The two-dimensional Hubbard model in the Hartree-Fock approximation

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The students interested in the study of strongly correlated electron systems normally feel, in the beginning of their studies, a great difficulty in understanding the complex correlations of these systems. We consider that for these students it is very important to have texts that analyze pedagogically the theoretical research methods of the subject. We show how to determine the thermodynamic properties of the Hubbard model for the two-dimensional square lattice, utilizing the Hartree-Fock approximation. All the procedures and peculiarities which lead to the determination of the thermodynamic properties and to the comprehension of the meaning of the Hartree-Fock approximation applied to models of strongly correlated electron systems are pedagogically presented in detail. We obtain the magnetization, the magnetic susceptibility, the internal energy, the specific heat, and also a magnetic phase diagram of the studied system. Our approach clearly shows that the use of the Hartree-Fock approximation, in this case, is very simple.

Keywords: Hubbard model, square lattice, Hartree-Fock approximation, thermodynamic properties.

Os estudantes interessados no estudo de sistemas de elétrons fortemente correlacionados sentem, normalmente, no começo de seus estudos, uma grande dificuldade em compreender as complexas correlações desses sistemas. Nós consideramos que para esses estudantes, é muito importante que existam textos que analisem didaticamente os métodos de pesquisa teórica do assunto. Nós mostramos como determinar as propriedades termodinâmicas do modelo de Hubbard para a rede quadrada, utilizando a aproximação de Hartree-Fock. Todos os procedimentos e peculiaridades que levam à determinação das propriedades termodinâmicas e à compreensão do significado da aproximação de Hartree-Fock aplicada a modelos de sistemas de elétrons fortemente correlacionados são apresentados em detalhes didáticos. Nós obtemos a magnetização, a susceptibilidade magnética, a energia interna, o calor específico e, também, um diagrama de fases magnéticas do sistema estudado. Nossa abordagem mostra claramente que o uso da aproximação de Hartree-Fock, neste caso, é muito simples.

Palavras-chave: modelo de Hubbard, rede quadrada, aproximação de Hartree-Fock, propriedades termodinâmicas.

1. INTRODUCTION

The Hubbard model [1] was created to describe the effect of correlations for d-electrons in transition metals. The Hamiltonian model,

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

consists of two contributions, a kinetic term describing the motion of electrons between neighboring sites, and an on-site term, which approximates the interactions among electrons, whose strength is given by the parameter U. The hopping integral T_{ij} is usually restricted to nearest-neighbors, and is assumed translationally invariant, namely $T_{ij} = -t$, $t > 0$ [2]. $c_{i\sigma}^{+}$ ($c_{i\sigma}$) is the electron creation (annihilation) operator on the site i with spin σ, $\sigma = \pm 1$, or $\uparrow, \downarrow$, and $n_{i\sigma} = c_{i\sigma}^{+} c_{i\sigma}$.

The Hamiltonian (1) is thought to be appropriate to describe the main features of electron correlations in narrow energy bands, leading to collective effects as itinerant magnetism and metal-insulator transition, and has been often used to describe real materials exhibiting these phenomena [2, 3].

The interest in the Hubbard model and, in general, in the field of strongly correlated electron systems, has been stimulated by the discovery of heavy fermions and high-*Tc* superconductors [2, 4]. The applications related to superconductivity have stimulated the achievement of new results concerning the properties of the model, especially for the two-dimensional case [2].

A considerable amount of work has been devoted to the solution of the Hubbard model since its creation. Nevertheless, exact results are still very rare, and their validity is mainly confined to the one-dimensional case [2, 3]. In more than one-dimension the model is not exactly solvable and a variety of approximate techniques have been used to study it, among others, the Hartree-Fock approximation.

In this work, we show how to determine the thermodynamic properties of the Hubbard model for the two-dimensional square lattice with nearest-neighbors hopping only, utilizing the Hartree-Fock approximation. We present, in pedagogical detail, all procedures and peculiarities that allow to determine the thermodynamic properties and to understand the meaning of the Hartree-Fock approximation applied to models of strongly correlated electron systems.

We believe that our approach will be useful for students that are interested in advancing to the study of strongly correlated electron systems.

The paper is organized as follows. In Sec. 2 we describe the Hartree-Fock approximation, and the quantities that we calculate are defined. In Sec. 3 the results are presented. We close with the conclusions in Sec. 4.

2. HARTREE-FOCK APROXIMATION

We discuss in this paper a particularly simple case of the Hartree-Fock approximation which may represent non-ferromagnetic or ferromagnetic states only. In the case of the Hubbard Hamiltonian this amounts to simply replacing the term $n_{i\sigma}n_{i-\sigma}$ by $n_{i\sigma}\langle n_{i-\sigma}\rangle + \langle n_{i\sigma}\rangle n_{i-\sigma}$, where $\langle n_{i\sigma}\rangle$ is the average of the expectation of $n_{i-\sigma}$ over a grand canonical ensemble at some temperature T [1].

The Hartree-Fock Hamiltonian is found to be

$$H_{HF} = \sum_{i,j,\sigma} T_{ij} c_{i\sigma}^{+} c_{j\sigma} + U \sum_{i,\sigma} \langle n_{i-\sigma} \rangle c_{i\sigma}^{+} c_{i\sigma} . \tag{2}$$

Attention will now be restricted to the class of solutions for which

$$\langle n_{i\sigma} \rangle = n_{\sigma} \text{ for all i.} \tag{3}$$

Then Eq. (2) becomes

$$H_{HF} = \sum_{i,j,\sigma} T_{ij} c_{i\sigma}^{+} c_{j\sigma} + U \sum_{i,\sigma} n_{-\sigma} c_{i\sigma}^{+} c_{i\sigma} \tag{4}$$

Now let $c_{\mathbf{k}\sigma}^{+} c_{\mathbf{k}\sigma}$ be the creation (annihilation) operator for electrons in the Bloch state $(\mathbf{k},\sigma)$, then one can also write

$$c_{i\sigma} = \frac{1}{\sqrt{Ns}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_i} c_{\mathbf{k}\sigma} , \tag{5}$$

$$c_{i\sigma}^{+} = \frac{1}{\sqrt{Ns}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}i} c_{\mathbf{k}\sigma}^{+} , \tag{6}$$

where N_s is the number of sites.

Relations (5) and (6) can now be used to rewrite the Hamiltonian (4) as

$$H_{HF} = \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}} + U n_{-\sigma}) c_{\mathbf{k}\sigma}^{+} c_{\mathbf{k}\sigma} = \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}} + U n_{-\sigma}) n_{\mathbf{k}\sigma} \tag{7}$$

which is simply the Hamiltonian for a collection of non-interacting electrons with a slightly modified band structure, the energy of the $(\mathbf{k},\sigma)$ state being $\varepsilon_k + Un_{-\sigma}$. The k sum runs over the first Brillouin zone, and the single-particle eigenstates for the non-interacting case (U = 0) have energies [1].

$$\varepsilon_{\mathbf{k}} = \frac{1}{Ns}\sum_{i,j} e^{-i\mathbf{k}\cdot(\mathbf{R_i}-\mathbf{R_j})} T_{ij} \tag{8}$$

Following the usual procedure of the grand canonical method of statistical mechanics, we calculate for the Hamiltonian (7) the average number of electrons in the state $(\mathbf{k},\sigma)$ with the Fermi-Dirac function

$$\langle n_{\mathbf{k}\sigma} \rangle = \frac{1}{e^{\beta(\varepsilon_{\mathbf{k}} + U n_{-\sigma} - \mu)} + 1} \tag{9}$$

where μ is the chemical potential and must be determined by imposing

$$n = n_{\uparrow} + n_{\downarrow}, \tag{10}$$

where

$$n_{\sigma} = \frac{1}{Ns}\sum_{\mathbf{k}} \langle n_{\mathbf{k}\sigma} \rangle \tag{11}$$

and n is the average number of electrons per site.

One possible solution of Eqs. (9) to (11) is that for which

$$n_{\uparrow} = n_{\downarrow} = \frac{n}{2} \tag{12}$$

which represents a non-ferromagnetic state of the system. Thus, it is simpler to determine μ by

$$\frac{n}{2} = \frac{1}{Ns}\sum_{\mathbf{k}} \frac{1}{e^{\beta\left(\varepsilon_{\mathbf{k}} + U\frac{n}{2} - \mu\right)} + 1} \tag{13}$$

In the magnetic case one must solve a self-consistent equation for m, the average magnetization per site (in Bohr magnetons),

$$m = n_{\uparrow} - n_{\downarrow} \tag{14}$$

with μ still being determined by Eq. (13).

In the presence of a magnetic field h in the z-direction, the Hamiltonian (7) is modified for

$$H_{HF} = \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}} + U n_{-\sigma} - \mu_B h\sigma) n_{\mathbf{k}\sigma} \tag{15}$$

where μ_B is Bohr magneton.

With Eq. (15) the magnetic susceptibility χ is calculated from

$$\chi = \lim_{h\to 0}\left(\frac{m(h) - m(0)}{h}\right) \tag{16}$$

The internal energy per site u is determined by

$$u = \frac{1}{Ns}\langle H_{HF} \rangle = \frac{1}{Ns}\sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}} + U n_{-\sigma} - \mu_B h\sigma) \langle n_{\mathbf{k}\sigma} \rangle \tag{17}$$

or

$$u = \frac{1}{Ns}\sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} \langle n_{\mathbf{k}\sigma} \rangle + 2U n_{\uparrow} n_{\downarrow} - \mu_B h(n_{\uparrow} - n_{\downarrow}) \tag{18}$$

Finally, the specific heat c can be calculated by

$$c = \frac{du}{dT} \tag{19}$$

3. THERMODYNAMIC PROPERTIES

We only consider the two-dimensional square lattice with nearest-neighbor hopping and thus, $T_{ij} = -t$ and the single-particle eigenstates for the non-interacting case have energies [3]

$$\varepsilon_{\mathbf{k}} = -2t[\cos(k_x a) + \cos(k_y a)] \tag{20}$$

where $a = |R_i - R_j|$ is the magnitude of the primitive lattice vectors $\mathbf{a_1}$ and $\mathbf{a_2}$. In this work we adopt $a=1$. Thus,

$$\varepsilon_{\mathbf{k}} = -2t[\cos(k_x) + \cos(k_y)] \tag{21}$$

Figure 1 shows some points of the two-dimensional square lattice.

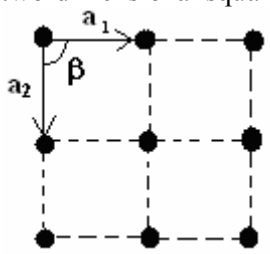

Figure 1. Some points of the two-dimensional square lattice, with |a1| = |a2| = a, and β = π/2.

The k sums, in this case, are interpreted as

$$\sum_{\mathbf{k}} \rightarrow \sum_{k_x, k_y}$$

with k_ν (ν = x, y) varying in the interval $-\pi$ until π. In practice, we consider, for effect of numerical calculation, a finite lattice with $Ns = L^2$, being that each $k\nu$ assumes L values through

$$k_\nu = \left(\frac{2n_\nu - L}{L}\right)\pi \quad , \quad n_\nu = 1, 2, 3, \ldots, L. \tag{21}$$

In this work we take $L = 50$.

The chemical potential μ is $U/2$ for a half-filled band, $n = 1.0$ [3], but in the general case it must be calculated by Eq. (13). Figure 2 shows the average number of electrons per site n versus μ/t, utilizing Eq. (13), for $T = 0.1t/k_B$ and $U = 6t$.

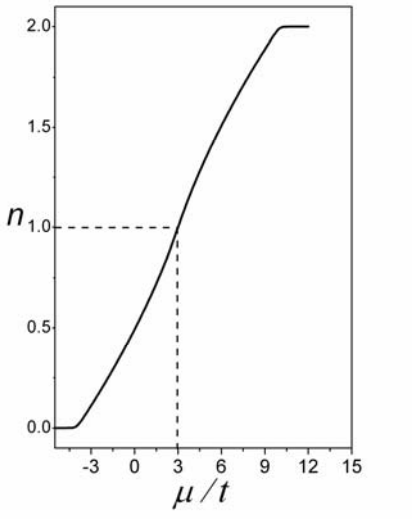

Figure 2. Average electron number per site versus μ/t, for T = 0.1t/kB and U = 6t.

The temperature dependence of the magnetization for null field, $h = 0$, is obtained from Eq. (14), under the constraint of Eq. (10), with Eqs. (11) and (9). Figure 3 shows a graph of the magnetization versus temperature for two different average electron numbers per site, $n = 1.0$ and $n = 0.8$, in which $U = 6t$. We observed that the critical temperature T_c, the temperature above which magnetization does not occur, is larger for $n = 1.0$.

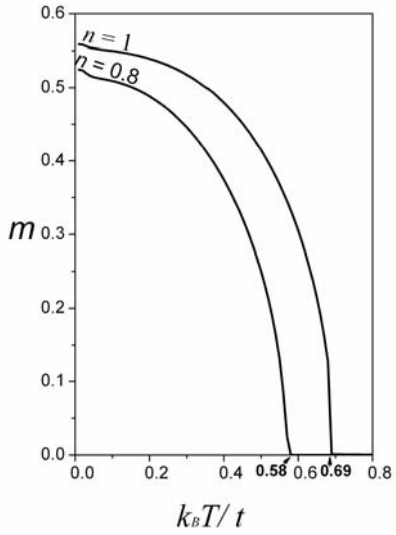

Figure 3. Magnetization versus temperature for n = 0.8 and 1.0, with U = 6t. $T_c = 0.58\ t/k_B$ for n = 0.8, and $T_c = 0.69\ t/k_B$ for n = 1.0.

Another interesting graph of the magnetization is shown in Fig. 4. In this case, the interaction U dependence of m is presented for $n = 0.8$ and 1.0, at $T = 0.1\ t/k_B$. We can verify in it the existence of critical interaction energy, U_c, below which magnetization does not occur and a U of saturation, above which the magnetization does not increase anymore, that is, it saturates. The maximum value of the magnetization, i.e., its saturation value, is $m = n$.

A simple phase diagram for ferromagnetic *(F)* and non-ferromagnetic *(NF)* phases can be obtained by plotting the U_c as a function of the average particle number per site n at fixed T. In Fig. 5 it is shown the phase diagram at $T = 0.1\ t/k_B$.

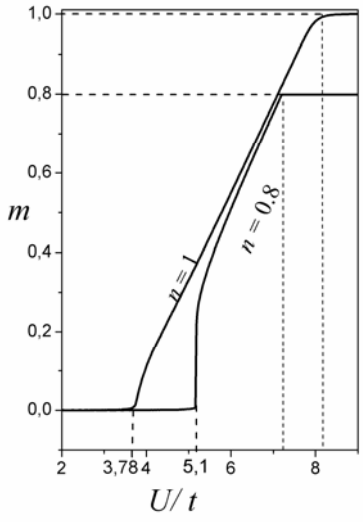

Figure 4. Magnetization versus U/t for n = 0.8 and for n = 1.0 at $T = 0.1\ t/k_B$. $U_c = 3.78t$ for n = 1.0, and $U_c = 5.1t$ for n = 0.8. The saturation value of the magnetization is m = n.

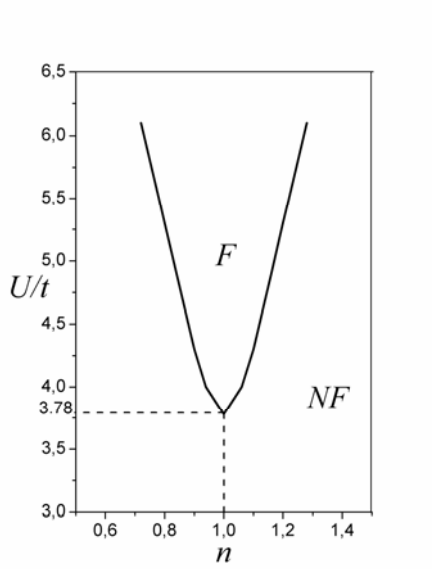

Figure 5. Phase diagram for two-dimensional Hubbard model in Hartree-Fock approximation. F and NF denote ferromagnetic and non-ferromagnetic phase at $T = 0.1t/k_B$, respectively.

The internal energy per site u can be determined from Eq. (18). Figure 6 shows u versus k_BT/t for $n = 1.0$, $h = 0$, and $U = 6t$. The occurrence of a phase transition with the temperature is evidenced by the inflection in u which occurs at $T_c = 0.69\ t/k_B$.

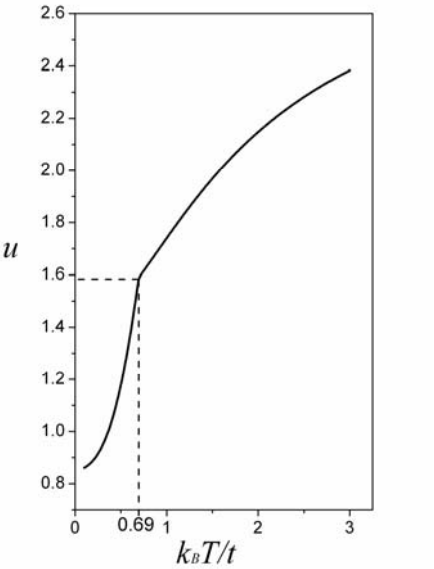

Figure 6. Internal energy per site u versus k_BT/t for n = 1, h = 0, and U = 6t. Tc = 0.69 t/k_B.

Calculating the derivative of the internal energy per site u as a function of temperature, Eq. (19), we easily get the graph of the specific heat as a function of temperature. Fig. 7 shows the specific heat c versus k_BT/t for $n = 1.0$, $h = 0$, and $U = 6t$, obtained from Figure 6. Note that at T_c=0.69 t/k_B, c presents a sharp peak. The form of the specific heat curve in Fig. 7 is the characteristic form of the specific-heat curve for two-dimensional square lattice magnetic models in the mean-field approximation [4, 5].

Finally, we determine the temperature dependence of the magnetic susceptibility χ from Eqs (16) and (15). Figure 8 shows χ versus k_BT/t for $n = 1.0$ and $U = 6t$. Observe that at critical temperature, $T_c = 0.69\ t/k_B$, a discontinuity occurs in χ.

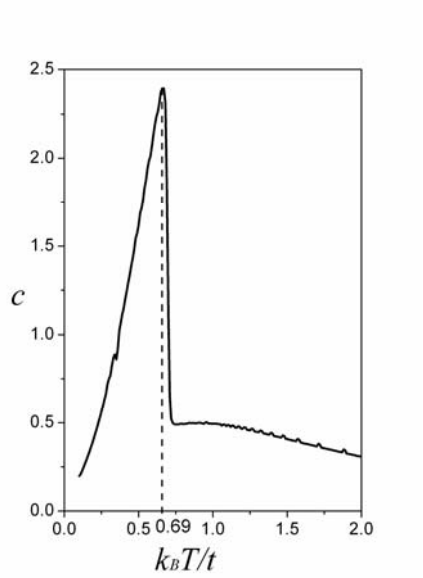

Figure 7. Specific heat c versus k_BT/t for n = 1.0, h = 0, and U = 6t. Tc = 0.69 t/k_B.

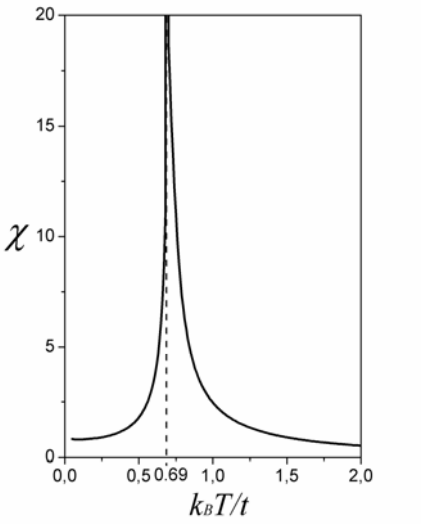

Figure 8. Magnetic susceptibility χ versus k_BT/t for n = 1.0 and U = 6t. T_c = 0.69 t/k_B.

4. CONCLUSIONS

We have studied, with a pedagogical approach, the thermodynamic properties of the two-dimensional Hubbard model on a square lattice using the Hartree-Fock approximation. The thermodynamic properties obtained in this work represent an important set of physical phenomena that are of ample interest in the study of strongly correlated electron systems.

We have shown how to obtain the magnetization, the magnetic susceptibility, the internal energy, the specific heat, and also a phase diagram for ferromagnetic and non-ferromagnetic phases of the studied system.

Our approach of the application of the Hartree-Fock approximation for the Hubbard model clearly shows that the use of the Hartree-Fock approximation in this case is very simple. The student can perceive how the ideas that involve the analysis of an ideal Fermi gas through the grand canonical method of statistical mechanics can be extended to an interacting system. The increase of the complexity only refers to the numerical problem of solving self-consistent equations.

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