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Critical study of the functional-integral method applied to the itinerant magnetism

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We have studied the Anderson model using the functional-integral technique within the static approximation and at the saddle points, with the hope of clarifying a few of the primary difficulties which have hindered the understanding of itinerant magnetism using this technique. The intra-atomic Coulomb repulsion term $Un_\uparrow n_\downarrow$ has been resolved into four different classes of quadratic forms of the electron number operator, representing a generalization of transformations previously proposed in the literature. In particular, we analyze in which conditions the use of such identities yield Anderson's Hartree-Fock result. We conclude that the application of the functional-integral method to the study of the Anderson and Hubbard models does not suffer from any arbitrariness, or ambiguity, as has been claimed in the literature.

I. INTRODUCTION

There has been a great effort in using functional-integral (FI) methods to understand the basic properties of itinerant electron magnetism over the last decade.[1–19] The main stream is to formulate a consistent theory able to reconcile both the localized and itinerant aspects found in the magnetic properties of the transition metals and alloys. However, many attempts to provide a unified picture have been hindered by difficulties in including the major aspects of the real physics of the problem, and by a proper comprehension in handling the formalism mentioned above. The purpose of the present paper is to discuss these various points, with the aim of shedding some light on a few of the primary difficulties.[20]

The basic features of itinerant magnets are thought to be contained in the Hubbard model,[21] while those related to the formation of localized moments in nonmagnetic metals are described by the so-called Anderson model.[22] In both cases the basic electron interaction is a local repulsive Coulomb interaction between electrons of opposite spins, namely, $Un_\uparrow n_\downarrow$, where n_σ is the electron number operator of spin σ ($=\uparrow$ or $\downarrow$) and U is the coupling strength.

The application of the FI method is based on the use of the Hubbard-Stratonovich transformation.[23] With this identity, one can exactly transform the problem of the interacting d^1 electrons to one of free electrons moving in space- and time-varying fields, the fields being averaged over with Gaussian weight. The arduousness after that is the calculation of a partition function in which both lattice position (wave vector) and time (frequency) are present.

In the literature, it is often pointed out[13,18–20] that the ambiguity of the method arises from the fact that it may be possible to resolve the electron interaction into quadratic forms of the electron number operator (properly applying the Hubbard-Stratonovich transformation) in more than one way. If the partition function is calculated exactly, the final result is obviously independent of the decomposition used. However, in the literature we find that different decompositions, which have been exploited by different approximations, lead to distinct results. As a consequence, the method has been termed "arbitrary" and "ambiguous." In our point of view the arbitrariness and ambiguity claimed in the literature is because of an improper understanding of the formalism as applied to the Hubbard and Anderson models. We share the opinion of Castellani and Di Castro[20] that a clarification of the formal apparatus in which this problem has been formulated, is preliminary to any practical application to a specific physical situation. With that in mind, but with practical concerns, we have studied the Anderson model, within

the static approximation (SA) and at the saddle points, by the FI technique using many representative classes of decompositions. We find that only one of the classes investigated has the property that its members (decompositions) reproduce the same result. Furthermore, as it should, at this level of approximation the result is equivalent to the original Anderson solution,[22] i.e., the Hartree-Fock (HF) approximation. Although several authors have anticipated the latter fact, there were severe doubts concerning its universality when using different decompositions for the interacting term. In this paper we show that these doubts are unfounded. Finally, we should mention that the use of the Anderson model in this study is to be understood as a device, with the hope of producing information for more general applications of the method. In fact, the basic properties of this model have been fully described by the renormalization-group technique in a very recent investigation.[24] However, the study of ferromagnets with local-moment behavior above the critical temperature can, to lowest order, be considered the problem of a collection of one-center problems.[3] Recently, this concept has been successfully explored by Hasegawa.[16,17] He regarded a single atom of a pure magnetic metal as an "impurity" embedded in the "host" pure metal. The self-consistency condition for the impurity and host atoms determines the physical properties of the metal in both the ferromagnetic and paramagnetic states. In spite of its simplicity, application[17] of this scheme to iron and nickel yields results for various thermodynamic properties, which are in qualitatively, or semiquantitatively good agreement with the experimental data.

The outline of the rest of the present paper is as follows: In Sec. II we derive four classes of identities for the intra-atomic Coulomb repulsion term $Un_\uparrow n_\downarrow$. In Sec. III we use these identities to calculate the partition function of this model within the SA and at the saddle points. In particular, we analyze in which conditions the use of such identities yield Anderson's HF result for $\langle n_\sigma \rangle$. At this level of approximation, the HF result is often required[5,18,19] as an essential prerequisite to proceeding to more elaborate theories. Finally, Sec. IV is devoted to a discussion of the results obtained in the previous sections.

II. MODEL HAMILTONIAN AND TRANSFORMATIONS

Let us consider the one-center problem defined by the Anderson Hamiltonian[22]

$$\mathscr{H}=\mathscr{H}_0+\mathscr{H}_1 , \tag{1}$$

with

$$\mathscr{H}_0=\sum_{\vec{k},\sigma} E_{\vec{k}} n_{\vec{k}\sigma}+\sum_\sigma E_d n_\sigma + \sum_{\vec{k},\sigma} (V_{\vec{k}d} C^\dagger_{\vec{k}\sigma} C_\sigma + \text{H.c.}) \tag{2}$$

and

$$\mathscr{H}_1=Un_\uparrow n_\downarrow , \tag{3}$$

where the first term of Eq. (2) represents the band of the metallic host, the second is the d level of the impurity, and the last one is the hybridization term between the host band and the d level. $\mathscr{H}_1$ is the intra-atomic Coulomb repulsion $n_\sigma = C^\dagger_\sigma C_\sigma$, and C_σ ($C^\dagger_\sigma$) is the annihilation (creation) operator of an electron with spin σ in the d level [$C_{\vec{k}\sigma}$ ($C^\dagger_{\vec{k}\sigma}$) denotes the same for an electron with wave vector $\vec{k}$ and spin σ in the metallic band].

In order to evaluate the partition function of the system using the FI method, we shall decompose the interaction term $\mathscr{H}_1$ in appropriate quadratic forms of $n_\uparrow$ and $n_\downarrow$. This fact has led to the appearance of many such decompositions in the literature, which in turn have created uncertainties and doubts about the effectiveness of the method.

If one wants to bring effective spin and charge fields associated with $(n_\uparrow - n_\downarrow)$ and $(n_\uparrow + n_\downarrow)$, respectively, into the problem, the most naive transformation for $\mathscr{H}_1$ is

$$Un_\uparrow n_\downarrow = rU(n_\uparrow^2+n_\downarrow^2)-\tfrac{1}{4}(2r-1)U(n_\uparrow+n_\downarrow)^2 - \tfrac{1}{4}(2r+1)U(n_\uparrow-n_\downarrow)^2 , \tag{4}$$

where r is an arbitrary parameter. The first term in Eq. (4) appears just to cancel out terms proportional to $n_\uparrow^2$ and $n_\downarrow^2$ coming from the last two terms associated with charge and spin fields. The necessity of canceling out these contributions arises because they represent spurious interactions among electrons with the same spin (thus violating Pauli's principle) not present in the initial Hamiltonian. A particular case of (4) is Hamann's decomposition,[5] with the choice $r=0$. It is the simplest transformation if both spin and charge fields are to be engaged.

Now, by using the fermion property $n_\sigma^2=n_\sigma$, identity (4) can be rewritten in the form

$$Un_\uparrow n_\downarrow = rU(n_\uparrow+n_\downarrow)-\tfrac{1}{4}(2r-1)U(n_\uparrow+n_\downarrow)^2 - \tfrac{1}{4}(2r+1)U(n_\uparrow-n_\downarrow)^2 . \tag{5}$$

In this case, the choice $r=\frac{1}{2}$ gives the Wang,

Evenson, and Schrieffer decomposition.[1] It has the apparent advantage of just retaining the effective spin field. However, we should notice that although Eq. (5) is a true property for fermion operators, this would not occur if n_σ would be a c number, since in the latter case there would be no algebraic cancelation of terms proportional to $n_\uparrow^2$ and $n_\downarrow^2$ in the right-hand side of (5).

The above identities were termed[13] Ising-like transformations because of the spin reprsentation of fermion operators $S^z=\frac{1}{2}(n_\uparrow-n_\downarrow)$. However, by using $S^+=C_\uparrow^\dagger C_\downarrow$, $S^-=C_\downarrow^\dagger C_\uparrow$, where $S^\pm=S^x\pm iS^y$, and the commutation relation for fermion operators, we have

$$\vec{S}\cdot\vec{S}=\tfrac{1}{4}(n_\uparrow-n_\downarrow)^2+\tfrac{1}{2}(n_\uparrow+n_\downarrow)-n_\uparrow n_\downarrow \ . \tag{6}$$

By completing the square in (6), Gomes and Lederer[13] found the identity

$$Un_\uparrow n_\downarrow=\frac{U}{4}(n_\uparrow+n_\downarrow)+\frac{U}{8}(n_\uparrow+n_\downarrow)^2-\frac{U}{2}\vec{S}\cdot\vec{S} \ . \tag{7}$$

On the other hand, by using $n_\sigma=n_\sigma^2$ in the second term of Eq. (6) we obtain $(S^z)^2=\frac{1}{4}(n_\uparrow-n_\downarrow)^2=\frac{1}{3}\vec{S}\cdot\vec{S}$. Thus, the last term of both Eqs. (4) and (5) can be rewritten in a form in which spin rotational invariance appears explicitly. In this latter form they were termed[13] Heisenberg-like transformations. In fact, if we set $r=\frac{1}{4}$ and $\frac{1}{4}(n_\uparrow-n_\downarrow)^2=\frac{1}{3}\vec{S}\cdot\vec{S}$, in Eq. (5), we find Eq. (7) which was obtained before[13] without using $n_\sigma=n_\sigma^2$.

In concluding this section we should state that four basic classes of transformations have been derived, namely Eqs. (4), (5), and the Heisenberg-type versions of these identities. In Sec. III, use will be made of these identities to calculate the partition function of the Anderson model within the SA and at the saddle points.

III. RESULTS USING THE FUNCTIONAL-INTEGRAL METHOD

In this section we shall outline the main steps in calculating the partition function and the desired thermodynamic properties. Using identity (4) the partition function of the system is written as

$$Q=\int d\xi\, d\eta\, d\Phi\, d\chi \exp[-\beta F(\xi,\eta,\Phi,\chi)] \ , \tag{8}$$

with

$$\beta F(\xi,\eta,\Phi,\chi)=\pi(\xi^2+\eta^2+\Phi^2+\chi^2)-\ln Z(\xi,\eta,\Phi,\chi) \ , \tag{9}$$

where ξ, η, Φ, and χ are fluctuating fields associated with $(n_\uparrow-n_\downarrow)$, $(n_\uparrow+n_\downarrow)$, $n_\uparrow$, and $n_\downarrow$ respectively, and

$$Z(\xi,\eta,\Phi,\chi)=\mathrm{Tr}\exp\left[-\beta\mathscr{H}_0-\sum_\sigma V_\sigma n_\sigma\right] . \tag{10}$$

Here

$$V_\sigma=-[\sigma a\xi+b\eta+c(\delta_{\sigma,\uparrow}\Phi+\delta_{\sigma,\downarrow}\chi)] \tag{11}$$

and

$$a=[(2r+1)\pi\beta U]^{1/2} \ , \tag{12}$$

$$b=[(2r-1)\pi\beta U]^{1/2} \ , \tag{13}$$

$$c=(-4r\pi\beta U)^{1/2} \ . \tag{14}$$

We should stress that four effective fields have been invoked in this case.

In order to calculate Z one may introduce[1] Z_λ obtained from Eq. (10) by the replacement $V_\sigma\to\lambda V_\sigma$, where λ is a parameter. In this way we can write

$$\frac{\partial\ln Z_\lambda}{\partial\lambda}=-\sum_\sigma V_\sigma\langle n_\sigma\rangle_\lambda \ , \tag{15}$$

where the thermodynamic average $\langle\ \rangle_\lambda$ is calculated using the density matrix

$$\rho=\frac{\exp\left[-\beta\mathscr{H}_0-\lambda\sum_\sigma V_\sigma n_\sigma\right]}{Z_\lambda} \ . \tag{16}$$

Now, to evaluated $\langle n_\sigma\rangle_\lambda$, we can write

$$\langle n_\sigma\rangle_\lambda=\lim_{\delta\to0}\sum_n e^{i\delta\omega_n}G_\sigma^\lambda(\omega_n) \ , \tag{17}$$

where δ is a positive convergence factor, ω_n are the usual Matsubara frequencies, and $G_\sigma^\lambda(\omega_n)$ is given by

$$G_\sigma^\lambda(\omega_n)=\frac{1}{(G^0)^{-1}-\lambda V_\sigma} \ . \tag{18}$$

Here G^0 is the Anderson-type d-electron Green's function[22]

$$G^0=\frac{1}{i\omega_n-\beta E_d+i\beta\Delta\,\mathrm{sgn}(\omega_n)} \ , \tag{19}$$

where $\Delta\approx\pi\rho(E_d)\,|\,V_{\vec{k}d}\,|_{av}^2$ is the width of the d state and $\rho(E_d)$ is the density of states of the conduction electrons in the host metal at the energy of the resonance level. The frequency sum of Eq. (17) can be evaluated[7] giving

$$\langle n_\sigma\rangle_\lambda=\frac{1}{2}+\frac{1}{\pi}\mathrm{Im}\Psi\left[\frac{1}{2}+\frac{\beta\Delta}{2\pi}-\frac{i}{2\pi}(\beta E_d+\lambda V_\sigma)\right], \tag{20}$$

where Ψ is the digamma function, defined by $\Psi(x)=(d/dx)\ln\Gamma(x)$, $\Gamma(x)$ being the gamma function. Taking $\beta\Delta>>1$, we can write $\Gamma(x)\to(2\pi)^{1/2}x^{x-1}e^{-x}$, valid for large x, and obtain

$$\langle n_\sigma\rangle_\lambda=\frac{1}{2}-\frac{1}{\pi}\tan^{-1}\left[\frac{\beta E_d+\lambda V_\sigma}{\beta\Delta}\right]. \tag{21}$$

Returning now to Eq. (15), and using (21), we have after integration[25] ($Z_{\lambda=1}\equiv Z$ and $Z_{\lambda=0}\equiv Z_0$)

$$\begin{aligned}\ln\left[\frac{Z}{Z_0}\right]=&b\eta+\tfrac{1}{2}c(\Phi+\chi)\\&-\sum_\sigma\left\{\frac{\beta\Delta}{2\pi}\ln\left[1+\left[\frac{\beta E_d+V_\sigma}{\beta\Delta}\right]^2\right]-\frac{1}{\pi}(\beta E_d+V_\sigma)\tan^{-1}\left[\frac{\beta E_d+V_\sigma}{\beta\Delta}\right]\right\}\\&-\frac{\beta\Delta}{\pi}\ln\left[1+\left[\frac{E_d}{\Delta}\right]^2\right]+\frac{2\beta E_d}{\pi}\tan^{-1}\left[\frac{E_d}{\Delta}\right].\end{aligned} \tag{22}$$

Finally, at the saddle points, where $(\partial F/\partial\xi)=(\partial F/\partial\eta)=(\partial F/\partial\Phi)=(\partial F/\partial\chi)=0$, we obtain, from Eq. (10), the relationships between the effective fields and the average number of d electrons ($\langle n_\sigma\rangle_{\lambda=1}\equiv\langle n_\sigma\rangle$)

$$\bar{\xi}=\frac{a}{2\pi}\sum_\sigma\sigma\langle n_\sigma\rangle, \tag{23}$$

$$\bar{\eta}=\frac{b}{2\pi}\sum_\sigma\langle n_\sigma\rangle, \tag{24}$$

$$\bar{\Phi}=\frac{c}{2\pi}\sum_\sigma\delta_{\sigma,\uparrow}\langle n_\sigma\rangle, \tag{25}$$

and

$$\bar{\chi}=\frac{c}{2\pi}\sum_\sigma\delta_{\sigma,\downarrow}\langle n_\sigma\rangle. \tag{26}$$

Equations (11) and (21)–(26) form the self-consistent set of equations of the problem. From it the expression for $\langle n_\sigma\rangle$ can be cast in the form

$$\begin{aligned}\langle n_\sigma\rangle=\frac{1}{\pi}\cot^{-1}(\{E_d+U[\langle n_{-\sigma}\rangle-2r\langle n_\sigma\rangle\\+2r\langle n_\sigma\rangle(\delta_{\sigma,\uparrow}+\delta_{\sigma,\downarrow})]\}/\Delta),\end{aligned} \tag{27}$$

where the contributions of the auxiliary fields Φ and χ appear explicitly in the last term in the argument of the arc cotangent. As we see, it cancels out the spurious contribution proportional to r, coming from the charge and spin fields. In this way, Eq. (27) can be rewritten in the form

$$\langle n_\sigma\rangle=\frac{1}{\pi}\cot^{-1}[(E_d+U\langle n_{-\sigma}\rangle)/\Delta], \tag{28}$$

which is Anderson's Hartree-Fock result.[22] Further, we can study the free energy F [see Eq. (9)] as a function of the auxiliary spin field ξ by using Eq. (22) and the values of η, Φ, and χ at the saddle points [Eqs. (24)–(26)]. Assuming the so-called symmetric case where $E_d=-U/2$, we obtain: For $(\pi\Delta/U)>1$ the minimum of F occurs in $\xi=0$, corresponding in the limit $(\pi\Delta/U)>>1$ to weakly exchange-enhanced Pauli paramagnetism.[1–5] For $(\pi\Delta/U)<1$ minima develop symmetrically about the origin. When $(\pi\Delta/U)<<1$ we reach the strongly localized-moment regime, the two minima corresponding to the up and down spin states.[1–5]

Let us proceed to apply the other three identities to study the same model. Using, for example, transformation (5), we obtain an equation for $\langle n_\sigma\rangle_\lambda$ similar to (21), where $E_d\to E_d+rU$ and $V_\sigma=-(\sigma s\xi+b\eta)$. We should point out that the renormalization of the energy of the d level is due to the first term in the right-hand side of (5), which is absorbed in $\mathscr{H}_0$ and thus treated exactly. Therefore, only two auxiliary fields are necessary. Now, following the same procedure as before, we find

$$\begin{aligned}\langle n_\sigma\rangle=\frac{1}{\pi}\cot^{-1}\{[E_d+U(r-2r\langle n_\sigma\rangle\\+\langle n_{-\sigma}\rangle)]/\Delta\}.\end{aligned} \tag{29}$$

In this case there is not a natural cancelation

among terms proportional to r, and we get (28) for just one value of r, namely $r=0$. It is not surprising since for this value of r both identities (4) and (5) are exactly the same.

To further clarify the problem of using identity (5) we have studied the diagram $n=\langle n_\uparrow\rangle+\langle n_\downarrow\rangle=2\pi\bar{\eta}/b$ [from Eq. (24)] versus $\pi\Delta/U$ where regions of magnetic and nonmagnetic behavior appear. At these "transitions", where $m=\langle n_\uparrow\rangle-\langle n_\downarrow\rangle=2\pi\bar{\xi}/a=0$ [from (23)], we have $\partial^2F/\partial\xi^2(\xi=0,\eta)=0$, and the following equation results:

$$\pi\Delta/U=(2r+1)\sin^2(\pi n_c/2)\ , \tag{30}$$

where n_c is the value of n where $\langle n_\uparrow\rangle=\langle n_\downarrow\rangle$. In Fig. 1 we show such a diagram for three values of r. For a given value of r, the area where the system exhibits magnetic behavior is equal to $2r+1$. As is easily deduced, no formation of localized moment occurs for $r\le-\frac{1}{2}$. This is clear and strong evidence that we have no confidence in the final result when using identity (5) in the present approximation.

Finally, let us investigate the Heisenberg-type versions of identities (4) and (5). Now, apart from the charge field η and the spin field ξ associated with the longitudinal part (z components) of $\vec{S}\cdot\vec{S}$, we have to introduce two new fields to account for the transversal part of $\vec{S}\cdot\vec{S}$. In this case, we have the Green's function

$$G_\sigma(\omega_n)=\frac{1}{(G^0)^{-1}-V_{\sigma,\sigma}-\{V_{\sigma,-\sigma}V_{-\sigma,\sigma}/[(G^0)^{-1}-V_{-\sigma,-\sigma}]\}}\ , \tag{31}$$

where

$$V_{\sigma,\sigma'}=-\left[\frac{\sigma}{\sqrt{3}}a\xi+b\eta+c(\delta_{\sigma,\uparrow}\Phi+\delta_{\sigma,\downarrow}\chi)\right]\delta_{\sigma,\sigma'}-\frac{a}{\sqrt{3}}\bar{\xi}^\sigma\delta_{\sigma,-\sigma'}\ , \tag{32}$$

and G^0 is defined by Eq. (19). However, for $\beta\Delta>>1$, the contribution of the transversal part to $G_\sigma(\omega_n)$ is negligible, and Eq. (18) is recovered [with $a\to a/\sqrt{3}$ in Eq. (11)] for $\lambda=1$. This means that the auxiliary fields associated with the transversal part give no contribution, i.e., at the saddle points

$$\bar{\xi}^\sigma=\frac{a}{\pi\sqrt{3}}\langle C_\sigma^\dagger C_{-\sigma}\rangle=0\ .$$

Again, following the same steps as in the Ising case, we find for the Heisenberg-type version of Eq. (4),

$$\langle n_\sigma\rangle=\frac{1}{\pi}\cot^{-1}(\{E_d+\tfrac{2}{3}U[(r+\tfrac{1}{2})\langle n_\sigma\rangle+(1-r)\langle n_{-\sigma}\rangle]\}/\Delta)\ . \tag{33}$$

The Hartree-Fock result is obtained only for $r=-\frac{1}{2}$. This is a trivial case in which the $\vec{S}\cdot\vec{S}$ term proportional to $(2r+1)$ is not present, reducing to a particular case of Eq. (4) (no spin field component).

Using now the Heisenberg-type version of Eq. (5), we obtain

$$\langle n_\sigma\rangle=\frac{1}{\pi}\cot^{-1}\left\{\left[E_d+U\left[r-\frac{(4r-1)}{3}\langle n_\sigma\rangle+\tfrac{2}{3}(1-r)\langle n_{-\sigma}\rangle\right]\right]/\Delta\right\}\ . \tag{34}$$

It is clear from the equation above that for $r\neq\frac{1}{4}$, contributions of spurious interactions are present. On the other hand, for $r=\frac{1}{4}$ we get a HF-like equation [see (28)] with renormalized d-electron en-

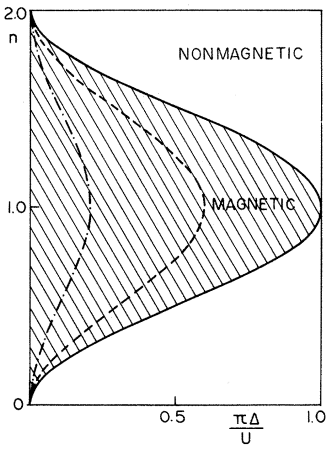

FIG. 1. Illustration of regions of magnetic and nonmagnetic behavior using identity (5). The full line is for $r=0$ [which is the result when using identity (4) for any value of r], the dashed line is for $r=-0.2$ and the dashed-dot line is for $r=-0.4$. The curves give n_c vs $\pi\Delta/U$ for the three values of r.

ergy and Coulomb coupling given by $\tilde{E}_d = E_d + \frac{1}{4}U$ and $\tilde{U} = U/2$, respectively. It is important to remember that for this value of r a Heisenberg-type transformation is derived without using $n_\sigma^2 = n_\sigma$, and therefore, no violation of Pauli's principle occurs, contrary to the suggestion of Ref. 19.

Finally, we should mention that if we perform a HF approximation ($n_\sigma n_{\sigma'} \rightarrow n_\sigma \langle n_{\sigma'} \rangle + n_{\sigma'} \langle n_\sigma \rangle$ and $\vec{S}\cdot\vec{S} \rightarrow 2S^z\langle S^z \rangle + S^+\langle S^- \rangle + S^-\langle S^+ \rangle$), directly to the interaction Hamiltonian $\mathscr{H}_1$ after the transformations of Sec. II are used, we get the same results for $\langle n_\sigma \rangle$ which have been obtained in this section using the FI technique. Therefore, both approaches are consistent at this level of approximation.

IV. DISCUSSION AND CONCLUSIONS

We have studied the Anderson model using the FI formalism within the SA and at the saddle points, with the hope that the results so obtained will clarify a few of the primary difficulties which have hindered the understanding of itinerant magnetism using this technique. The interaction Hamiltonian has been resolved into four different classes of quadratic forms of the electron number operator, representing a generalization of transformations previously proposed in the literature.

The results derived in the last section permit us to summarize the following: (i) The application of the FI method to the Anderson model yields, within the SA and at the saddle points, the same results of Anderson's HF theory for the whole class of identities defined by Eq. (4). For an arbitrary value of the parameter r, it was very clear that the effect of spurious interactions existing in the spin- and chargelike terms are canceled out by contributions of the auxiliary fields associated to $n_\uparrow^2$ and $n_\downarrow^2$. For $r=0$, the latter auxiliary fields are not present but the conjugate action of the spin and charge fields is free of these problems. (ii) The use of $n_\sigma^2 = n_\sigma$ to obtain (5) from (4), or the use of $n_\sigma = n_\sigma^2$ to deduce $(S^z)^2 = \frac{1}{3}\vec{S}\cdot\vec{S}$, and thus generating the Heisenberg-type versions of (4) and (5), are sources of spurious interactions whose effects persist toward the final result [see Eqs. (29), (33), and (34)]. This can also be understood by noticing that in a HF-like approximation n_σ^2 is replaced by $2\langle n_\sigma \rangle n_\sigma$, which is not identical to n_σ. Therefore, the same problem should appear when using the FI method within the SA and at the saddle points if identities such as (5) are used. (iii) The question of using transformation (7), i.e., a Heisenberg-type version of (5) for $r = \frac{1}{4}$, deserves a separate discussion. In its derivation use was not made of $n_\sigma^2 = n_\sigma$, which explains the HF-like result with renormalized d-electron energy and Coulomb coupling.

In the following, we shall try to combine the results sketched above with others existing in the literature, so that some general conclusions can be drawn which are not restricted to the level of approximation used in this paper: (a) Result (i) teaches us that there is not a true "superiority" of a given transformation as suggested in Ref. 8 (but rather a convenience) since an infinite number of such transformations yield the same result. Notice also that these transformations may differ in a number of basic aspects. For instance, by varying the value of r in Eq. (4), one may obtain transformations with four, three, or two auxiliary fields. Therefore, we have found at least one class of transformations [see Eq. (4)] such that the effect of spurious interactions, not present in the initial Hamiltonian $Un_\uparrow n_\downarrow$, are canceled out in any level of approximation in which all contributing terms are treated on the same footing. (b) On the other hand, it is clear form (ii) that when using approximations based on poor truncations, as in the case of HF, the majority of classes of transformations may lead to illogical results, as was demonstrated in Sec. III. Using these transformations, the contributing terms may not be treated on the same footing and, in consequence, effects of spurious interactions do appear at the end. However, if a perturbative method is carried out to all orders of perturbation, these effects may be ruled out, or drastically diminished from the final results, as was evidenced by Keiter.[7] A very recent example is the work of Ref. 24. There, a transformation similar to Eq. (5) but with no spin field, is introduced with a convenient charge field in which a background of a unit of charge is subtracted. In this case the renormalization group technique is powerful enough to produce sensible results. (c) As far as Heisenberg-like transformations are concerned we have the following comments: It is usually required[2,12–14,18,19] that the spin-like term should display spin-rotational invariance explicitly, so that the derived magnetic properties would explicitly contain the symmetry of the original system. However, we should not disregard the contribution of the chargelike terms to the magnetic properties. In that sense, a combining effect of both spin- and chargelike terms (or even transformations contain-

ing chargelike terms alone), could provide a final result with the right symmetry of the original system. If one decides to use a Heisenberg-type transformation, the best one available is Eq. (7), which gives a HF-like result as discussed in (iii). We are now investigating the universality of the results when using different transformations in more elaborated schemes, by comparing a recent study[13,14] of critical phenomena in itinerant magnets, using Eq. (7), with one employing Eq. (4). Finally, we should mention that attempts to introduce Heisenberg-like transformations have recently been made[18,19] in which a Hartree-Fock (Stoner) result could be recovered in the SA and at the saddle points. This has been obtained with a kind of average procedure which would be equivalent to replacing $(S^z)^2 \rightarrow \vec{S}\cdot\vec{S}$ [instead of $(S^z)^2 \rightarrow \frac{1}{3}\vec{S}\cdot\vec{S}$] and $r=0$ in Eq. (4). This imposition in obtaining HF may be a source of spurious results in more elaborate approximations. However, the method may be adequate in building an effective theory in treating degenerate d bands, in which the couplings associated to the spin- and chargelike terms are replaced by effective couplings with no *ab initio* relation between one another, as one naturally obtains in the case of the single-band Hubbard model.

In conclusion, we would like to stress that the application of the FI method to the study of the Anderson and Hubbard models, does not suffer of any arbitrariness or ambiguity as has been claimed in the literature. However, care must be exercised when a given transformation for the interacting term is used and a specific approximation is made, as has been fully evidenced in this paper.

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[25]If one uses (20) instead of (21) the following expression is obtained:

$$\ln(Z/Z_0) = -\sum_{\sigma}\left[\frac{1}{2}V_\sigma + 2\ln\left|\Gamma\left[\frac{1}{2}+\frac{\beta\Delta}{2\pi}-\frac{i}{2\pi}(\beta E_d+V_\sigma)\right]\Big/\Gamma\left[\frac{1}{2}+\frac{\beta\Delta}{2\pi}-\frac{i}{2\pi}(\beta Ed)\right]\right|\right],$$

which reduces to (22) in the limit $\beta\Delta >> 1$.