Revista Mexicana de Física **42**, *No. 4 (1996) 617–627*

Anisotropic charge density waves in the electron gas

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Recibido el 31 de enero de 1996; aceptado el 20 de febrero de 1996

ABSTRACT. The analysis of the formation of anisotropic charge density waves for an electron gas system embedded in a deformable jellium model at finite temperature is presented. The formulation of the problem is based on unrestricted temperature-dependent Hartree-Fock equations. In the present work we focus our discussion in studying the instability condition against the formation of 3D anisotropic charge density waves. The phase diagram for different values of the anisotropy parameter is constructed and zones of stability are shown.

RESUMEN. En el presente trabajo se hace un análisis sobre la formación de ondas de densidad de carga anisotrópica en el modelo de gas de electrones deformables a temperaturas cero y finita. El problema se resuelve dentro de la aproximación de Hartree-Fock dependiente de la temperatura. Se discute en particular el estudio de ondas de densidad de carga anisotrópica en 3 dimensiones. Se construye el diagrama de fases para los diferentes valores del parámetro de anisotropía, mostrando las zonas de estabilidad para la onda de densidad de carga.

PACS: 71.45.Lr, 65.40.–f, 71.10.+x

1. INTRODUCTION

The study of the electron gas system has played a fundamental role in the understanding of several physical properties in condensed matter. During the last decades this model has been widely used for the description of important applications. Among those phenomena that have attracted a lot of attention in recent years the problem on the formation of a charge density wave [1–3] deserves a special and careful analysis. Evidence of this collective effect has been found through optical and dielectric measurements in some organic materials and in the pseudo-organic compound potassium platinocyanide (KCP) [4]. Various inorganic compounds have been also found that exhibit CDW with nonlinear transport phenomena, being perhaps the potassium-molybdenum-bronzes $K_{0.3}MoO_3$ (the blue

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bronze) one of the best examples [5]. There have been also some researches concerning a possible influence a CDW might have on high T_c superconductors. Experiments of positron annihilation on polycrystalline samples of $Y_1Ba_2Cu_3O_{7-x}$ suggested that the redistribution in momentum space of valence electrons in the superconducting state is consistent with the formation of a static CDW in the Cu-O chains [6,7].

The existence of a spatially modulated electron density implies that its period might be incommensurated with the spacing of the underlying lattice, loosing in that case truly periodicity in the crystal. Most of the discussions concerning the origin of the phase transition to a state in which the electron density presents periodic modulation have been made for low dimensional systems [8]. It has been shown however that the existence of CDW is not restricted to those sytems [9–13]. In fact, within the Hartree-Fock (HF) theory or density functional formalism [14], the study of the jellium model predicts the existence, for certain values of the electron density, of a state with a non uniform density with lower binding energy than the plane wave. At low electron densities, Wigner predicted the formation of a state where the electrons arrange in a crystalline phase. In such a phase the electrons do not move freely but they are confined to the sites of a lattice with small oscillations about their mean positions corresponding to quantum mechanical zero point motions [15, 16]. The existence of the Wigner crystal has been found experimentally on the electron gas formed at the interface of GaAs and AlGaAs layers of a modulated-doped heterojunction subjected to strong magnetic fields [17, 18]. Although CDW instabilities have been widely discussed at zero [19–22] and finite [23, 24] temperatures there are still many interesting questions to be answered concerning their behavior at finite temperature.

In this work we present the results of studying the instability condition for a three dimensional electron gas within a deformable jellium model for the formation of an anisotropic CDW as a function of density and temperature. The analysis is based on comparing the stability condition of the plane wave solution against the correlated charged density wave within the temperature-dependent Hartree-Fock model. The use of the HF approximation is then justified since we are using a trial wave function that already contains the collective effects [25]. We formulate our model in Sect. 2 and discuss the instability condition against the formation of an anisotropic charge density wave. Here it is shown how given the anisotropy parameter, the present model may be used in a systematic way to calculate the temperature and density dependence of the HF solution. In Sect. 3 we present our results and show the phase diagrams for a three dimensional electron gas system for different values of the anisotropy parameter. Here we show the zones in an energy, temperature and density diagram where a 3D charge density waves is stable. Sect. 4 gives a brief summary of our results.

2. DESCRIPTION OF THE MODEL

We study the ground state of a many electron system by considering the stability condition of a deformable jellium model. In this model the electrons move against a deformable positive background allowing the background density $\eta(\mathbf{R})$ to adjust in order to have local neutrality.

The stability condition is analyzed by comparing the energy of the system with uniform electron density with that corresponding to a spatially modulated one. All this analysis is made within a temperature dependent Hartree-Fock model (TDHF).

The hamiltonian for the jellium model is given by

$$H = H_{ee} + H_{bb} + H_{eb}, \tag{1}$$

where

$$H_{ee} = \sum_{\mathbf{k}} T_{\mathbf{kk}}\, a_{\mathbf{k}}^{+}\, a_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{kk'}} V_{\mathbf{kk'kk'}}\, a_{\mathbf{k}}^{+}\, a_{\mathbf{k'}}^{+}\, a_{\mathbf{k'}} a_{\mathbf{k}}, \tag{2}$$

$$H_{bb} = \frac{1}{2} \int \eta(\mathbf{R})\, V(\mathbf{R} - \mathbf{R}')\, \eta(\mathbf{R}')\, d\mathbf{R}\, d\mathbf{R}', \tag{3}$$

corresponding to the electronic and background hamiltonians in second quantization formalism respectively, where $a_{\mathbf{k}}^{+}$, $a_{\mathbf{k}}$ are the creation and anhilation electron operators and $\mathbf{k}$ is the 3 dimensional wave vector. The electron-background hamiltonian is

$$H_{eb} = -\sum_{\mathbf{k}} \int V_{\mathbf{kk}}(\mathbf{R})\, \eta(\mathbf{R})\, d\mathbf{R}\, a_{\mathbf{k}}^{+}\, a_{\mathbf{k}}. \tag{4}$$

The matrix elements for the electron kinetic energy, the electron-electron interaction and the electron-background interaction $T_{\mathbf{kk}}$, $V_{\mathbf{klmn}}$ and $V_{\mathbf{kk}}$respectively, are expressed in terms of the single particle electron wave function $\phi_{\mathbf{k}}(\mathbf{r})$ through the usual relations:

$$T_{\mathbf{kk}} = \int \phi_{\mathbf{k}}^{*}(\mathbf{r})\, T \phi_{\mathbf{k}}(\mathbf{r})\, d\mathbf{r}, \tag{5}$$

$$V_{\mathbf{klmn}} = \int \phi_{\mathbf{k}}^{*}(\mathbf{r})\, \phi_{\mathbf{l}}^{*}(\mathbf{r}')\, V(\mathbf{r} - \mathbf{r}')\, \phi_{\mathbf{m}}(\mathbf{r})\, \phi_{\mathbf{n}}(\mathbf{r}')\, d\mathbf{r}'\, d\mathbf{r}, \tag{6}$$

$$V_{\mathbf{kk'}}(\mathbf{R}) = \int \phi_{\mathbf{k}}^{*}(\mathbf{r})\, V(\mathbf{r} - \mathbf{R})\, \phi_{\mathbf{k'}}(\mathbf{r})\, d\mathbf{r}. \tag{7}$$

In order to perform the HF calculation we take for the electron-electron interaction the screened coulomb potential

$$V(r) = \frac{e^{-\mu_0 r}}{r}, \tag{8}$$

where the screening parameter $\mu_0 = 0.815/\sqrt{r_s}$ is determined by the Thomas-Fermi model.

It can be shown that for the above hamiltonian, the energy per particle in the thermodynamic limit [26] is given by

$$E = \sum_{\mathbf{k}} T_{\mathbf{kk}} \langle n_{\mathbf{k}} \rangle_T - \frac{1}{2} \sum_{\mathbf{kk'}} V_{\mathbf{kk'k'k}} \langle n_{\mathbf{k}} \rangle_T \langle n_{\mathbf{k'}} \rangle_T . \tag{9}$$

As it is well known, within the jellium model the only contribution to the energy of the system comes from the electron kinetic energy and the exchange term of the electron-electron interaction. This is due to the fact that the direct term of the electron-electron interaction, the electron-background and the background-background interaction add up to zero. The temperature average of the occupation number $\langle n_{\mathbf{k}} \rangle_T$ has the general expression

$$\langle n_{\mathbf{k}} \rangle_T = \frac{1}{e^{\beta(\varepsilon_{\mathbf{k}} - \mu)} + 1}, \tag{10}$$

where $\beta = 1/k_B T$. This last expresion in the low temperature regime can be expressed by the Sommerfeld approximation

$$\langle n_{\mathbf{k}} \rangle_T \approx \theta(\varepsilon_F - \varepsilon_{\mathbf{k}}) - \frac{\pi^2}{6\beta^2} \frac{d}{d\varepsilon_{\mathbf{k}}} \delta(\varepsilon_F - \varepsilon_{\mathbf{k}}), \tag{11}$$

where $\theta(\varepsilon)$ is the Heavyside function and $\delta(\varepsilon)$ is the Dirac function, ε_F is the energy of the Fermi level and $\varepsilon_{\mathbf{k}}$ is the energy of the $\mathbf{k}$ level which in our case corresponds to a free particle. Equation (11) is valid for r_s values as high as 60 and temperatures up to the order of 60 K.

The variation of the energy given by Eq. (9) with respect to the orbitals with the usual orthonormalization condition, gives us the reduced Hartree-Fock equations:

$$T\phi_{\mathbf{k}}(\mathbf{r}) - \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}(\mathbf{r}) \langle n_{\mathbf{k}} \rangle_T \, \phi_{\mathbf{k}}(\mathbf{r}) = \epsilon_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{r}), \tag{12}$$

where $V_{\mathbf{k}\mathbf{k}'}(\mathbf{r})$ is defined by Eq. (7).

In order to study the stability condition for the electron gas we perform in this work an analysis of the HF solutions with a Bloch type function

$$\phi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{v}} e^{-i\mathbf{k}\cdot\mathbf{r}} \sum_{\mathbf{n}=-\mathbf{N}_1}^{\mathbf{N}_1} c_{\mathbf{n}} \, e^{i\mathbf{q}\cdot\mathbf{r}}, \tag{13}$$

where $\mathbf{q} = (n_x q_{0x}, n_y q_{0y}, n_z q_{0z})$ with n_x, n_y, n_z integers, $q_{0j} > 2k_F$ is the wave vector in the j direction, k_F is the Fermi radius and v is the electron gas volume. With this trial wave function, the HF Eq. (12) leads to an equation for the coefficients $c_{\mathbf{n}}$, given by

$$\sum_{\mathbf{n}_3} \left[\sum_{\mathbf{k}_1} T_{\mathbf{k}_1+\mathbf{n}_1, \mathbf{k}_1+\mathbf{n}_3} \langle n_{\mathbf{k}_1} \rangle_T - \sum_{\mathbf{n}_2 \mathbf{n}_4} \sum_{\mathbf{k}_1 \mathbf{k}_2} c_{\mathbf{n}_2} V_{\mathbf{k}_1+\mathbf{n}_1, \mathbf{k}_2+\mathbf{n}_2, \mathbf{k}_2+\mathbf{n}_4, \mathbf{k}_1+\mathbf{n}_3} c_{\mathbf{n}_4} \langle n_{\mathbf{k}_1} \rangle_T \langle n_{\mathbf{k}_2} \rangle_T \right] c_{\mathbf{n}_3} = \epsilon c_{\mathbf{n}_1}, \tag{14}$$

where the eigenvalue matrix equation for the coefficients has to be solved self-consistently, taking into account normal spin occupancy. Hence the geometrical properties of the electron gas, *i.e.* the instability against the formation of a CDW will be analyzed through the behavior of the vector $\mathbf{q}$ whose components are found from the solution of Eq. (14).

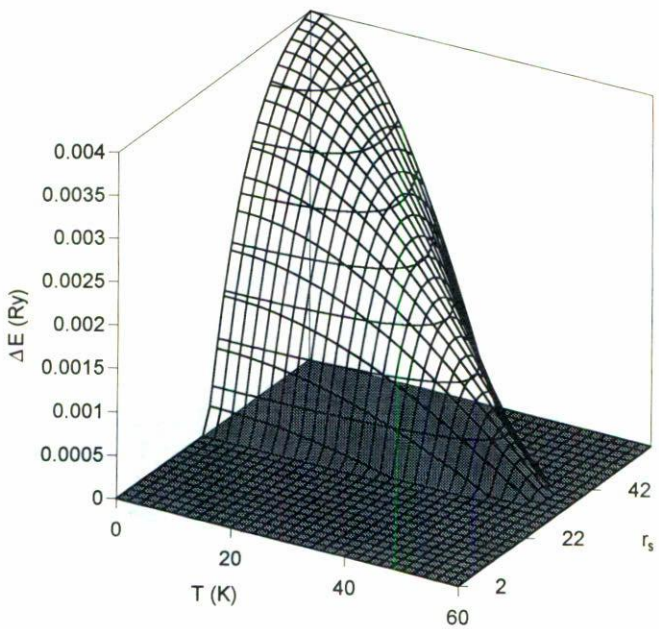

FIGURE 1. (a)

3. INSTABILITY CONDITION

The instability condition for an electron gas against the formation of a charge density wave is studied from the knowledge of the phase diagram constructed from the solution of the temperature dependent HF equations as a function of the electron density and for specific values of the anisotropy parameter $\alpha = q_{0x}/q_{0z}$. We have chosen for the present discussion a model with tetragonal symmetry *i.e.* $q_{0x} = q_{0y} \neq q_{0z}$. The phase diagram is constructed by plotting the binding energy difference between plane wave and the most stable solution for the HF equation versus density and temperature. Hence those points on the plane which correspond to zero energy difference determine the region for which the plane wave is stable, and bumps in the difference energy surface correspond to the regions of plane wave instability, that is when the CDW is present. In Fig. 1 we show the phase diagram for different α values. For the sake of comparison we also present the homogenous case ($\alpha = 1$). As can be seen from Fig. 1, as we increase the anisotropy parameter, the region where the CDW exists decreases. This means that in order to have a CDW for large anisotropy, we must go to lower temperatures and larger r_s values (smaller densities). It should be noted that the lowest r_s value for which we found a plane wave instability is $r_s = 26$ and correspond to the isotropic case $\alpha = 1$. We should note also how the maximum temperature for which we can have a CDW decreases as α increases. In particular we can see how for $\alpha = 1.10$ a CDW does not exist for $T \geq 28$ K

Another feature coming out from our calculation and that can be seen from Fig. 1 is that whereas at $T = 0$ we can have a CDW for all r_s values above the threshold, at $T \neq 0$ this is not longer true. This is more evident at higher temperatures where the region of instability for a given temperature is well localized in r_s. This is connected with the

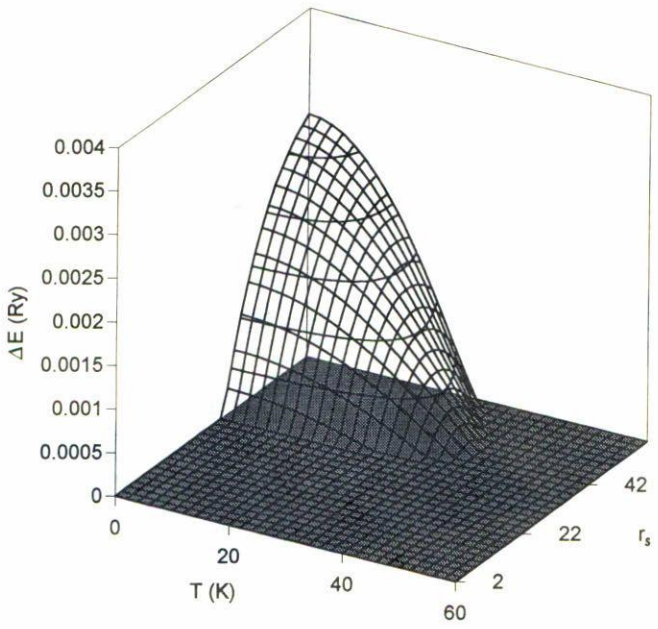

FIGURE 1. (b)

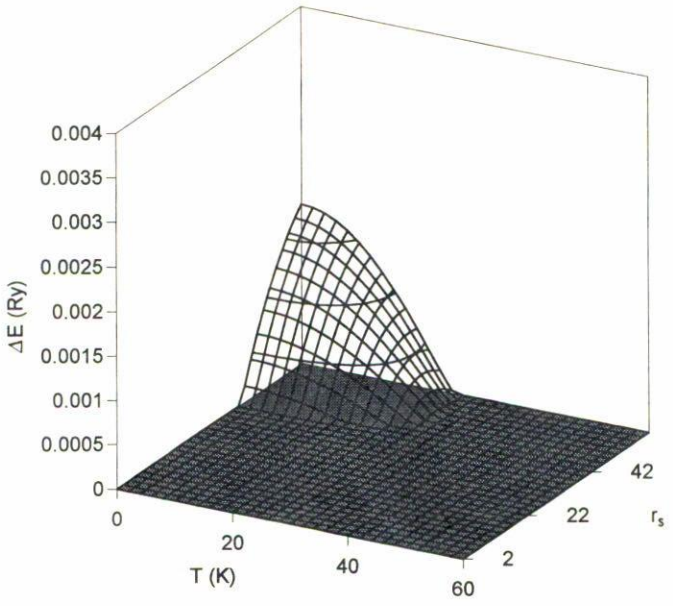

FIGURE 1. (c)

FIGURE 1. Phase diagram for the 3 dimensional electron gas system for several anisotropy parameters α. The vertical axis is defined as the energy difference per particle between the plane wave and the most stable HF solution $\Delta E(T, r_s) = E_{\mathrm{PW}} - E_{\mathrm{CDW}}$. The bumps correspond to the instability region for the PW solution leading to the formation of a CDW. Graphs (a), (b) and (c) correspond to $\alpha = 1.0$, 1.05 and 1.1, respectively.

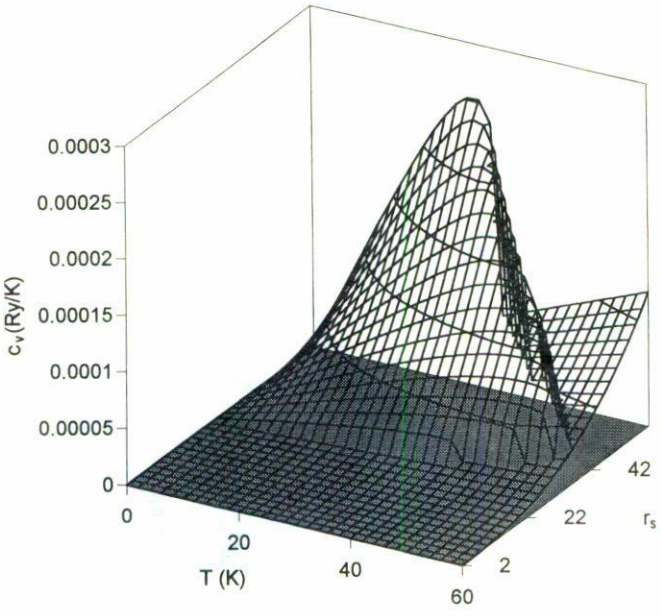

FIGURE 2. (a)

existence of a Wigner crystal. At $T = 0$ as we decrease the density (increase r_s) we go from plane wave to CDW which eventually becomes at sufficiently low densities a Wigner crystal. As we go to $T \neq 0$ moving along the r_s axis we have basically the same situation, that is we go from PW to CDW, the difference is now that thermal motion might upset the formation of a Wigner crystal, getting back a plane wave solution for the electron gas.

In Fig. 2 we show the behavior of the specific heat as a function of T and r_s for the three dimensional system discussed above. As can be seen on the region of plane wave stability, the specific heat corresponds to the free electron gas (*i.e.* $c_v \sim T$). What is worth discussing is its behavior on the instability region. Fig. 3 shows the projection of the c_v on a r_s constant plane (*i.e.* $c_v = c_v(T)$), for different values of the anisotropy parameter α. It is clear from these figures that c_v presents a discontinuous jump, showing a characteristic behavior of a second order phase transition. In Fig. 4 we show a more detailed calculation of c_v around the transition temperature. It is clear from this figure how in fact c_v presents a discontinuity at the transition temperature.

4. CONCLUSIONS

We have presented the use of a temperature dependent Hartree-Fock model for studying the stability condition of the three-dimensional electron gas. In particular we have focussed the present discussion to the stability condition against a CDW formation as a function of the anisotropy parameter. It is found, for a given anisotropy parameter α, that the smallest r_s value for such instability to occur increases with temperature and also increases as α

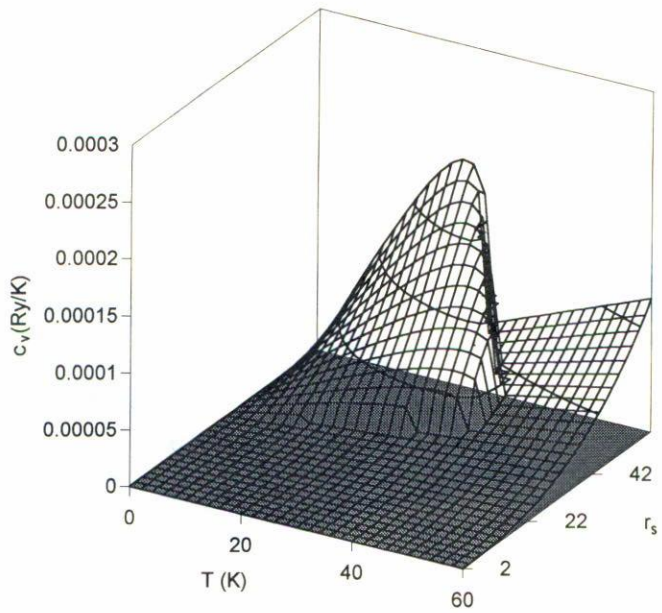

FIGURE 2. (b)

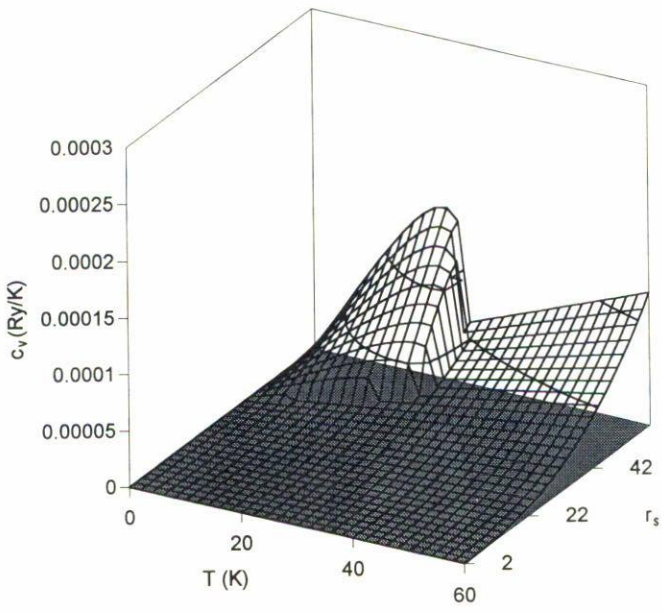

FIGURE 2. (c)

FIGURE 2. Specific heat behavior for the 3 dimensional electron gas system as a function of T and r_s for several values of the anisotropy parameter α. The bumps over the surface correspond to the CDW state. Graphs (a), (b) and (c) correspond to $\alpha = 1.0$, 1.05 and 1.1, respectively.

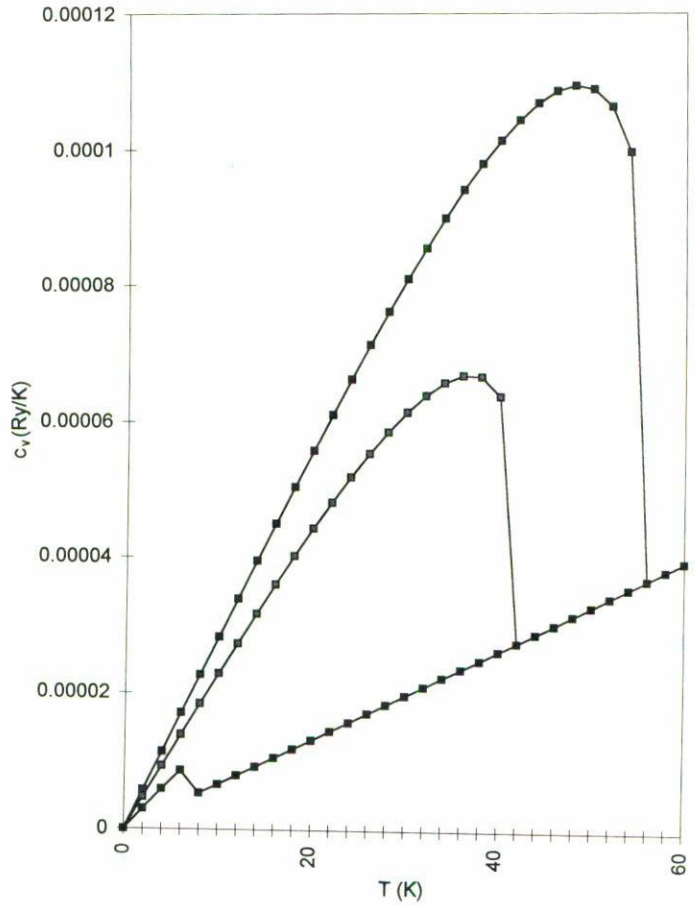

FIGURE 3. $c_v(T)$ for three different values of the anisotropy parameter. These curves correspond to the projection of $c_v(T, r_s)$ of Fig. 2 on the $r_s = 40$ plane for the same α values.

increases. In general it is found that as we increase α, the region on the r_s–T plane where a CDW exists gets smaller. At $T = 0$, the HF solution shows an instability threshold at $r_s = 26$ and remains unstable for larger r_s values. At $T \neq 0$ the behavior is completely different and there is a well defined range of r_s values for which the instability of plane wave solution against a CDW exists. Hence whereas at $T = 0$, we have the formation of a Wigner crystal, at $T \neq 0$ the existence of such a phase is limited by thermal effects.

The change of phase from plane wave to CDW was analyzed through the behavior of the specific heat. The theoretical calculation shows the characteristic gap of a second order phase transition.

Finally, we would like to mention that a typical copper-oxide superconductor like YBCO has an anisotropy parameter of the order of 3 ($\alpha \approx 3$) which according to our model calculation should not show the existence of a 3D CDW, ruling out the possibility of having a 3D CDW state connected with high T_c superconductivity in a broad range of densities.

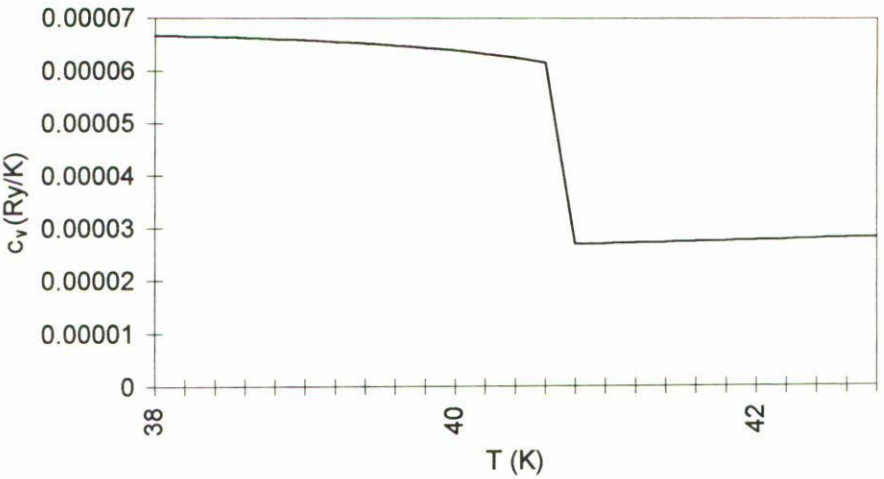

FIGURE 4. A detailed calculation for $c_v(T)$ around the transition temperature for $\alpha = 1.05$ and $r_s = 40$.

Although we have presented the analysis for the anisotropic 3D CDW, the formalism here discussed can be applied to systems that show CDW in 1D and 2D.

ACKNOWLEDGMENTS

This work was supported by CONACyT under contract No. 3910–E9402, by DGAPA-UNAM under contract IN-104694, and DGSCA-UNAM under contract CRAY-I200994, México. E.Y. acknowledges partial support from Cofaa-IPN.

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