Phase diagrams of the two-dimensional Hubbard model

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The magnetism of strongly correlated electrons in narrow energy bands is a relevant phenomenon for several technologically important materials. In this paper, we investigate the conditions for ferromagnetism of the two-dimensional Hubbard model by the functional-integral method. Using the static and uniform approximation for the partition function of the system we have determined the functional free energy for a squared lattice. Thus we have obtained magnetic phase diagrams equivalent to the Hartree-Fock approximation ones. We have observed the existence of a critical temperature (T_C) and of a critical onsite Coulombian electrons interaction (U_C) for occurrence of spontaneous magnetization in the context of our approximations. We have obtained several phase diagrams relating T, U and n (average number of electrons per site). We graphically verified the dependence of T_C and U_C with respect to n, besides the dependence of T_C with respect to n and U simultaneously. In the half-filled-band case (n=1) we have obtained an analytical expression for U_C, for some given temperatures. The determination of T_C and U_C for the spontaneous magnetization occurrence contributes to show the functional characteristics of this method. The shape of the curves relative to temperature agrees qualitatively with that expected for itinerant electrons magnetic systems. We have shown that besides the existence of a minimum value for the Coulombian interaction energy for occurrence of spontaneous magnetization, there is a saturation point, that is, a limiting value for the magnetization increase, as expected.

Keywords: functional integral method, Hubbard model, magnetism of itinerant electrons

1. INTRODUCTION

The development of a consistent theory for magnetism of strongly correlated electron systems has challenged statistical physics since the 30's. During all this time there were important progresses about the microscopic origin, but safe theoretical methods have not been attained for determining the thermodynamics properties of such systems in consonance with the extraordinary available experimental results.

The functional integral method was created[1,2] to study strongly correlated electrons systems at the end of the 50's, and was largely theoretically developed[3-7] at the 70's and 80's. The method presents innovative aspects concerning electron correlations since it converts complex interactions in quanta fields which spatially and temporally fluctuates over electrons which hypothetically do not interact with each other.

In this paper, we use the model introduced by Hubbard in order to deal with electron correlations in narrow energy bands, which is well known as Hubbard model[8].

Let $\phi(\mathbf{r} - \mathbf{R_i})$ be the atomic wave function for an electron in an atom at a site $\mathbf{R_i}$, and $c_{i\sigma}^+$ ($c_{i\sigma}$) the creation (annihilation) operator for an electron at the site $\mathbf{R_i}$, where $\sigma = \pm 1$, or $\uparrow$ and $\downarrow$, is the spin label. In the "tight binding" approximation the Hamiltonian can be written

$$H = \sum_{ij,\sigma} T_{ij} c_{i\sigma}^+ c_{j\sigma} + \frac{1}{2} \sum_{i,j,k,l} \sum_{\sigma,\sigma'} \langle ij | \frac{1}{r} | kl \rangle c_{i\sigma}^+ c_{j\sigma'}^+ c_{l\sigma'} c_{k\sigma} , \qquad (1)$$

where

$$T_{ij} = \int \phi^*(\mathbf{r} - \mathbf{R}_i) \left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \phi(\mathbf{r} - \mathbf{R_j}), \qquad (2)$$

and

$$\langle ij|\frac{1}{r}|kl\rangle = e^2 \int \phi^*(\mathbf{r}-\mathbf{R_i})\phi^*(\mathbf{r}-\mathbf{R_j}) \times \frac{1}{|\mathbf{r}-\mathbf{r}'|}\phi(\mathbf{r}-\mathbf{R_k})\phi(\mathbf{r}-\mathbf{R_l})d\mathbf{r}d\mathbf{r}'. \qquad (3)$$

In (2) V represents the nuclear potential acting over the electrons, Tij is a matrix element related to two sites (hopping integral). Thus, the first term in (1) is actually the ordinary Hamiltonian band. Eq. (3) represents the interaction among electrons.

Now we can perform the more important approximation: to disregard all terms in (3) different from $U = \langle ii|\frac{1}{r}|ii\rangle$, that is, to consider only interactions at the same site.8 Thus (1) becomes

$$H = \sum_{i,j,\sigma} T_{ij}c^+_{i\sigma}c_{j\sigma} + \frac{1}{2}U\sum_{i,\sigma} n_{i,\sigma}n_{i,-\sigma}, \qquad (4)$$

which is the well known Hubbard Hamiltonian.

Supposing that there is a magnetic field B applied to the system, the Zeeman term can be written as

$$-\sum_i g\mu_B B\frac{1}{2}(n_{i\uparrow} - n_{i\downarrow}) = -\sum_{i,\sigma}\sigma\frac{1}{2}g\mu_B Bn_{i\sigma}, \qquad (5)$$

where g is the Landé´s factor and μ_B is the Bohr magneton.

Including the Zeeman term (5), the Hamiltonian can be written as

$$H = H_0 + H_1, \qquad (6)$$

where

$$H_0 = \sum_{i,j,\sigma} T^{\sigma}_{ij}c^+_{i\sigma}c_{j\sigma}, \qquad (7)$$

$$H_1 = \sum Un_{i\uparrow}n_{i\downarrow}, \qquad (8)$$

and

$$T^{\sigma}_{ij} = T_{ij} - \sigma\frac{1}{2}g\mu_B B\delta_{ij}. \qquad (9)$$

This model describes electron correlation effects in a hypothetically crystalline lattice regarding the band as a narrow one.

The magnetic behavior of strongly correlated electrons systems is of great interest and thus several investigations have been performed to determine, for example, spontaneous magnetization phases. Here we delineate such phases by means of parameters such as temperature, average number of electrons per site and Coulombian on-site electrons interaction energy. Performing the static and uniform approximation for the development of the functional-integral related to the partition function of the system, we have calculated its functional free energy, which gave rise to all results that we have obtained.

Nowadays there is plenty of technological and scientific research about itinerant magnetism mostly because of the discovery of new superconductings and semiconducting materials whose microscopic mechanisms present itinerant electrons[9,10].

This paper is organized as follows. In Sec. 2 the methodology is introduced; in Sec. 3 our results are presented and discussed. Sec. 4 summarizes the conclusions of the work.

2. METHODOLOGY

2.1 Functional Integral Method

The grand partition function is given by

$$Z = \mathrm{Tr}\exp(-\beta H). \tag{14}$$

The model we chose here to represent the physical properties of magnetic systems of itinerant electrons is the Hubbard model for a non-degenerated orbital in which only interactions between electrons at the same site are admitted. Since we are working in the grand canonical ensemble, we add a new term related to the chemical potential in (7):

$$H_0 = \sum_{i,j}\sum_{\sigma} T_{i,j}^{\sigma}c_{i,\sigma}^{+}c_{j,\sigma} - \sum_{i}^{N}\sum_{\sigma}\mu n_{i,\sigma}. \tag{15}$$

Representing the partition function by the interaction representation

$$Z = Z_0\langle T\tau \times \exp\left[-\int_0^1 d\tau\beta H_1(\tau)\right]\rangle_{H_0}, \tag{16}$$

where Z_0 is the partition function for H_0, $T\tau$ is the time ordered, and $H_1(\tau)$ is defined in the interaction representation by

$$H_1(\tau) = e^{\beta H_0\tau}H_1 e^{-\beta H_0\tau}. \tag{17}$$

The functional-integral method formulation for the Hubbard model requires the Coulombian interaction in terms of squares of one-body charge and spin operators representation. We adopt the following identity:[7]

$$n_{i\uparrow}n_{i\downarrow} = -\frac{1}{2}(b_0 - 1)n_i - b_0\left(S_i^0\right)^2 - b_1\left(S_i^z\right)^2 - b_2\left(S_i^x\right)^2 - b_3\left(S_i^y\right)^2, \tag{18}$$

with

$$b_0 + b_1 + b_2 + b_3 = 2,$$

where

$$S_i^z = \frac{1}{2}\left(n_{i\uparrow} - n_{i\downarrow}\right), \tag{19.a}$$

$$S_i^x = \frac{1}{2}\left(S_i^+ + S_i^-\right), \tag{19.b}$$

$$S_i^y = -\frac{i}{2}\left(S_i^+ - S_i^-\right), \tag{19.c}$$

in which $S_i^+ = c_{i\uparrow}^{+}c_{i\downarrow}$, and $S_i^- = c_{i\downarrow}^{+}c_{i\uparrow}$. S_i^0 is defined by

$$S_i^0 = \frac{i}{2}\left(n_{i\uparrow} + n_{i\downarrow}\right). \tag{19.d}$$

Substituting (18) in (15), the Hubbard Hamiltonian can be rewritten as

$$H = \overline{H}_0 + \overline{H}_1, \tag{20.a}$$

with

$$\overline{H}_0 = \sum_{i,j}\sum_{\sigma}\overline{T}_{ij}^{\sigma}c_{i\sigma}^{+}c_{i\sigma} \quad, \quad \overline{T}_{ij}^{\sigma} \equiv T_{ij}^{\sigma} - \left[\mu + \frac{1}{2}(b_0 - 1)U\right]\delta_{i,j}, \tag{20.b}$$

and

$$\overline{H}_1 = -U\sum_{i}\left[b_0\left(S_i^0\right)^2 + b_1\left(S_i^z\right)^2 + b_2\left(S_i^x\right)^2 + b_3\left(S_i^y\right)^2\right]. \tag{20.c}$$

The single body term in (18) was included in $\overline{H}_0$. The term $\overline{H}_0$ now, as before, represents the Hamiltonian term of a single body and the term $\overline{H}_1$ represents the Hamiltonian term of two bodies. Thus, an analogy with (16) can be made and one can express the partition function in the interaction representation defined by $\overline{H}_0$ as[7]

$$Z = \overline{Z}_0\langle T\tau\exp\left[-\int_0^1 d\tau\beta\overline{H}_1(\tau)\right]\rangle_{H_0}, \tag{21}$$

where $\overline{Z}_0 = Tr\left[\exp(-\beta\overline{H}_0)\right]$, and $\langle...\rangle$ is the thermal average related to $\overline{H}_0$.

In equation (20), for each interval $d\tau$, one can use Hubbard-Stratonovich identity[1,2] which is valid for any real or complex operator a

$$e^{\pi a^2} = \int\limits_{-\infty}^{\infty} dx e^{-\pi x^2 + 2\pi a x} \quad . \tag{22}$$

The main usage of this identity is to substitute the squared exponential operators by an integral of linear operators.

The application of the functional-integral method in strongly correlated electrons systems is based upon this transformation (22).

Hence one can rewrite the grand partition function in this way[7]:

$$Z = Z_0 \int D\xi_q^\alpha \exp\left[-\frac{1}{2}\sum_{\alpha,q}\xi_q^\alpha \xi_{-q}^\alpha + \underset{k,\sigma}{Tr}\ln\left(1-VG^0\right)\right], \tag{23}$$

with

$$V_{k,k'}^{\alpha,\alpha'} = -\left(\frac{2\beta U}{N}\right)^{1/2}\sum_\alpha (b_\alpha)^{1/2}\xi_{k-k'}^\alpha S_{\sigma,\sigma'}^\alpha. \tag{24}$$

In (23), Z_0 is the partition function of the non-interacting system and ξ_q^α are Fourier transforms for auxiliary fields; $q \equiv (q, \omega_v)$ [$k \equiv (k, \omega_n)$] represent wave vectors and Matsubara frequencies for bosons [fermions]; N is the site number and G_0 is the non-interacting Green function of an electron.

From calculation of (23) and (24) the system thermodynamic properties can be determined.

2.2 Functional free energy determination by the static and uniform approximation

As written in (18), the term $n_{i\uparrow}n_{i\downarrow}$ can be represented by

$$n_{i\uparrow}n_{i\downarrow} = -\left(S_i^0\right)^2 - \left(S_i^z\right)^2 \tag{25}$$

The partition function Z in wave vectors and Matsubara frequencies space is7

$$Z = Z_0 \int \prod_{\mathbf{q}}\prod_{v} d\xi_{\mathbf{q}v}^0 d\xi_{\mathbf{q}v}^z \exp\left[-\sum_{\overrightarrow{\mathbf{q},v}}\pi\left(\xi_{\mathbf{q}v}^0\xi_{-\mathbf{q}-v}^0 + \xi_{\mathbf{q}v}^z\xi_{-\mathbf{q}-v}^z\right)\right]\exp\left[Tr\ln\left(1-VG^0\right)\right] \tag{26}$$

where V, defined by (24), obeys the dependence relation $V_{\mathbf{kk'},nn'}^{\sigma\sigma'} = V_{\mathbf{k-k'},n-n'}^{\sigma\sigma'}$.

Doing k-k'= q and n-n'= v, and recalling the definition (24) we have

$$V_{\mathbf{q},v}^{\sigma\sigma'} = -2\left(\pi\beta U \middle/ N\right)^{1/2}\left(\xi_{\mathbf{q}v}^0 S_{\sigma\sigma'}^0 + \xi_{\mathbf{q}v}^z S_{\sigma\sigma'}^z\right) . \tag{27}$$

Matsubara`s Green function in (26) can be expressed as

$$G_{\mathbf{kk'},nn'}^{0\sigma\sigma'} = G_\sigma^0(\mathbf{k},\omega_n)\delta_{\mathbf{k},\mathbf{k'}}\delta_{n,n'}\delta_{\sigma,\sigma'} , \tag{28}$$

where

$$G_\sigma^0(\mathbf{k},\omega_n) = \frac{1}{i\omega_n - \beta\varepsilon_{\mathbf{k}\sigma}},$$

in which

$$\varepsilon_{\mathbf{k}\sigma} = \varepsilon_{\mathbf{k}} - \sigma\mu_B B - \mu , \tag{29}$$

and

$$\varepsilon_{\mathbf{k}} = -2t\sum_{i=1}^{d}\cos(\mathbf{k}_i) . $$

Performing the static and uniform approximation, which consists in the approximation of V in (26) by V_0.

$$Z_0 \exp\left[Tr\ln\left(1-VG^0\right)\right] \cong Z_0 \exp\left[Tr\ln\left(1-V_0 G^0\right)\right] . \tag{30}$$

At this point, all auxiliary fields in the functional integral $(\xi_{\mathbf{q}\nu}^0, \xi_{\mathbf{q}\nu}^z)$ whose moments or frequencies different from zero are all discarted;

Thus, $V_{\mathbf{kk'},nn'}^{\sigma\sigma'} = V_{0,0}^{\sigma\sigma'}\delta_{\mathbf{kk'}}\delta nn' = V_{0,0}^{\sigma}\delta_{\mathbf{kk'}}\delta_{nn'}\delta_{\sigma\sigma'}$ and

$$V_{0,0}^{\sigma} = -\left(\pi\beta U\Big/N\right)^{1/2}\left(i\xi_0^0 + \sigma\xi_0^z\right).\tag{31}$$

Calculating the generic matrix element (V0G0), we obtain

$$(V_0 G^0)_{\mathbf{kk'},nn'}^{\sigma\sigma'} = \sum_{\mathbf{k}1}\sum_{n1}\sum_{\sigma1}V_{\mathbf{kk}1,nn1}^{\sigma\sigma1}G_{\mathbf{k}1\mathbf{k'},n1n'}^{\sigma1\sigma'},$$

$$(V_0 G^0)_{\mathbf{kk'},nn'}^{\sigma\sigma'} = \sum_{\mathbf{k}1}\sum_{n1}\sum_{\sigma1}V_0^{\sigma}\delta_{\mathbf{kk}1}\delta_{nn1}\delta_{\sigma\sigma1}G_{\sigma1}^0(\mathbf{k}1,\omega_{n1})\delta_{\mathbf{k}1\mathbf{k'}}\delta_{n1n'}\delta_{\sigma1\sigma'}$$

$$= V_0^{\sigma}G_{\sigma}^0(\mathbf{k},\omega_n)\delta_{\mathbf{kk'}}\delta_{nn'}\delta_{\sigma\sigma'}.\tag{32}$$

Thus, the matrix $(V_0 G^0)$ is diagonal, and so its trace is equal to the summation of all its elements;

$$Z(\xi_0^0, \xi_0^z) = Z_0 \exp\left[Tr\ln(1 - V_0 G^0)\right] = Z_0 \exp\left\{\sum_{\mathbf{k},n,\sigma}\ln\left[1 - V_0^{\sigma}G_{\sigma}^0(\mathbf{k},\omega_n)\right]\right\},\tag{33}$$

where

$$\ln\left\{\frac{Z(\xi_0^0, \xi_0^z)}{Z_0}\right\} = \sum_{\mathbf{k},n,\sigma}\ln\left[1 - V_0^{\sigma}G_{\sigma}^0(\mathbf{k},\omega_n)\right]$$

$$= \sum_{\mathbf{k},n,\sigma}\int_0^1 d\theta\frac{\partial\ln\left[1 - \theta V_0^{\sigma}G_{\sigma}^0(\mathbf{k},\omega_n)\right]}{\partial\theta} = -\lim_{\delta\to 0}\sum_{n,\mathbf{k},\sigma}V_0^{\sigma}\int_0^1\frac{\exp(i\omega_n\delta)d\theta}{i\omega_n - \beta\varepsilon_{\mathbf{k}\sigma} - \theta V_0^{\sigma}}.$$

Using the identity [11]:

$$\lim_{\delta\to 0}\sum_n\frac{\exp(i\omega_n\delta)}{i\omega_n - x} = \frac{1}{e^x + 1};$$

we have

$$\ln\left\{\frac{Z(\xi_0^0, \xi_0^z)}{Z_0}\right\} = -\sum_{\mathbf{k},\sigma}V_0^{\sigma}\int_0^1\frac{d\theta}{\exp(\beta\varepsilon_{\mathbf{k}\sigma} + \theta V_0^{\sigma}) + 1};$$

and thus,

$$\ln\left\{\frac{Z(\xi_0^0, \xi_0^z)}{Z_0}\right\} = \sum_{\mathbf{k},\sigma}\left\{-V_0^{\sigma} + \ln\left[1 + \exp(\beta\varepsilon_{\mathbf{k}\sigma} + V_0^{\sigma})\right] - \ln\left[1 + \exp(\beta\varepsilon_{\mathbf{k}\sigma})\right]\right\}.$$

As all auxiliary fields related to frequencies or moments different from zero are disregarded, the productories are simplified in (26) and the partition function (Z) can now be written as

$$Z = \int d\xi_0^0 d\xi_0^z \exp\left[-\pi(\xi_0^{0^2} + \xi_0^{z^2})\right]Z(\xi_0^0, \xi_0^z).\tag{34}$$

On the other hand, one can make

$$Z = \int d\xi_0^0 d\xi_0^z \exp\left[-\beta F(\xi_0^0, \xi_0^z)\right],\tag{35}$$

where $F(\xi_0^0, \xi_0^z)$ is the functional free energy of the system. Comparing (34) with (35), we have

$$\beta F(\xi_0^0, \xi_0^z) = \pi(\xi_0^{0^2} + \xi_0^{z^2}) - \ln\left[Z(\xi_0^0, \xi_0^z)\right] =\tag{36}$$

$$\pi(\xi_0^{0^2} + \xi_0^{z^2}) - \sum_{\mathbf{k},\sigma}\left\{-V_0^{\sigma} + \ln\left[1 + \exp(\beta\varepsilon_{\mathbf{k}\sigma} + V_0^{\sigma})\right] - \ln\left[1 + \exp(\beta\varepsilon_{\mathbf{k}\sigma})\right]\right\} - \ln Z_0.\tag{37}$$

The most relevant terms in Z occur for a minimum value of the functional free energy. It has been proved3 in the static and uniform approximation, that the resulting phase diagrams are

equivalent to those corresponding obtained by the well-known Hartree-Fock method. For the most relevant terms which we mentioned above we have

$$\frac{\partial F}{\partial \xi_0^0}=0 \quad \text{and} \quad \frac{\partial F}{\partial \xi_0^z}=0\;;$$

$$\frac{\partial F}{\partial \xi_0^0}=\frac{2\pi\overline{\xi}_0^0}{\beta}-\sum_{\mathbf{k},\sigma}\left\{\frac{i}{\beta}\left(\frac{\pi\beta U}{N}\right)^{\!\frac12}-\frac{\exp(\beta\varepsilon_{\mathbf{k}\sigma}+\overline{V}_0^{\sigma})i\left(\pi\beta U/N\right)^{\!\frac12}}{\beta+\beta\exp(\beta\varepsilon_{\mathbf{k}\sigma}+\overline{V}_0^{\sigma})}\right\}=0\;;\quad(38)$$

$$\frac{\partial F}{\partial \xi_0^z}=\frac{2\pi\overline{\xi}_0^z}{\beta}-\sum_{\mathbf{k},\sigma}\left\{\frac{\sigma}{\beta}\left(\frac{\pi\beta U}{N}\right)^{\!\frac12}-\frac{\exp(\beta\varepsilon_{\mathbf{k}\sigma}+\overline{V}_0^{\sigma})\sigma\left(\pi\beta U/N\right)^{\!\frac12}}{\beta+\beta\exp(\beta\varepsilon_{\mathbf{k}\sigma}+\overline{V}_0^{\sigma})}\right\}=0\;.\quad(39)$$

From (36) $\quad\beta F(\xi_0^0,\xi_0^z)=\pi(\xi_0^{0^2}+\xi_0^{z^2})-\ln\left\{Tr\exp\left[-\beta H_0-\sum_{\mathbf{k},\sigma}V_0^{\sigma}n_{\mathbf{k}\sigma}\right]\right\}\;;$

$$\frac{\partial F}{\partial \xi_0^0}=\frac{2\pi\overline{\xi}_0^0}{\beta}-\frac{Tr\left\{\exp\left[-\beta H_0-\sum_{\mathbf{k},\sigma}V_0^{\sigma}n_{\mathbf{k}\sigma}\right]\left[\sum_{\mathbf{k},\sigma}i\sqrt{\frac{\pi\beta U}{N}}n_{\mathbf{k}\sigma}\right]\right\}}{\beta Tr\exp\left[-\beta H_0-\sum_{\mathbf{k},\sigma}V_0^{\sigma}n_{\mathbf{k}\sigma}\right]}=0\;;\quad(40)$$

$$\frac{\partial F}{\partial \xi_0^z}=\frac{2\pi\overline{\xi}_0^z}{\beta}-\frac{Tr\left\{\exp\left[-\beta H_0-\sum_{\mathbf{k},\sigma}V_0^{\sigma}n_{\mathbf{k}\sigma}\right]\left[\sum_{\mathbf{k},\sigma}\sigma\sqrt{\frac{\pi\beta U}{N}}n_{\mathbf{k}\sigma}\right]\right\}}{\beta Tr\exp\left[-\beta H_0-\sum_{\mathbf{k},\sigma}V_0^{\sigma}n_{\mathbf{k}\sigma}\right]}=0\;;\quad(41)$$

One can observe, from (40) and (41), that ξ_0^0,ξ_0^z can be written as thermal averages of the occupation number ($n_{\mathbf{k}\sigma}$):

$$2\pi\overline{\xi}_0^0=i\sqrt{\frac{\pi\beta U}{N}}\sum_{\mathbf{k},\sigma}\langle n_{\mathbf{k}\sigma}\rangle\;;\qquad 2\pi\overline{\xi}_0^z=\sqrt{\frac{\pi\beta U}{N}}\sum_{\mathbf{k},\sigma}\sigma\langle n_{\mathbf{k}\sigma}\rangle\;.$$

Performing an exchange of variables we have

$$\xi_0^z=\frac{\sqrt{\pi\beta NU}}{2\pi}z\;.\quad(42)$$

Notice that $\overline{z}=n_\uparrow-n_\downarrow$ when $\xi_0^z=\overline{\xi}_0^z$, that is, the new variable z is proportional to the magnetization when, keeping ξ_0^0 constant, the functional free energy has a minimum value.

At this moment we will perform the calculation of the functional free energy as a function of ξ_0^z, keeping ξ_0^0 constant and equal to $\overline{\xi}_0^0$. V_0^{σ} and $\varepsilon_{\mathbf{k}\sigma}$ will be substituted in (37) by the values given by (31) and (29), respectively. With

$$h=\mu_B B\;;\quad \beta F_0=-\ln Z_0\quad\text{and}\quad \overline{V}_0^{\sigma}=-\frac{\beta U}{2}(z\sigma-n)\text{ we obtain}$$

$$\beta F(z)=\frac{\beta NU}{4}(z^2-n^2)+\beta NUn-\sum_{\mathbf{k}}\{\;\ln[1+\exp(\beta[\varepsilon_{\mathbf{k}}-h-\mu-U(z-n)/2])]$$
$$+\ln[1+\exp(\beta[\varepsilon_{\mathbf{k}}+h-\mu+U(z+n)/2])]-\ln[1+\exp(\beta[\varepsilon_{\mathbf{k}}-h-\mu])]$$
$$-\ln[1+\exp(\beta[\varepsilon_{\mathbf{k}}+h-\mu])]\;\}+\beta F_0\quad(43)$$

Calling S_k for the argument of the summation above, we have for the functional free energy

$$\frac{F(z)}{N} = \frac{U}{4}\left(z^2 - n^2\right) + Un - \frac{1}{\beta N}\sum_{\mathbf{k}} S_{\mathbf{k}} + \frac{F_0}{N} \tag{44}$$

3. RESULTS AND DISCUSSION

With (43), we plot the functional free energy as a function of *z*. One observes that, for constant temperature and constant average number of electrons per site (*n*), there is a critical Coulombian interaction energy (U_C). For *U* larger than U_C, the system presents spontaneous magnetization and for *U* lower than U_C it does not. The graphic in figure 1 presents this behavior. We worked in the half-filled band case (average number of electrons per site equal to 1), and temperature kept at 0,1 t/k_B. The graphic shows the behavior of the functional free energy for three values of *U*; U_C being equal to 3,78t. Here, the *F(z)* terms which are independent of z are all disregarded, in order to have a better comparative analysis. In the same way we now keep *U* constant and equal to *6t*, and verify the functional free energy dependence in relation to z for three different temperatures, T_C being 0.69 t/k_B, as shown in figure 2.

In case of paramagnetic behavior, the second derivative of the functional free energy in relation to z at the point $z = 0$ must be positive. On the other hand, for ferromagnetic behavior, it must be negative. Thus we can determine critical parameters for spontaneous magnetization occurrence making the second derivative of the functional free energy in relation to z at the point $z = 0$ equal to zero. The parameters that can be determined are, for example, T_C for a given *n* or U_C for a given n.

From (41), the second derivative of the functional free energy in relation to z at the point $z = 0$ is

$$\frac{\partial^2 F}{\partial z^2} = \frac{U}{2} - \frac{\beta U^2}{2N}\sum_{\mathbf{k}}\left\{\frac{\exp\left(\beta\left[\varepsilon_{\mathbf{k}} - \mu + \frac{Un}{2}\right]\right)}{\left(1 + \exp\left(B\left[\varepsilon_{\mathbf{k}} - \mu + \frac{Un}{2}\right]\right)\right)^2}\right\} \ . \tag{45}$$
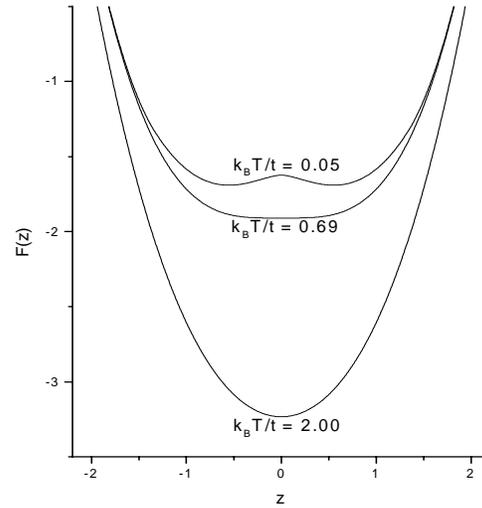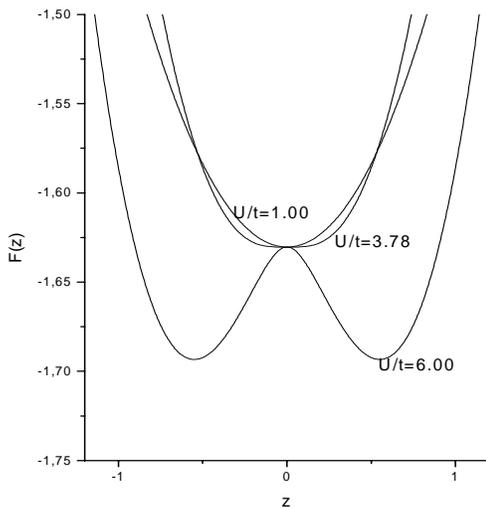

Figure 1: Functional free energy as a function of the auxiliary field which acts in the electrons spins for three different values of U; temperature kept constant (T= 0,1 t/kB)

Figure 2: Functional free energy as a function of the auxiliary field which acts in the electrons spins for three different values of T; U kept constant (U=6t)

A notable case of this calculation is the half-filled band (n = 1), because in this situation the chemical potential (μ) is equal to $U/2$. This fact, well known in the literature, makes Eq (45) much easier. Thus (45) can be rewritten as

$$\frac{\partial^2 F}{\partial z^2} = \frac{U}{2} - \frac{\beta U^2}{2N} \sum_{\mathbf{k}} \left\{ \frac{\exp(\beta \varepsilon_{\mathbf{k}})}{(1+\exp(B\varepsilon_{\mathbf{k}}))^2} \right\}.$$

Making the first term equal to zero, one gets UC for the half-filled band case as

$$U_C = \frac{N}{\beta S_{\mathbf{k}}} ; \quad \text{where} \quad S_{\mathbf{k}} = \sum_{\mathbf{k}} \left\{ \frac{\exp(\beta \varepsilon_{\mathbf{k}})}{(1+\exp(\beta \varepsilon_{\mathbf{k}}))^2} \right\}. \quad (46)$$

For temperature equal to 0.1t/k_B, we found U_C equal to 3,7859t, which is shown figure 1.

In the same way, we can make (45) equal to zero and determine, by iteractive numerical calculation, U_C and T_C for each given n, making a phase diagram of the system. Figure 3 shows U_C as a function of n with the temperature being kept constant and equal to 0.1t/k_B. Figure 4 shows T_C as a function of n, U being kept constant and equal to 6t. In both cases, the regions denoted by F and P correspond to ferromagnetic and paramagnetic behavior; respectively. From (39) and taking into account the exchange of variables (42), we have

$$\bar{z} = \frac{1}{N} \sum_{\mathbf{k},\sigma} \sigma \left\{ \frac{1}{1+\exp\left[\beta\left(\varepsilon_{\mathbf{k}\sigma} + Un/2 - \sigma U\bar{z}/2\right)\right]} \right\} = n_\uparrow - n_\downarrow.$$

Thus we plot $\bar{z}$ as a function of U and $\bar{z}$ as a function of T. In both cases the average number of electrons per site was kept equal to 1 (half-filled band). Figure 5 shows $\bar{z}$ as function of U; the temperature being kept equal to 0.1 t/k_B. It is important to notice the existence of a critical value for U, that is, it is not allowed the occurence of magnetization for values of U lower than the critical value. On the other hand, there is a saturation value for U, and for values of U larger than this value the magnetization does not increase any more. These results are in perfect agreement with those that would be expected because as it was explained before, U_C in half-filled band case at 0.1 t/k_B, is equal to 3.78, which can be seen in figure 5. Besides that, since $n_\uparrow + n_\downarrow = 1$, $(n_\uparrow - n_\downarrow)_{máx} = 1$, one can notice that there is a natural limit for increase in the magnetization, which justifies the existence of a saturation value for U.
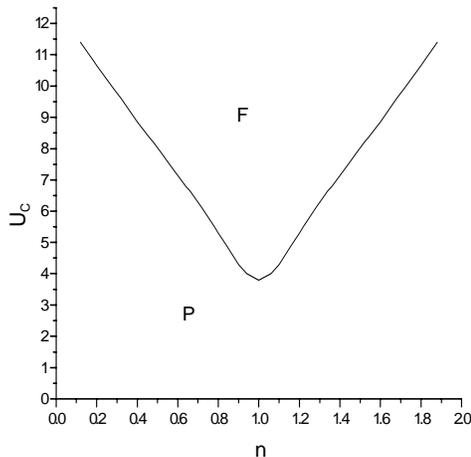

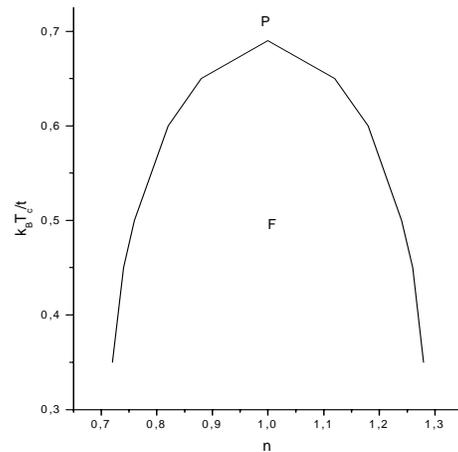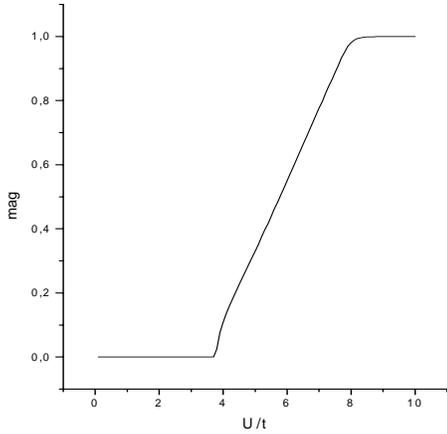Figure 3: U_C as a function of n (T = 0.1 t/k_B)   Figure 4: T_C as a function of n (U=6t)

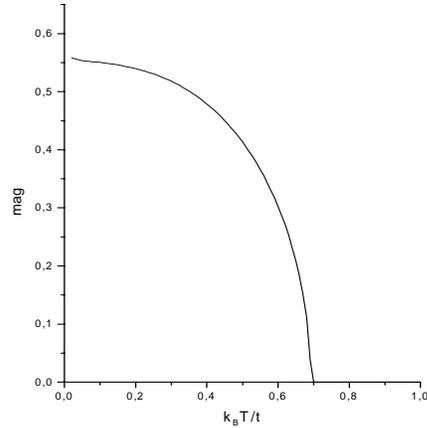*Figure 5: Mag as a function of U. There are a critical value and a saturation value for U(T = 0.1 t/kB)*

Figure 6: Mag as a function of T; (U = 6t).

Figure 6 shows the graphic of $\bar{z}$ as a function of *T*; *U* being kept equal to 6t. The figure shows a critical value for the temperature, and for temperatures larger than the critical temperature the magnetization is not allowed. These results are in agreement with figure 2 and its shape is well known for ferromagnetic materials. In both graphics, $\bar{z}$ is denoted by *mag*.

Considering yet the half-filled band case and using (46) one can determine a magnetic phase diagram relating *U* and *T*. It is represented in figure 7. A more generic result is the three-dimensional phase diagram which is shown in figure 8, relating *U*, *T* and n.
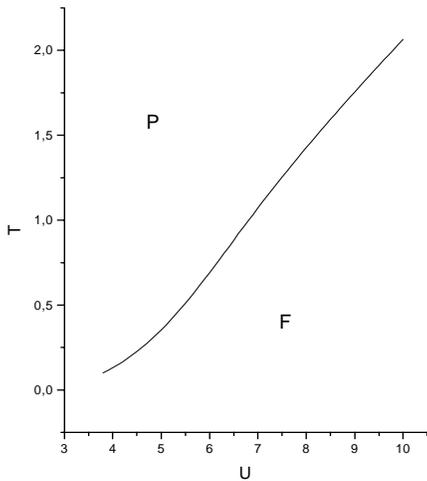

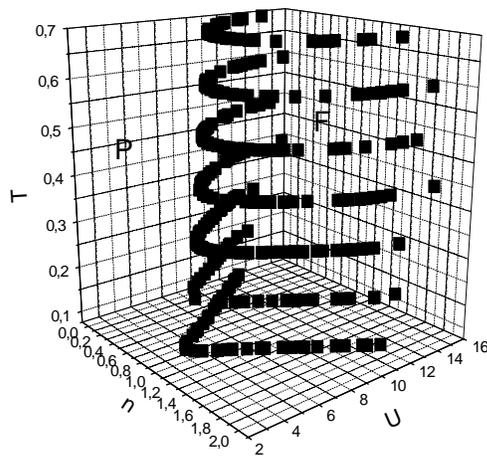*Figure 7: Phase diagram relating T and U in the half-filled band case.*

Figure 8: Three-dimensional phase diagram relating T, U and n. The volume inside the surface of points corresponds to ferromagnetic behavior. The other one, outside, corresponds to paramagnetic behavior

4. CONCLUSIONS

The most innovative aspect of the functional-integral method is the fact that it transforms, by means of a mathematical identity, the electronic interactions systems into a system of non-interacting electrons subjected to space-and time-varying auxiliary fields.

By means of calculation of the functional free energy, here attained with the static and uniform approximation in the functional-integral, and taking into account the most relevant terms of the energy, we defined spontaneous magnetization regions in several diagrams of magnetic phases equivalent to Hartree-Fock results.

The determination of critical values for the Coulombian interaction energy and temperature for the occurance of spontaneous magnetization contributes to present the functional caracteristics of this method. The shape of curves related to temperature qualitatively agrees with those that would be expected. We have shown that besides the existence of a minimum value for the Coulombian interaction energy for occurrence of spontaneous magnetization, there is a saturation point, that is, a limiting value for the magnetization increase, as expected.

5. ACKNOWLEDGMENTS

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