=\sum_{i\sigma}\epsilon_0\hat{n}_{i\sigma}+\sum_{ij\sigma}V_{ij}a_{i\sigma}^\dagger a_{j\sigma}+U\sum_i\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, \quad (1.1)$$

where the sites $\{i\}$ form a lattice: σ takes two values, $+1$ for spin up and -1 for spin down; ϵ_0 is a constant, V_{ij} is usually taken (for simplicity) as a constant V for i, j nearest neighbors and zero otherwise; $a_{i\sigma}^\dagger, a_{i\sigma}$ are operators creating and annihilating electrons at a local Wannier state $|i\sigma\rangle$ centered around the site i with spin σ; and, finally $\hat{n}_{i\sigma}$ is the number operator $a_{i\sigma}^\dagger a_{i\sigma}$. The last term in (1.1) describes the interaction of two electrons located at the same site. Note that the Hamiltonian (1.1) allows interactions only between electrons located at the same site and this restriction may prove a serious drawback for small values of U/V.[10] Besides U/V, another parameter characterizing this model is the number of electrons per site n. Here we confine ourselves to the special case $n=1$, which has been studied extensively; however, our methods can be extended to treat the case $n\neq 1$.

Hubbard[8] (Fukuyama and Ehrenreich,[11] for example, have also used this scheme to calculate the susceptibility of the model) replaced the last term in (1.1) by the random potential $\sum_{i\sigma}\epsilon_{i\sigma}\hat{n}_{i\sigma}$, where the quantities $\epsilon_{i\sigma}$ are independent random variables with a common binary probability distribution. In particular, each $\epsilon_{i\sigma}$ was taken as either U or 0 with equal probability. This simple substitution incorporates fluctuations but not correlations among different sites and, thus, the possibility of magnetic ordering is completely omitted. Furthermore, although this approximation is exact at the atomic limit, $V=0$, it steadily worsens as U/V decreases due to the increasingly rapid switching of $\epsilon_{i\sigma}$ back and forth between U and 0. This gradual dynamic elimination of the effective fluctuations (randomness) has been termed motional narrowing by Hubbard. The above static approximation omits the motional narrowing effects completely and, as a result, the Fermi surface is not well defined in the metallic limit $U/V=0$ with $U\neq 0$.

Several authors[7,12-15] have since managed to partly include motional narrowing effects by assuming that $\epsilon_{i\sigma}$ can take the values Un_+ or Un_- where $n_+ + n_- = 1$ and $n_+ \geqslant n_-$. The quantities n_+, n_- were determined by a generalized Hartree-Fock approximation derived in the framework of the Gaussian random field formulation of the problem [approach (ii) above] and it was found that in the atomic limit $n_+=1$ and $n_-=0$ while in the metallic limit $n_+=n_-=\frac{1}{2}$. Thus, both limits were produced exactly at zero temperature. However, for $T\neq 0$, the atomic limit is not reproduced correctly, and, in addition, the possibility of magnetic ordering, one of the important aspects of the model, was omitted altogether. Some recent attempts have been made to rectify this latter problem. Thus, Plischke[16] and Gupta *et al.*[17] have examined the question of magnetic ordering by introducing imperfect long-range order. This is not a satisfactory way to treat magnetic ordering, however, since the long-range order should actually develop through short-range correlations. So, e.g., the common case of absence of long-range order while short-range order is still present is left out in these treatments. Furthermore, neither of these approaches include motional narrowing effects, and so suffer from the type of problems mentioned above in the metallic regime. On the other hand, Lacour-Gayet and Cyrot[18] have evaluated the exchange integrals J_{ij}; however, their calculation was in general not self-consistent since these integrals were obtained by employing an electronic spectrum that did not include the effects of partial magnetic ordering.

In the present work we will present a random potential approximation which is exact in both the atomic and metallic limits for all temperatures, and incorporates magnetic ordering in a self-consistent, and, we believe, satisfactory manner for the first time. The usual way of obtaining the magnetic properties[18] assumes an electronic motion that corresponds to either perfect magnetic ordering or no magnetic ordering at all, out of which an exchange or superexchange interaction J_{ij} is calculated, which is then used in an appropriate spin Hamiltonian to produce the magnetic effects. Such an approach omits the feedback of the actual imperfect magnetic ordering on the electronic motion and consequently it is not self-consistent. This lack of self-consistency has negligible effects for very low temperatures ($k_BT \ll |J|$, where the order is almost perfect) or very high temperatures ($k_BT \gg |J|$, where the order disappears altogether).

In many cases for the entire range of temperatures of interest either $k_BT \ll |J|$ or $k_BT \gg |J|$ and thus there is no actual need for a self-consistent treatment. However, when $k_BT \sim |J|$, a self-consistent treatment is necessary since the reduction of magnetic ordering as temperature is increased has a profound effect on the electronic spectrum, as has been shown in the limit ($V \neq 0$, $U \to \infty$) by the detailed many-body treatment of Brinkman and Rice.[19] We have found that the electronic spectrum depends strongly on magnetic ordering not only in this limit but for other values of U as well. This change in the electronic density of states, due to destruction of magnetic ordering will have important physical effects if the spectrum is thermally sampled at temperatures approximately equal to $|J|$, i.e., when $k_BT \sim J \sim |E_i - \mu|$ (μ is the chemical potential and E_i is a typical energy in the vicinity of μ where the density of states changes substantially with the destruction of ordering) a self-consistent treatment like ours is indispensable. In this instance several physical quantities exhibit an anomalous temperature dependence, e.g., the resistivity is dropping precipitously. To the best of our knowledge this point has not been recognized in the literature and no satisfactory calculational scheme is available to treat it. Yet it seems to be important in view of the fact that several materials such as NiS,[20,21] $LaVO_3$,[22] oxides of V (Ref. 23), and Ti (Ref. 24), and some quasi-one-dimensional organic metals[25] exhibit a behavior qualitatively similar to that predicted by our self-consistent inclusion of magnetic ordering. It should be pointed out that the above discussion is not restricted to the case of magnetic ordering only, but also, for example, applies to charge density ordering or Peierls distortion in problems of electron-phonon interaction. The present scheme explicitly takes into account the effects of the destruction of magnetic ordering on the quasielectron spectrum for all values of T and U/V and self-consistently determines the magnetic properties.

We have calculated the conductivity σ_c of the system and found, as expected, that the destruction of magnetic ordering with increasing temperature affects the temperature dependence of σ_c and that this effect is more pronounced when $U/ZV \sim 1$; Z is the coordination number of the lattice.

In Sec. II we introduce concepts and relations pertinent to the present work. Then in Sec. III we introduce and develop one of our two basic original contributions, namely, the incorporation of magnetic ordering and its self-consistent treatment. Next, in Sec. IV we express various quantities of physical interest in terms of the totally and partially averaged Green's functions. Finally, in the last section we summarize our formalism and we introduce our second basic contribution to the subject, namely, the approximate inclusion of dynamical processes.

II. *AD HOC* RANDOM POTENTIAL APPROACH

The spirit of this approach is to approximate the many-body $\mathcal{G}_\sigma$ by $\langle \hat{G}_\sigma \rangle$, where $\hat{G}_\sigma(E) = (\hat{E} - \hat{H}_\sigma)^{-1}$ and $\hat{H}_\sigma$ is a one-body random Hamiltonian obtained from (1.1) by replacing the many-body part by an appropriate random one-electron part, i.e.,

$$U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \approx \epsilon_{i\sigma}\hat{n}_{i\sigma}\,, \tag{2.1}$$

where the quantities $\{\epsilon_{i\sigma}\}$ are random statistically correlated variables.

This *ad hoc* procedure can be justified formally by employing the Gaussian random field method.[5,6,18] Accordingly, the free energy of the system can be expressed as a functional integral over the quantities $\{\epsilon_{i\sigma}\}$, which are functions of a "time" variable s.[5,6] Then one introduces the first approximation of this work, termed the *static approximation,* which omits the time dependence of the quantities $\{\epsilon_{i\sigma}\}$; the functional integral is then transformed to an ordinary integral over the variables $\{\epsilon_{i\sigma}\}$. The integration can then be performed by the saddle-point approximation which picks out the values of $\{\epsilon_{i\sigma}\}$ which makes the integrand maximum. The final result is that the free energy F has the same form which would have been obtained by employing Eq. (2.1) with each quantity $\epsilon_{i\sigma}$ satisfying a generalized Hartree-Fock equation

$$\epsilon_{i\sigma} = U\bar{n}_{i-\sigma}\,, \tag{2.2}$$

where the bar indicates a quantum-mechanical and thermal average. Note that Eq. (2.2) can be obtained by employing (2.1), assuming that the quantities $\{\epsilon_{i\sigma}\}$ are time independent, calculating the free energy F, and then choosing the $\{\epsilon_{i\sigma}\}$ so to minimize F with respect to their variations.

It is well known that the Coulomb repulsion term suppresses strongly charge fluctuations. For this reason we introduce a second approximation which eliminates such possibilities altogether, i.e.,

$$\bar{n}_{i\uparrow} + \bar{n}_{i\downarrow} = 1\,. \tag{2.3}$$

Combining Eqs. (2.2) and (2.3), one can show that

$$\epsilon_{i\sigma} = \tfrac{1}{2}U(1 - \sigma\mu_{i\sigma})\,, \tag{2.4}$$

where

$$\mu_{i0} = \bar{n}_{i\uparrow} - \bar{n}_{i\downarrow}\,. \tag{2.5}$$

Equation (2.5) is derived in the Appendix by employing the Gaussian random-field approach.

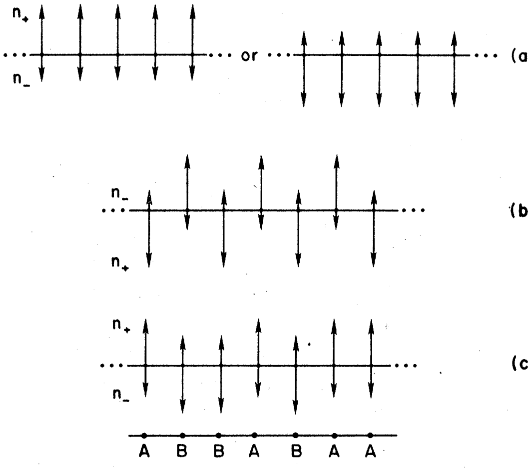

FIG. 1. (a) Vectors pointing up (down) represent the quantities $\bar{n}_{i\uparrow}$ ($\bar{n}_{i\downarrow}$) at each site i of the 1 D lattice shown. The vector sum at each site is the local moment. Two symmetric uniform configurations are shown; (b) alternating periodic (antiferromagnetic) configuration; (c) random configuration, where the up (down) vectors represent $\langle\bar{n}_{i\uparrow}\rangle_i^\alpha$ ($\langle\bar{n}_{i\downarrow}\rangle_i^\alpha$), $\alpha = A, B$.

Each quantity μ_{j0} can be interpreted as the z component of a moment located at the site j. These moments are produced by electrons that are neither completely localized at every site i nor of the Bloch type; instead they move in the self-consistent potential defined by (1.1) and (2.1). If the set $\{\mu_{j0}\}$ satisfies Eq. (2.5) so does the set $\{-\mu_{j0}\}$ because of the updown spin symmetry. A solution to (2.5) can be easily obtained if one assumes that $\mu_{j0} = \mu_0$, independent of j. Then, there are in fact three solutions: one with $\mu_0 = 0$ corresponding to a maximum, not a minimum, in F, and two genuine symmetric solutions, $\mu_0 = \pm|\mu_0|$, corresponding to a minimum in F. These are the ordinary Hartree-Fock solutions which neglect fluctuations altogether. They are shown schematically in Fig. 1 (a) where it is clear that they correspond to a ferromagnetic arrangement of the moments. Another possibility corresponding to an antiferromagnetic arrangements of the moments is shown in Fig. 1(b). In this case fluctuations are allowed but completely correlated so as to produce again a periodic arrangement, but now with double spacing. Observe that the self-consistent magnitude $|\mu_0|$ is not the same in cases (a) and (b) of Fig. 1 because the corresponding Green's functions $G_{i\sigma}$ are different. One may consider still another example where all μ_{j0} have the same absolute value $\tilde{\mu}$ but their signs are random. In this instance we can call A sites those with $\mu_{j0} > 0$ and B sites those with $\mu_{j0} < 0$, as is done in Fig. 1(c). Thus, the electronic motion can be thought of as a random AB alloy. With this random system, it is not possible to satisfy Eq. (2.5) at each site, and instead one can try to satisfy it on the average, i.e.,

$$N_A\tilde{\mu} = \sum_{j\in A}(\bar{n}_{j\uparrow} - \bar{n}_{j\downarrow})\,, \tag{2.6a}$$

$$-N_B\tilde{\mu} = \sum_{j\in B}(\bar{n}_{j\uparrow} - \bar{n}_{j\downarrow})\,, \tag{2.6b}$$

where $N_A(N_B)$ is the total number of $A(B)$ sites. The quantities μ_{j0} can be considered as random variables where the probability distribution P_0 of each μ_{j0} is determined from the ensemble of values of μ_{j0} as j runs over all lattice sites. In the present case

$$P_0(\mu_{j0}) = \tfrac{1}{2}\delta(\mu_{j0} - \tilde{\mu}) + \tfrac{1}{2}\delta(\mu_{j0} + \tilde{\mu})\,. \tag{2.7}$$

Equation (2.6) can then be written in a more elegant form

$$\mu^{\alpha}=\langle\bar{n}_{j\uparrow}\rangle_j^{\alpha}-\langle\bar{n}_{j\downarrow}\rangle_j^{\alpha}, \quad \alpha=A \text{ or } B, \tag{2.8}$$

where the symbol $\langle\ \rangle_j^{\alpha}$ denotes an average over all μ_{i0}, $i\neq j$, with $\mu_{j0}=\mu^{\alpha}$, $\alpha=A, B$; $\mu^A\equiv+\tilde{\mu}$, $\mu^B\equiv-\tilde{\mu}$. We denote by n_+ the quantity $\langle\bar{n}_{i\uparrow}\rangle_i^A$ and by n_- the quantity $\langle\bar{n}_{i\uparrow}\rangle_i^B$; then $\tilde{\mu}=n_+-n_-$ and $\mu_{j0}=\pm(n_+-n_-)$ as shown in Figs. 1(a)– 1(c). From Eq. (2.3) it follows that $n_++n_-=1$. Keep in mind that μ_{j0} can be though of as the z component of a local moment operator $\vec{\mathrm{m}}_j=\tilde{\mu}\vec{\sigma}_j$, where $\vec{\sigma}_j$ is the Pauli matrix operator. Thus the site j being A (B) is equivalent to σ_{jz} having the eigenvalue 1 (-1). In what follows we will use both the alloy picture and this equivalent local moment picture.

Obviously the above scheme can be generalized by starting with a more complicated probability density for μ_{j0}, e.g.,

$$P_0(\mu_{j0})=\sum_{\alpha}P_{\alpha}\delta(\mu_{j0}-\mu_{\alpha}),$$

and then determining the quantities μ_{α} from self-consistency equations of the type (2.8). Note that the probabilities P_{α} must be found from symmetry requirements and by minimizing the total free energy of the system if necessary. An approach of this sort could prove superior to the present binary one, although the practical implementation of such a general scheme is far from trivial.

Here we restrict ourselves to the simplest but still reasonable case where $P_0(\mu_{j0})$ is taken as in Eq. (2.7). This random "binary alloy" approximation is clearly the simplest one which allows fluctuations and it has the additional advantage of being able to reproduce exactly both the atomic and metallic limits, and thus will interpolate between these two extremes.

The quantity $\tilde{\mu}$ can be thought of physically as a time average of $n_{i\uparrow}(t)-n_i(t)$ in a specially prepared system, i.e.,

$$\tilde{\mu}\approx\frac{1}{\tau}\int_0^{\tau}[\bar{n}_{i\uparrow}(t)-n_{i\downarrow}(t)]\,dt, \tag{2.9}$$

where the system at $t=0$ has been prepared in such a way that $\bar{n}_{i\uparrow}(0)=1$, and τ is of the order of Hubbard's switching time.[8]

The self-consistency condition (2.5) or its approximate form (2.8) develops a serious flaw for high T for all values U/ZV above a certain critical value. Let us for convenience consider the atomic limit $(V=0)$. Then Eq. (2.5) takes the form

$$\tilde{\mu}=\frac{1}{e^{-(\beta U\tilde{\mu}/2)}+1}-\frac{1}{e^{(\beta U\tilde{\mu}/2)}+1}. \tag{2.10}$$

The self-consistent solution of (2.10) starts with $\tilde{\mu}=1$ at $T=0$ and drops monotonically with increasing T until $k_BT=U$. For $k_BT>U$, $\tilde{\mu}=0$. One can easily check that the thermodynamics is not correctly reproduced by (2.10) and in addition, a phase transition is forced by this self-consistency condition at $T=U/k_B$ which is clearly spurious. The physical origin of this problem is the incompatibility of the local nature of Eq. (2.5) and the *thermal equilibrium* averaging involved in (2.5): That is, through the thermal averaging, configurations associated with other sites are automatically included [as in (2.10)] in calculating $\bar{n}_{j\uparrow}-\bar{n}_{j\downarrow}$, and thus the μ_{j0}, and hence the effective fluctuations, are spuriously reduced in size. A possible solution to this problem is to utilize a thermal ensemble possessing only partial equilibrium, i.e., one for which the chemical potentials are not all equalized. The formalism then becomes very complicated and impractical. In the next section we will present an *ad hoc* solution of this difficulty which although not completely satisfactory, is very convenient and seems to work reasonably well.

III. MAGNETIC ORDERING

In this section we introduce one of the main ideas of this work and develop the corresponding formalism. Magnetic ordering can be incorporated very conveniently within the binary AB alloy approximation since the latter is equivalent to local spin$\frac{1}{2}$ moments. All we have to do is to consider the z component of the local moments at different sites as statistically dependent. This statistical dependence arises from short range interactions among the z component of the local moments as in the Ising model.[26] It is important to note that these interactions can produce long-range correlations as well due to the connectivity of the lattice. To simplify the problem we will assume that all correlations result from a basic nearest-neighbor correlation; more explicitly, we assume that the probability of any site being of type A or B outside a fixed configuration shell consisting of all the nearest neighbors of a given central site is independent of the character (A or B) of this central site. This assumption is equivalent to only nearest-neighbor coupling in the Ising model. Of course, real systems have interactions beyond nearest neighbors which are weak and decay with increasing relative distance. As a matter of fact the Hubbard Hamiltonian implies interactions beyond nearest neighbors.[18] However, the incorporation of these additional features produces only minor quantitative changes while making the formalism complicated. For this reason we describe the correlations through a single parameter P referring to a pair of nearest neighbors.[27] This parameter can be expressed, as we shall see, in terms of the nearest-neighbor coupling J of the equivalent Ising model and is defined as the probability of a given site i being of type A (i.e., having $\mu_{i0} = \tilde{\mu}$) under the condition that a nearest-neighbor site is of type B (i.e., it has $\mu_{j0} = -\tilde{\mu}$). Thus, $0 \leq P \leq 1$. The value $P=0$ corresponds to the perfect ferromagnetic configuration shown in Fig. 1(a) while $P=1$ describes the perfect antiferromagnetic order shown in Fig. 1(b). Obviously $P > \frac{1}{2}$ implies that local antiferromagnetic ordering exists while $P < \frac{1}{2}$ corresponds to local ferromagnetic ordering and $P = \frac{1}{2}$ is the pure paramagnetic case. It should be stressed that when P exceeds a critical value P_c or when P is below another critical value P_c', long-range order exists in the system which is created out of the short range correlations. Both P_c and P_c' depend on the lattice topology and for the one-dimensional (1D) case, one can easily show that $P_c' = 0$ and $P_c = 1$. For the two-dimensional (2D) square lattice, $P_c \approx 0.85$ and $P_c' \approx 0.15$, so in this instance, when $0 \leq P \lesssim 0.15$, we have both long- and short-range ferromagnetic order, but for P such that $0.15 \lesssim P < \frac{1}{2}$, we have only short-range ferromagnetic order. When $\frac{1}{2} < P \lesssim 0.85$ only short-range order is still present but now it is of antiferromagnetic character. Finally, when $0.85 \lesssim P \leq 1$, both short- and long-range antiferromagnetic order appear.

P will be determined by minimizing the total free energy of the system, i.e., from the condition

$$\left(\frac{\partial F}{\partial P}\right)_{T,\tilde{\mu}} = 0\,. \tag{3.1}$$

Thus we need to express F as a function of P. The partition function can be written

$$Z = e^{-\beta F_e} \sum_{\{\mu_{i0}\}}\,, \tag{3.2}$$

where F_e is the value of the free energy for any set $\{\mu_{i0}\}$ satisfying Eqs. (2.7 and 2.8) and the sum $\sum\{\mu_{i\sigma}\}$ extends over all the sets of $\{\mu_{i0}\}$ minimizing F. For $P=0$, corresponding to Fig. 1(a), $\sum\{\mu_{i\sigma}\} = 2$, since there are only two sets minimizing F; similarly, for $P=1$ [shown in Fig. 1(b)], $\sum\{\mu_{i0}\} = 2$; when $P = \frac{1}{2}$, $\sum\{\mu_{i0}\} = 2^N$, where N is the total number of sites, each one being either of type A or B. However, in general, $\sum\{\mu_{i\sigma}\}$ depends on P in a complicated way. The free energy of the system $F = -(1/\beta)\ln Z$ can be written, using Eq. (3.2), as

$$F = F_e - k_B T \ln \sum_{\{\mu_{i\sigma}\}}\,. \tag{3.3}$$

We define the quantity $S_l = k_B \ln \sum\{\mu_{i\sigma}\}$, which depends only on P, as the "lattice" or "magnetic" entropy. Denoting by A' the $\lim_{N\to\infty} A/N$, where A is any extensive thermodynamic quantity, we can then write (3.3) as

$$F' = F_e' - TS_e'\,. \tag{3.4}$$

$S_l'(P)$ goes to zero when $P = 0, 1$ and has a maximum at $P = \frac{1}{2}$ and finding its explicit P dependence is a problem mathematically equivalent to solving the Ising model with nearest-neighbor coupling only. For the 1D case,

$$S_l'(P) = -k_B[P\ln P + (1-P)\ln(1-P)]\,, \tag{3.5}$$

a result which can be verified immediately if one notes that the bonds (but not the sites) can be assigned independently the values P and $1-P$. For the 2D square lattice one can use the Onsager's solution[26] to find $S_l'(P)$. This is achieved by first noting that both the Ising entropy per site S_I' (which is identical to S_l') and the Ising energy per site H_I', are solely functions of βJ and J; i.e., $S_I' = f_1(\beta J)$ and $H_I' = J f_2(\beta J)$. Further, H_I' is directly related to P through the relation $H_I' = ZJ(P - \frac{1}{2})$ where Z is the coordination number of the lattice. Thus P is a function of βJ only and so by eliminating this quantity between $S_I' = f_1(\beta J)$ and

$$P = \tfrac{1}{2} + (1/Z) f_2(\beta J)\,, \tag{3.6}$$

we can obtain $S_l'(P)$. If P is known at a given temperature one may invert Eq. (3.6) to find the exchange coupling of the equivalent Ising model. Note though that for three-dimensional (3D) lattices the function $S_l'(P)$ can be found only approximately. In Fig. 2, $S_l'(P)$ is shown for the 1D chain, the 2D square lattice, and approximately for the 3D simple cubic lattice. Note also that S_l' is an analytic function of P in the range $0 < P < 1$ for the 1D case. For the 2D case S_l' is not analytic at $P = P_c \approx 0.855$ or at $P = P_c' = 1 - P_c \approx 0.145$ where a logarithmic singularity develops corresponding to a second-order phase transition associated with the onset of long-range order. Singularities appear also in the 3D case, although exact results are not available. Note that the Bethe-Peierls approximation[26] used to obtain the 3D result shown in Fig. 2 increases the values of S_l' for high values of $P - \frac{1}{2}$ and shifts the value of P_c, P_c' towards $\frac{1}{2}$.

We need also to obtain F_e' for any value of P, which means that the Green's function $G_{i\sigma}(E)$ should be calculated in the presence of partial ordering as described by P. This is not an easy problem and probably the lack of a satisfactory solution to it has been the main obstacle delaying the proper incorporation of magnetic ordering up to now. To overcome this difficulty we have developed[28,29] a generalized coherent-potential approximation which is very successful in incorporating effects associated with partial ordering. This method is presented in detail in Ref. 28.

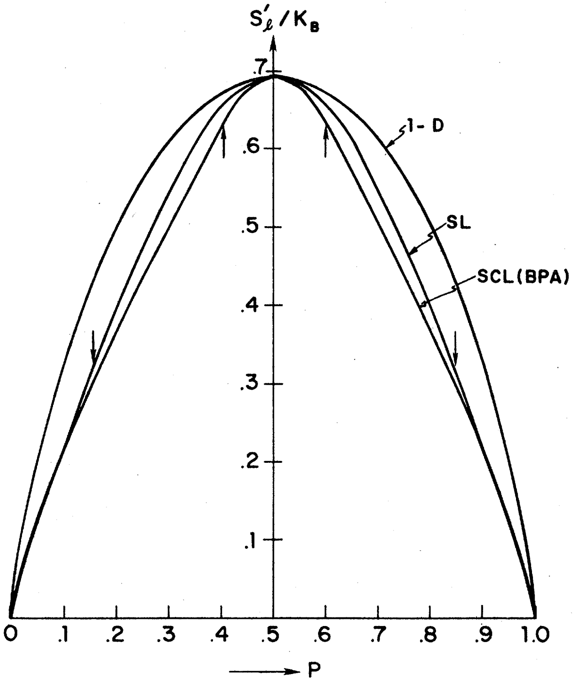

FIG. 2. Lattice entropy per site (see text) S'_l as a function of the correlation parameter P for the 1D lattice, 2D square lattice (SL), and the 3D simple cubic lattice (SCL), according to the Bethe-Peierls approximation (BPA) [SCL(BPA)]. Arrows indicate the critical points.

The basic Eq. (3.1) can be written

$$\left(\frac{\partial F'_e}{\partial P}\right)_{T,\tilde{\mu}} = T\,\frac{dS'_l}{dP}, \tag{3.7}$$

Since the average Ising energy $\overline{H}'_l = ZJ(P-\frac{1}{2})$, we can write

$$\frac{dS'_l}{dP} = ZJ\left(\frac{\partial S'_l}{\partial \overline{H}'_l}\right)_J = \frac{ZJ}{T}. \tag{3.8}$$

Thus the basic Eq. (3.7) can be rewritten in terms of the exchange coupling J of the equivalent Ising problem as[30]

$$J = \frac{1}{Z}\left(\frac{\partial F'_e}{\partial P}\right)_{T,\tilde{\mu}}. \tag{3.9}$$

If one eliminates P between Eqs. (3.6) and (3.9) one can find J as a function of T. Note that it was not necessary at all to introduce J; i.e., everything could be expressed in terms of P. Nevertheless, we have introduced J since it is a more familiar quantity, and also because as it turns out, the numerical solution of Eq. (3.7) is somewhat facilitated by considering the equivalent set of Eqs. (3.6) and (3.9). From Eq. (3.9) one can easily show that

$$J \xrightarrow[T\to 0]{} -\Delta\overline{H}_n/2n, \tag{3.10}$$

where ΔH_n is the change in the total ground-state energy when n of the $\frac{1}{2}NZ$ AB bonds become AA or BB. Equation (3.10) coincides with the usual definition of J.

At this point it is reasonable to summarize our results: The many-body Green's function G_σ corresponding to the Hamiltonian (1.1) can be approximated by $\langle G_\sigma\rangle$, where

$$\hat{G}_\sigma(E) = (E-\hat{H}_\sigma)^{-1}, \tag{3.11}$$

and the angular brackets $\langle\ \rangle$ denote configurational averaging. $\hat{H}_\sigma$ is defined as

$$\hat{H}_\sigma = \sum_i (\epsilon_0+\epsilon_{i\sigma})\hat{n}_{i\sigma} + \sum_{ij} V_{ij}a^\dagger_{i\sigma}a_{j\sigma}, \tag{3.12}$$

with $\epsilon_{i\sigma}$ given by (2.4) and $\{\mu_{i\sigma}\}$ having a binary probability distribution characterized by two quantities: $\tilde{\mu}$ [see Eq. (2.7)] and P. The quantity $\tilde{\mu}$ is determined from the self-consistency condition

$$\tilde{\mu}_0 = \langle\overline{n}_{i\uparrow}\rangle^A_{i,T=0} - \langle\overline{n}_{i\downarrow}\rangle^A_{i,T=0}. \tag{2.8$'$}$$

Note that Eq. (2.8′) is not identical to (2.8); the difference is that in Eq. (2.8′) $\tilde{\mu}_0$ is determined self-consistently for each P at zero temperature only and then used for all temperatures. The subscript 0 has been introduced to emphasize this difference. The advantages of this *ad hoc* modification are: (a) the thermodynamics in the atomic limit are reproduced exactly; (b) there is no spurious phase transition at high temperatures as with Eq. (2.8); (c) the high-temperature entropy in the intermediate U/V regime essentially reduces to the correct result in contrast to what would be obtained by using Eq. (2.8); (d) the calculational effort is considerably reduced. It should be noted that the quantity $\tilde{\mu}_0$ as determined by Eq. (2.8′) can be interpreted as a local moment only at $T=0$, and that $\tilde{\mu}_0$ depends on T implicitly through P.

The quantity P is determined by minimizing the free energy with respect to P or by the equivalent set of Eqs. (3.6) and (3.9).

As already mentioned, we have developed[28,29] an approximate method which allows us to obtain $\langle G_{i\sigma}\rangle$ where $G_{i\sigma} = (\sigma i|(E-\hat{H}_\sigma)^{-1}|i\sigma)$ and $\hat{H}_\sigma$ is the self-consistent random Hamiltonian (3.12). In the next section we express quantities of physical interest in terms of this and subsidiary quantities.

IV. QUANTITIES OF INTEREST

A. Density of states

The partially averaged density of states (DOS) is given by

$$\rho^\alpha_\sigma(E) = -(1/\pi)\,\mathrm{Im}\langle G_{i\sigma}(E^+)\rangle^\alpha_i;\quad \alpha = A, B. \tag{4.1}$$

It is easy to see that $\rho^A_\uparrow(E) = \rho^B_\downarrow(E)$ and $\rho^A_\downarrow(E) = \rho^B_\uparrow(E)$.

The totally averaged DOS can be written in terms of these quantities as

$$\rho(E) = -(1/\pi)\,\mathrm{Im}\langle G_{i\sigma}(E^+)\rangle$$
$$= \tfrac{1}{2}[\rho_\uparrow^A(E) + \rho_\downarrow^A(E)]\,. \qquad (4.2)$$

The DOS $\rho(E)$ is very important because every physical quantity depends on it; its determination permits at least an approximate calculation of any observable quantity of the system. In particular, we are interested in the U, V, and T dependence of ρ, where the latter arises from the temperature dependence of the magnetic parameter P. Knowledge of the density of states ρ at or about the Fermi level is extremely important because this information allows a qualitative prediction of the physical behavior of the system.

The partially averaged density of states ρ^α, $\alpha = A$ or B is a useful quantity also because it provides some information about the nature of the eigenstates: namely, what percentage of them are associated with sites of a given type (A or B).

B. Local moment

At zero temperature the local moment $\tilde{\mu}_0$ is a function of U/ZV starting from zero at $U/ZV = 0$ and going to one at $U/ZV = \infty$. For finite temperatures we can define[31] the local moment $m^*(T)$ so that $1 - m^{*2}(T) = \overline{4n_{i\uparrow}n_{i\downarrow}}$. The quantity $\langle 4n_{i\uparrow}n_{i\downarrow}\rangle_{\mathrm{av}}$ can be evaluated within the framework of our approach by taking into account Eqs. (2.1), (2.4), and (2.7), which leads to the result

$$4\overline{n_{i\uparrow}n_{i\downarrow}} = \frac{4}{U}\langle \epsilon_{i\sigma}\bar{n}_{i\sigma}\rangle = 1 - m(T)m(0)\,, \qquad (4.3)$$

where

$$m(T) = \langle \bar{n}_{i\uparrow}\rangle_i^A - \langle \bar{n}_{i\downarrow}\rangle_i^A\,. \qquad (4.4)$$

The quantity $\langle n_{i\sigma}\rangle_i^\alpha$ is given by

$$\langle \bar{n}_{i\sigma}\rangle_i^\alpha = \int dE\, f(E)\rho_\sigma^\alpha(E), \quad \alpha = A, B\,. \qquad (4.5)$$

Similarly,

$$\langle n_{i\sigma}\rangle_{i,T=0}^\alpha = \int_{-\infty}^0 dE\,\rho_\sigma^\alpha(E)\,, \quad \alpha = A, B\,. \qquad (4.6)$$

Thus, $m^*(T)$ can be expressed as

$$m^*(T) = [\tilde{\mu}_0 m(T)]^{1/2}\,; \qquad (4.7)$$

obviously, $m^*(T) \to \tilde{\mu}_0$ as $T \to 0$.

C. Exchange coupling

The exchange coupling J of the equivalent Ising Hamiltonian is of great physical interest because it controls the magnetic behavior of the system. We would like to obtain J not only as a function of U/ZV, but also as a function of temperature through our self-consistent approach. If J turns out to be temperature dependent, the conventional Ising treatments should be modified.

D. Various thermodynamic quantities

The energy can be obtained by considering first its expression in terms of the many body Green's function

$$\overline{H}' = \frac{1}{N}\sum_{\vec{k}}\int \frac{dE}{\pi}\,\tfrac{1}{2}(E + E_{\vec{k}})\, f(E)\, i\,\mathrm{Im}\,\mathcal{G}(E^+, \vec{k})\,, \qquad (4.8)$$

and then replacing $\mathcal{G}(E, \vec{k})$ by $\langle G(E, \vec{k})\rangle$. Explicitly the unperturbed one particle energy $E_{\vec{k}}$ is given in the present case by $E_{\vec{k}} = \sum_l V_{0l}e^{i\vec{k}\cdot\vec{l}}$; going into the Wannier representation, and taking into account the equation $(\hat{E} - \hat{H}_\sigma)\hat{G}_\sigma = \hat{1}$ one can show after some lengthy but straightforward algebra that

$$\overline{H}' = \sum_\sigma \int dE\, f(E)E\rho(E) - \tfrac{1}{4}U[1 - \tilde{\mu}_0 m(T)]\,, \qquad (4.9)$$

where we have taken $\epsilon_0 + \frac{1}{2}U = 0$, and $m(T)$ is defined by Eq. (4.4). The result (4.9) can be easily interpreted physically by first rewriting it as $\overline{H}' = \sum_\sigma \overline{H}'_\sigma - \langle \epsilon_{i\sigma}\bar{n}_{i\sigma}\rangle$ and then noting that the last term corrects the double counting of the electron-electron interaction in the first term.

To determine the other thermodynamic quantities we can use the general relation

$$\overline{\frac{\partial \hat{H}}{\partial\lambda}} = \left(\frac{\partial F}{\partial \lambda}\right)_{T,N}\,, \qquad (4.10)$$

where λ is any parameter in the Hamiltonian and F is the free energy. Taking $\lambda = U$, we obtain

$$\left(\frac{\partial F}{\partial U}\right)_{P,T} = \sum_i \overline{n_{i\uparrow}n_{i\downarrow}} \approx \tfrac{1}{4}[1 - m^{*2}(T)]\,, \qquad (4.11)$$

which allows us to write

$$F' = -TS'_l(P) + F'_e(U=0) + \tfrac{1}{4}\int_0^U dU'[1 - m^{*2}(T)] \qquad (4.12')$$

$$= -TS'_l(P) + F'_e(U=\infty) + \frac{1}{4}\int_\infty^U dU'[1 - m^{*2}(T)]\,, \qquad (4.12)$$

where Eq. (4.12) is more convenient for low U/ZV and Eq. (4.12′) more appropriate for high U/ZV. The first term in Eqs. (4.12) is the "lattice" or "magnetic" free energy and the rest is the "electronic" free energy. The total entropy is given by

$$S' = -\frac{dF'}{dT} = -\left(\frac{\partial F'}{\partial T}\right)_P = S'_l + S'_e\,, \qquad (4.13)$$

where S_e' is obtained by differentiating the last two terms of (4.12). Expressions (4.12) and (4.13) are not convenient for numerical calculations because the integral over U requires solution of the problem for many U. Besides, we were not able to show in general that S', F', $\bar{H}'$ as given by Eqs. (4.13), (4.12), and (4.9), respectively, satisfy the basic identity $\bar{H}' = F' + TS'$; after a rather complicated and lengthy derivation we did prove though that this identity is obeyed in the limits $T \to 0$, $P \to 1$ as well as in the atomic and metallic limits.

One can follow a different path however to find the entropy. In particular, having a reliable and convenient expression for $\bar{H}'$ one can obtain S_e' from the thermodynamic identity $T(\partial S_e'/\partial T)_P = (\partial \bar{H}'/\partial T)_P$ which is obtained from Eq. (4.13) and $\bar{H}' = F' + TS'$. Then S_e' is given by

$$S_e' = -k_B \sum_\sigma \rho_\sigma(E)[f \ln f + (1-f)\ln(1-f)]\, dE + k_B \tfrac{1}{4} U \tilde{\mu}_0 \int \frac{dE}{E} [\rho_\uparrow^B - \rho_\uparrow^A] \times [f \ln f + (1-f)\ln(1-f)] + \phi(P), \tag{4.14}$$

where $\phi(P)$ is an unknown function of P which should approach zero as $P \to 1$. We have chosen $\phi(P) = 0$, which makes S' exact in the atomic and metallic limits for all T and highly accurate everywhere else. For $E = 0$, $\rho_\uparrow^A = \rho_\uparrow^B$; thus, the integral in Eq. (4.14) is well defined. However, in some special cases $(\rho_\uparrow^A - \rho_\uparrow^B)$ may be appreciable for E close to zero; then the factor E^{-1} magnifies any numerical or other error and the expression (4.14) may become unreliable. In these instances, one can use Eq. (4.12) instead. Within numerical accuracy, both Eqs. (4.12) and (4.14) lead to the same physical results.

The specific heat C' is given by the relation

$$C' = \frac{d\bar{H}'}{dT} = \left(\frac{\partial \bar{H}'}{\partial T}\right)_P + \left(\frac{\partial \bar{H}'}{\partial P}\right)_T \frac{dP}{dT}. \tag{4.15}$$

Using the basic thermodynamic identities and the fact that P is a function of βJ only as can be seen from (3.6) we can reexpress C' as

$$C' = C_e' + C_I' - C_I' \frac{dJ}{dT} \frac{T}{J} \left(2 - \frac{T}{J} \frac{dJ}{dT}\right), \tag{4.16}$$

where $C_e' = (\partial \bar{H}'/\partial T)_P$ is the "electronic" contribution to the specific heat and C_I' is the Ising contribution which equals $J(\partial f_2/\partial T)_J$.

E. Response functions

The calculation of the response functions is in general a considerably more difficult problem, since they depend not only on the density of states, as the thermodynamic quantities do, but on details of the eigenfunctions.

The present scheme provides an approximate way of calculating response functions as a sum of a magnetic part and an electronic part; the latter can be obtained by considering only its dependence on the density of states and omitting other dependencies. This is not as bad as it may seem, since already incorporated into our density of states is information about correlations and fluctuations. This approach can be applied, e.g., in determining the Pauli susceptibility χ which is given by

$$\chi = 2\mu_B^2 \int \left(-\frac{\partial f}{\partial E}\right) \rho(E)\, dE + \chi_m, \tag{4.17}$$

where χ_m is the susceptibility of an Ising model and μ_B is the Bohr magneton. Note that a more complete treatment of the magnetic susceptibility would require the reexamination of the entire problem in the presence of a magnetic field, taking into account the renormalization of $\tilde{\mu}_0$ due to this field, etc. These aspects were neglected in arriving at Eq. (4.17); however, we are presently investigating their inclusion.

As was noted in the Introduction, the present scheme provides a more sophisticated approach to the problem of calculating response functions. It is well known that most of the interesting response functions like the conductivity, dielectric functions, magnetic susceptibility, etc., depend on the two-particle Green's function $\mathcal{G}_2$. The latter can be approximated within our scheme as $\langle \hat{G}\hat{G} \rangle$. Since in general $\langle \hat{G}\hat{G} \rangle \neq \langle \hat{G} \rangle \langle \hat{G} \rangle$ this approach incorporates "vertex corrections" in addition to the "self-energy" corrections already present in $\langle \hat{G} \rangle$.

We have attempted to apply our formalism to the calculation of the static conductivity of the Hubbard model σ_0 which involves within the framework of our scheme, evaluating the average[32] $\sum_{ijkl} \langle V_{ij} G_{jk} V_{kl} G_{li} \rangle$. Within the ordinary coherent-potential approximation (CPA), Velicky[33] has shown that the vertex corrections do not contribute to σ_c and subsequently, he greatly simplified the final expression for σ_c, which was then recast by Chen *et al.*[9] into a form very convenient for numerical work.

Our way of calculating averages is more sophisticated and more accurate[28] than the ordinary CPA, and consequently, the vertex corrections contribute to the conductivity tending to reproduce at least approximately the reduction of $\sigma_c(E)$ in the region of the spectrum whose correlations and fluctuations are more prominent. Unfortunately the numerical effort needed to determine $\sum_{ijkl} \langle V_{ij} G_{jk} V_{kl} G_{li} \rangle$ by employing our generalized

CPA makes the calculation prohibitive. Thus we have omitted the vertex corrections, as in the ordinary CPA, and have written our result for $\sigma_{\text{CPA}}(E)$ in terms of a self-energy $\Sigma(E)$ defined from the relation $\langle G(E)\rangle = G^0(E - \Sigma(E))$ where G^0 is the Green's function for the periodic lattice. This last step was made in order to use the explicit formulas given in Ref. 9 that express $\sigma_{\text{CPA}}(E)$ in terms of the real and imaginary parts of Σ.

To partly remedy the omission of the vertex corrections and the subsequent overestimation of $\sigma_c(E)$, we have attempted to determine where the eigenstates of our approximate random Hamiltonian are localized. At an eigenenergy belonging to a localized region of the band we have taken $\sigma_c(E) = 0$ while for energies belonging to the extended spectrum $\sigma_c(E)$ was not modified, i.e., $\sigma_c(E) = \sigma_{\text{CPA}}(E)$. Note that the concept of a localized eigenstate has meaning only within our static approximation. Explicitly, if the omitted time dependence of our random potential is restored, the "localized" states would become delocalized, since the particle trapped in these states can now hop. This follows because of the time dependence of the capturing fluctuations varying from region to region in a way analogous to the phonon-assisted hopping which allows a localized state to contribute to the conductivity because of the time dependence of the lattice vibrations. Thus σ_c is not actually zero in the region of "localized" eigenstates although we expect it to be considerably lower than in the region of "extended" eigenstates. We think that $\sigma_{\text{CPA}}(E)$ probably overestimates the conductivity while $\sigma_c(E)$ as corrected above (by taking it equal to zero in the localized spectrum) underestimates it and thus the actual result lies somewhere in between. Note that in the one-dimensional case, all eigenstates are localized within the static approximation and thus the lower limit of $\sigma_c(E)$ is the trivial one, $\sigma_c(E) = 0$.

Having obtained $\sigma_c(E)$ one can find the conductivity as a function of temperature $\sigma_c(T)$ from the relation

$$\sigma_c(T) = \int \sigma_c(E)\left(\frac{-\partial f}{\partial E}\right) dE . \tag{4.18}$$

The temperature dependence of $\sigma_c(T)$ can then be used to define characteristic temperatures, e.g., temperatures at which $\sigma_c(T)$ is discontinuous, temperatures at which a metal-insulator transition takes place, etc.

In Paper III of this sequence[34] we present results for the conductivity obtained by employing the above approximations. We think that the problem of response functions should be examined in greater detail within the framework of our approach and we intend to do so.

V. CONCLUDING REMARKS

Using our statistically correlated random potential approach to the many-body problem, we were able to recast quantities of interest as consisting of an "electronic" part and a "lattice" or "magnetic" part. In other words, the elementary excitations of the system can be separated into two groups: (i) the "electronic" excitations associated with quasiparticles excited across the Fermi level leaving behind quasiholes; the effective quasiparticle density of states $\rho(E)$ is sufficient to describe quantitatively this part of the spectrum: (ii) the "lattice" or "magnetic" excitations associated with changes $\delta\rho$ in the thermally occupied quasiparticle spectrum; these changes $\delta\rho$ stem from modifications of the parameter P, which, together with $\bar{\mu}_0(P)$, determines the effective random one-body potential. Note that the "lattice" excitations could have been described quantitatively in terms of $\delta\rho$ and the number of equivalent configurations of the random one-body potential; however, a much more convenient and physically transparent description is achieved by noting the equivalence of the "lattice" excitations to the excitations of an Ising model

$$H_I = -J \sum_{i,\delta}{}' \sigma_{iz}\sigma_{(i+\delta)z} ,$$

with a properly defined, possibly temperature dependent J; $i+\delta$ is any nearest neighbor of i and the prime indicates that each pair should be counted only once. In the present work we have kept only nearest-neighbor magnetic couplings, although more generally

$$H_I = -\sum_{ij}{}' J_{ij}\sigma_{iz}\sigma_{jz} .$$

Thus, the determination of the quantities of physical interest has been reduced to obtaining the density of states $\rho(E; U, T)$, which describes the "electronic" excitations, and the coupling $J(U, T)$, which describes the "magnetic" excitations; we explained above, how these quantities are found self-consistently for each value of U and T.

After our present inclusion of "lattice" or "magnetic" ordering, there remains only one last physical ingredient omitted by our random potential approach to the many body problem: The time-dependent or dynamical nature of the effective one body potential. In what follows we describe in physical terms the expected modifications of our previous conclusions as a result of the time-dependent character of the effective random potential. Although much of the motional narrowing[8] processes have already been included in our self-consistently defined $\bar{\mu}_0$, still the random potential is not static. In other words, the configuration of A's and B's over the lattice sites [see Fig. 1(c)] is not frozen but changes with time, so that an A site can become B (and vice versa). Note that whenever a site changes from A to B, $A \rightarrow B$, another site should change from B to A, $B \rightarrow A$, so that the total number of electrons with spin up (or down) is conserved. Such processes can be described by a Hamiltonian ΔH of the form

$$\Delta H = \sum_{ij} t_{ij} \sigma_i^{\dagger} \sigma_j^{-} , \tag{5.1}$$

where $\sigma_i^{\dagger}$ is the usual Pauli matrix which changes a down local moment at i to up, or equivalently a B site to A [see Fig. 1(c)]; similarly σ_j^{-} makes the transformation $A \rightarrow B$ at the site j. Thus the time-dependent character is incorporated by adding the Hamiltonian ΔH to our self-consistent static random Hamiltonian. This addition will transform the Ising part of the latter $H_I = -\sum'_{ij} J_{ij} \sigma_{iz} \sigma_{jz}$ to

$$\begin{aligned} H_I + \Delta H &= -\sum_{ij}{}' J_{ij} \left(\sigma_{iz}\sigma_{jz} - \frac{t_{ij}}{2J_{ij}} (\sigma_{ix}\sigma_{jx} + \sigma_{iy}\sigma_{jy}) \right) \\ &= -\sum_{ij}{}' J_{ij} \vec{\sigma}_i \cdot \vec{\sigma}_j = H_H . \end{aligned} \tag{5.2}$$

In arriving at the last expression the isotropy of the Hubbard model has been used, which requires that

$$t_{ij} = -2J_{ij} . \tag{5.3}$$

Thus the time-dependent nature of the problem is equivalent to changing the character of the "magnetic" excitations from Ising to Heisenberg.

The replacement of the Ising by a Heisenberg Hamiltonian would modify in general the quantities $\rho(E; U, T)$, $J(U, T)$, $\tilde{H}_0(U, T)$ which were determined self-consistently using Ising-type magnetic excitations. This question will be examined in the following paper after specific results have been obtained and analyzed.

To conclude: We have incorporated in the static random potential approximation to the Hubbard model the possibility of magnetic ordering; the latter introduces Ising-like magnetic excitations and modifies the quasi-particle spectrum. We developed techniques to determine self-consistently both the magnetic coupling constant and the modified quasiparticle spectrum ρ for every value of U/ZV and T. Furthermore, it was shown that, if the static approximation is relaxed, the magnetic excitations will become Heisenberg-like; this will lead to some additional renormalization of the self-consistent magnetic coupling constant and the shape of the quasiparticle spectrum.

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APPENDIX: GAUSSIAN RANDOM-FIELD APPROACH

The partition function $Z = \mathrm{Tr}\exp(-\beta\hat{H})$ can be written[18]

$$Z = \int D\mu\, D\nu \exp\left(-\tfrac{1}{4} U \sum_i \int_0^{\beta} [\nu_i^2(s) + \mu_i^2(s)]\, ds \right) Z(\nu, \mu) , \tag{A1}$$

where $\hat{H}$ is given by (1.1), $\beta = 1/k_B T$,

$$Z(\nu, \mu) = \mathrm{Tr}\, T_0 \exp\left(-\int_0^{\beta} \hat{H}(s)\, ds \right) ; \tag{A2}$$

T_0 is a "time" s chronological-ordering operator,

$$\begin{aligned} \hat{H}(s) = &\sum_{i\sigma} \epsilon_0 \hat{n}_{i\sigma}(s) + \sum_{ij\sigma} V_{ij} \hat{a}_{i\sigma}^{\dagger}(s) \hat{a}_{j\sigma}(s) \\ &- \tfrac{1}{2} U \sum_{i\sigma} \left(i\nu_i(s) + \sigma\mu_i(s) \right) \hat{n}_{i\sigma}(s) \end{aligned} \tag{A3}$$

and $\int D\mu\, D\nu$ denotes functional integration over the functions $\{\nu_i(s)\}$, $\{\mu_i(s)\}$.

The static approximation is to omit the dependence on the "time" s and thus reduce the functional integral in (A1) to an ordinary integral.

One can then argue that the quantities ν_i, which represent charge densities[18] at each site i, have negligible fluctuations for positive U and consequently, can be replaced by a constant determined from the total number of electrons in the system.

Using these two approximations, and choosing for convenience $\epsilon_0 = -\frac{1}{2}U$ we can then write

$$Z = \int \prod_i d\mu_i \exp\left(-\frac{\beta U}{4} \sum_i (\mu_i^2 - 1) \right) \tilde{Z} , \tag{A4}$$

where

$$\hat{H}_{\sigma} = \sum_{ij} V_{ij} a_{i\sigma}^{\dagger} a_{j\sigma} + \tfrac{1}{2} U \sum_i \mu_{i\sigma} \tilde{n}_{i\sigma} , \tag{A5}$$

$$\mu_{i\sigma} \equiv -\sigma\mu_i , \tag{A6}$$

and

$$\tilde{Z} = \mathrm{Tr}\exp\left(-\beta \sum_{\sigma} \hat{H}_{\sigma} \right) . \tag{A7}$$

To evaluate $\tilde{Z}$ we first introduce the auxiliary quantity $\tilde{Z}(\lambda)$ which is obtained by replacing U everywhere by λU. [Thus, e.g., $\tilde{Z} = \tilde{Z}(1)$.] One can then easily show that

$$-\frac{1}{\beta}\ln\tilde{Z}=-\frac{1}{\beta}\ln\tilde{Z}(0)+\int_0^1 d\lambda\sum_{i\sigma}\tfrac{1}{2}U\mu_{i\sigma}\bar{n}_{i\sigma}(\lambda)\,, \qquad \text{(A8)}$$

where $\bar{n}_{i\sigma}(\lambda)$ is the thermodynamic average of $\hat{n}_{i\sigma}$ corresponding to the value λ and is given by

$$\bar{n}_{i\sigma}(\lambda)=-\frac{1}{\pi}\int \mathrm{Im}G_{i\sigma}(E^+;\lambda)f(E)\,dE\,. \qquad \text{(A9)}$$

The Green's function $G_{i\sigma}(z;\lambda)$ is defined the usual way:

$$G_{i\sigma}(z;\lambda)=\langle i\sigma\|[\hat{z}-\hat{H}_\sigma(\lambda)]^{-1}|\sigma i\rangle\,, \qquad \text{(A10)}$$

and E^+ denotes the limit $\lim_{s\to 0^+}(E+is)$ and f represents the Fermi distribution $f(E)=(e^{\beta E}+1)^{-1}$. Note, since we have assumed one electron per lattice site and taken $\epsilon_0=-\frac{1}{2}U$, the chemical potential μ is zero for all temperatures.

The partition function can be written by combining Eqs. (A4), (A7), and (A8) as

$$Z=\tilde{Z}(0)\int\prod_i d\mu_i\,\mathrm{e}^{-\beta\tilde{F}}\,, \qquad \text{(A11)}$$

with

$$\tilde{F}=\frac{U}{4}\sum_i(\mu_i^2-1)+\frac{U}{2}\sum_{i\sigma}\mu_{i\sigma}\int_0^1 d\lambda\,\bar{n}_{i\sigma}(\lambda)\,. \qquad \text{(A12)}$$

Equations (A9), (A10), (A11), and (A12) have actually reduced the many-body problem to a random one body one. The free energy $\tilde{F}$ can also be expressed as

$$\tilde{F}=\frac{U}{4}\sum(\mu_i^2-1)-\sum_{i\sigma}\int dE\,f(E)[D_{i\sigma}(E)-D^0_{i\sigma}(E)]\,, \qquad \text{(A12}'\text{)}$$

where $D_{i\sigma}$, is the cumulative density of states per site per spin,

$$D_{i\sigma}(E)=-\frac{1}{\pi}\int_{-\infty}^{E}\mathrm{Im}G_{i\sigma}(E'^+)\,dE'\,,$$

and $D^0_{i\sigma}\equiv D_{i\sigma}$ when $U=0$. Equation (A12′) can be derived from (A12) by introducing $D_{i\sigma}(E;\lambda)$ corresponding to λU instead of U and then showing that

$$-\sum_{i\sigma}\int dE\,f(E)\frac{\partial D_{i\sigma}(E;\lambda)}{\partial\lambda}=\frac{U}{2}\sum_{i\sigma}\mu_{i\sigma}\bar{n}_{i\sigma}(\lambda)\,.$$

The last step is based upon the general relations $\partial\hat{G}/\partial\chi=\hat{G}\partial\hat{H}/\partial\chi\hat{G}$ and $\partial\hat{G}/\partial E=-\hat{G}^2$, where $\hat{G}=(\hat{E}-\hat{H})^{-1}$ and χ is any parameter entering $\hat{H}$. Note that Eq. (A12) does not agree with the corresponding expression obtained by Cyrot.[7,18] The difference is due to the additional approximation. employed by Cyrot,[7,18] of omitting the change in $\hat{G}_{i\sigma}$ due to variations in μ_j for $j\neq i$. Note also that the general expression for the free energy of noninteracting quasiparticles is

$$F_{qp}=\mu N-\sum_{i\sigma}\int dE\,f(E)D_{i\sigma}(E)\,,$$

where $D_{i\sigma}(E)$ is the corresponding cumulative density of states per site. In our case the chemical potential $\mu=0$; the first term in the righthand side of Eq. (A12′) corrects automatically for the doublecounting of the interaction term in $\hat{H}_\sigma(\sigma=\pm 1)$; the last term is compensated by $\tilde{Z}(0)$. Thus, Eq. (A12′) has the expected form.

The integration in (A11) can be performed using the saddle-point approximation, which picks out the most probable values of $\{\mu_i\}$, which we will term μ_{i0}, corresponding to the minimum of F, i.e.,

$$\left(\frac{\partial F}{\partial\mu_i}\right)_{\mu_j=\mu_{j0}}=0\,. \qquad \text{(A13)}$$

Again employing the relation $\partial\hat{G}/\partial\chi=\hat{G}(\partial\hat{H}/\partial\chi)\hat{G}$, one can easily show that

$$\sum_{i\sigma}\mu_{i\sigma}\frac{\partial G_{i\sigma}}{\partial\mu_j}=\sum_\sigma(-\sigma)\frac{\partial G_{j\sigma}}{\partial\lambda}\lambda\,, \qquad \text{(A14)}$$

and finally by using this result in conjunction with Eqs. (A12) and (A9), we obtain Eq. (2.5) of the text

$$\mu_{i\sigma}=\bar{n}_{i\uparrow}-\bar{n}_{i\downarrow}\,. \qquad \text{(A15)}$$

Note that Eq. (A 15) is a generalized Hartree-Fock self-consistency condition since it states that the most probable local effective potential energy that an electron with spin σ experiences at the site j is equal to $\epsilon_0+U\bar{n}_{j-\sigma}$.

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