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THE PARAMAGNETIC SUSCEPTIBILITY OF A ONE DIMENSIONAL CRYSTAL WITH A SINUSOIDAL POTENCIAL

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ABSTRACT

The paramagnetic susceptibility of a one dimensional crustal with a sinusoidal potential is examined in the second quantized formulation where two electrons per lattice site are assumed to be under the influence of the potential. Electron-electron interactions via Coulomb repulsion are ignored. The Green's function equation of motion technique is utilized to obtain an exact expression for the paramagnetic susceptibility for k, the allowed linear momenta, restricted to the first two Brillouin zones. The expressions are numerically integrated with the aid of an electronic computer to obtain values of susceptibility as a function of the inverse absolute temperature.

RESUMEN

Se examina la susceptibilidad paramagnética de un cristal unidimensional con un potencial sinusoidal usando la formulación de la segunda cuantización, suponiendo que dos electrones por sitio de la red estén bajo la influencia del potencial. No se consideranlas interacciones repulsivas coulombianas entre electrones. Se utiliza la técnica de la función de Green de las ecuaciones de movimiento para obtener una expresión exacta para la susceptibilidad paramagnética con K, los momentos lineales permitidos, restringidos a las dos primeras zonas de Brillouin. Las expresiones son integradas numéricamente usando un computador electrónico para obtener valores de la susceptibilidad como función del inverso de la temperatura absoluta.

1. INTRODUCCTION

Recently(1), one of the present authors examined the electronic specific heat of a one-dimensional crystal with a sinusoidal potential and obtained results which showed semiconductor to metal behavior as a function of temperature and well depth of the sinusoidal potential. The present purpose is to examine the crystal to determine the semiconductor to metal behavior for the paramagnetic susceptibility. As in the previous article(1), it is assumed that two electrons per lattice site (one atom per site contributing the electrons) are under the influence of the potential. The momentum vector will be restricted to the first two Brillouin zones. The choice of two electrons per lattice site under the influence of the potential will automatically ensure that the first Brillouin zone is completely filled at temperature T=0. (In the previous article(1); the graphs of Figs. 2 and 3 should be interchanged, and the specific heat unit is ev/(cm-k).) The momentum vector has been restricted to two Brillouin zones in order to limit the amount of necessary calculations, but it is also assumed that for reasonable temperatures, the probability of an electron jumping energy gaps into a third or higher Brillouin zone is small.

2. ANALYSIS

For the one-dimensional, paramagnetic sample under consideration one has, in the first quantized formulation, the Hamiltonian for one electron to be

$$H = \frac{\hbar^2}{2m} \nabla^2 - \frac{U}{2} \left(1 - \cos 2\pi \frac{x}{a}\right) \pm \frac{1}{2} g_s \mu_B H_0 \quad . \qquad (1)$$

In Eq. (1), H_o is the applied magnetic field, g_s is the gyromagnetic ratio for spin of the electron, and μ_B is the Bohr magneton. All other symbols have their previous$^{(1)}$ meanings. One assumes that the matter field is quantized in plane wave form to be

$$\psi = \frac{1}{\sqrt{L}} \sum_{K,\sigma} a_{K,\sigma}\, e^{iKx}\, ((\sigma) \,, \qquad (2)$$

where L is the sample length, K is the linear momentum vector, σ is the spin angular momentum, $(\sigma$ is the single particle spin state and $a_{K\sigma}$ is the electron creation operator. One may then obtain the Hamiltonian for electrons in the second quantized formulation to be

$$\begin{aligned} H &= \sum_{K,\sigma} (\hbar^2 k^2/2m - U/2 - \mu)\, a^{+}_{K,\sigma}\, a_{K,\sigma} \\ &\quad - U/4 \sum_{K,\sigma} (a^{+}_{K,\sigma}\, a_{K-2\pi/a,\sigma} + a^{+}_{K-2\pi/a,\sigma}\, a_{K,}\sigma) \\ &\quad - 1/2\, g_s \mu_B H_o\, {}_K\Sigma\, (\overset{+}{a}_{K,\uparrow}\, a_{K,\uparrow} - \overset{+}{a}_{K,\downarrow}\, a_{K,\downarrow}) \quad , \qquad (3) \end{aligned}$$

where μ, the chemical potential, is introduced so that one may obtain Grand canonical ensemble results when using the Green's function technique of statistical mechanics. By using a procedure entirely analogous to that done previously, one may obtain the Green's function equation of motion to be

$$E<<A/B>> = -\, 1/2\pi <[A,B]_+> \; + <<[A,H]_-|B>> \quad .$$

With $A = a_{K1,\uparrow}$ and $B = a^{+}_{K_2,\uparrow}$, one obtains, using the above equation and some manipulations

$$(E - \Delta_{K_1} + 1/2\, g_s \mu_B H_o) \quad <<a_{K_1,\uparrow}{}^{\dagger} a_{K_2,\uparrow}>>$$

$$= - 1/2\ \delta_{K_1K_2} - U/4\ (\langle\langle a_{K_1-2\pi/a,\uparrow}|a^{+}_{K_2,\uparrow}\rangle\rangle$$

$$+ \langle\langle a_{K_1+2\pi/a,\uparrow}|a_{K_2,\uparrow}\rangle\rangle) \quad , \tag{4}$$

$$\text{where one has } \Delta_K = \hbar^2K^2/2m - U/2 - \mu \quad . \tag{5}$$

By a similar procedure, replacing A by $a_{K_1,\uparrow}$ and B by $a_{K_2,\downarrow}$, one can obtain

$$(E - \Delta_{K_1} - 1/2\ g_s\mu_BH_o)\ \langle\langle a_{K_1,\downarrow}|a^{+}_{K_2,\downarrow}\rangle\rangle$$

$$= - 1/2\ \delta_{K_1K_2} - U/4(\langle\langle a_{K_1-2\pi/a,\downarrow}|a^{+}_{K_2,\downarrow}\rangle\rangle$$

$$+ \langle\langle a_{K_1+2\pi/a,\downarrow}|a^{+}_{K_2,\downarrow}\rangle\rangle) \quad . \tag{6}$$

One now utilizes Eqs. (4) and (6) and appies them to the two band model where one has for the first Brillouin zone (first band) $- \frac{\pi}{a} < K < \frac{\pi}{a}$, and for the second Brillouin zone (second band), $\frac{\pi}{a} < K < \frac{2\pi}{a}$, $\frac{-2\pi}{a} < K < \frac{-\pi}{a}$. Any Green's function outside of the first two Brillouin zones will be neglected. Due to symmetry considerations and the fact that only wave numbers within the first two Brillouin zones are used, one can see that all of the needed Green's function can be obtained from Eqs. (4) and (6) for $K > 0$.

In Eq. (4) for $K_1 = K_2 = K$, one obtains

$$(E - \Delta_{K_1} + 1/2\ g_s\mu_BH_o)\langle\langle a_{K,\uparrow}|a^{+}_{K,\uparrow}\rangle\rangle \tag{7}$$

$$= - 1/2\pi - U/4\ \langle\langle a_{K-2\pi/a,\uparrow}|a^{+}_{K,\uparrow}\rangle\rangle \ .$$

For $K_1 = K$, $K_2 = K - \frac{2\pi}{a}$, one has

$$(E - \Delta_K + 1/2\ g_s\mu_B H_o) \langle\langle a_{K,\uparrow} | a^+_{K - 2\pi/a,\uparrow} \rangle\rangle$$

$$= - U/4 \langle\langle a_{K-2\pi/a,\uparrow} | a_{K - 2\pi/a,} \rangle\rangle \quad . \tag{8}$$

For $K_1 = K - \frac{2\pi}{a}$, $K_2 = K$, one has

$$(E - \Delta_{K-2\pi/a} + 1/2\ g_s\mu_B H_o) \langle\langle a_{K - 2\pi/a,\uparrow} | a^+_{K,\uparrow} \rangle\rangle$$

$$= - U/4 \langle\langle a_{K,\uparrow} | a^+_{K,\uparrow} \rangle\rangle \quad . \tag{9}$$

For $K_1 = K_2 = K - \frac{2\pi}{a}$, one has

$$(E - \Delta_{K - 2\pi/a} + 1/2\ g_s\mu_B H_o) \langle\langle a_{K - 2\pi/a,\uparrow} | a^+_{K - 2\pi/a,\uparrow} \rangle\rangle$$

$$= - 1/2\pi - U/4 \langle\langle a_{K,\uparrow} | a^+_{K - 2\pi/a,\uparrow} \rangle\rangle \ . \tag{10}$$

One can write Eq. (10) as

$$\langle\langle a_{K - 2\pi/a,\uparrow} | a^+_{K - 2\pi/a,\uparrow} \rangle\rangle =$$

$$- 1/2\pi \frac{1}{(E - \Delta_{K-2\pi/a} + 1/2\ g_s\mu_B H_o}$$

$$-U/4 \frac{\langle\langle a_{K,\uparrow} | a^+_{K-2\pi/a,\uparrow} \rangle\rangle}{(E - \Delta_{K - 2\pi/a} + 1/2\ g_s\mu_B H_o)} \tag{11}$$

Using Eq. (11) in Eq. (8), one obtains

$$<<a_{K,\uparrow}|a^{+}_{K - 2\pi/a,\uparrow}>> \tag{12}$$

$$= 1/2\pi \frac{U/4}{(E - \Delta_{K - 2\pi/a} + 1/2\ g_s\mu_B H_o)(E - \Delta_K + 1/2\ g_s\mu_b H_o) - (U/4)^2)} \cdot$$

One can write Eq. (7) as

$$<<a_{K,\uparrow}|a_{K,\uparrow}>>$$

$$= -\ 1/2\pi \frac{1}{(E - \Delta_K + 1/2\ g_s\mu_B H_o)} - U/4 \frac{<<a_{K - 2\pi/a}|a_{K,\uparrow}>>}{(E - \Delta_K + 1/2\ g_s\mu_B H_o)} \cdot \tag{13}$$

Substitution of Eq. (13) into Eq. (9) yields

$$<<a_{K - 2\pi/a,\uparrow}|a^{+}_{K,\uparrow}>> =$$

$$1/2\pi \frac{U/4}{(E - \Delta_{K - 2\pi/a} + 1/2\ g_s\mu_B H_o)(E\ \Delta_K + 1/2\ g_s\mu_B H_o) - (U/4)^2} \cdot \tag{14}$$

From Eqs. (12) and (14), one has

$$<<a_{K - 2\pi/a,\uparrow}|a^{+}_{K,\uparrow}>> = <<a_{K,\uparrow}|a^{+}_{K - 2\pi/a',\uparrow}>> \quad . \tag{15}$$

From Eqs. (7) and (9), eliminating $<<a_{K - \frac{2\pi}{a},\uparrow}|a_{K,\uparrow}>>$, one obtains

$$<<a_{K,\uparrow}|a^{+}_{K,\uparrow}>> = \tag{16}$$

$$-1/2\pi \frac{E - \Delta_{K - 2\pi/a} + 1/2\ g_s\mu_B H_o}{(E - \Delta_K - 1/2\ g_s\mu_B H_o)(E - \Delta_{K - 2\pi/a} + 1/2\ g_s\mu_B H_o) - (U/4)^2}$$

By using a similar procedure with Eq. (6), one obtains

$$<<a_{K,\downarrow}|a^{+}_{K,\downarrow}>> = \tag{17}$$

$$- 1/2\pi \frac{E - \Delta_{K - 2\pi/a} - 1/2\ g_s\mu_B H_o}{(E - \Delta_K - 1/2\ g_s\mu_B H_o)(E - \Delta_{K-2\pi/a} - 1/2\ g_s\mu_B H_o) - (U/4)^2} .$$

From Eq. (16), one may write

$$<<a_{K,\uparrow}|a^{+}_{K,\uparrow}>> =$$

$$-1/2\pi \frac{E - \Delta_{K -2\pi/a} + 1/2\ g_s\mu_B H_o}{(E - \Delta_K + 1/2\ g_s\mu_B H_o)(E - \Delta_{K -2\pi/a} + 1/2\ g_s\mu_B H_o) - (U/4)^2}$$

$$= - 1/2\pi \frac{E' - \Delta_{K - 2\pi/a}}{(E'^2 - (\Delta_K + \Delta_{K - 2\pi/a})\ E' + (\Delta_K\Delta_{K - 2\pi/a} - [U/4]^2))}$$

where one uses $E' = E + 1/2\ g_s\mu_B H_o$. One can now factor the denominator and write Eq. (17) as

$$<<a_{K,\uparrow}|a^{+}_{K,\uparrow}>> =$$

$$- 1/2\pi \frac{E' - \Delta_{K - 2\pi/a}}{(E' - D_1(K))\ (E' - D_2(K))} , \tag{18}$$

where one defines $D_1(K)$ and $D_2(K)$ to be

$$D_1(K) = 1/2\ (\Delta_K + \Delta_{K - 2\pi/a}) + \sqrt{1/4|\Delta_K - \Delta_{K - 2\pi/a}|^2 + (U/4)^2} ,$$

$$D_2(K) = 1/2(\Delta_K + \Delta_{K\ -2\pi/a}) - \sqrt{1/4|\Delta_K - \Delta_{K\ -\ 2\pi/a}|^2 + (U/4)^2}\ . \quad (19)$$

Decomposing the right hand side of Eq. (18) into partial fractions, one obtains

$$<<a_{K,\uparrow}|a^+_{K,\uparrow}>> =$$

$$-(1/2\pi)\frac{1}{D_1(K) - D_2(K)}\left[\frac{(D_1(K) - \Delta_{K-2\pi/a}}{(E' - D_1(K))} - \frac{(D_2(K) - \Delta_{K\ -\ 2\pi/a})}{(E' - D_2(K))}\right]\ . \quad (20)$$

Similarly, one can write Eq. (17) as

$$<<a_{K,\downarrow}|a^+_{K,\downarrow}>>$$

$$-(1/2\pi)\ \frac{1}{D_1(K)-D_2(K)}\ \left[\frac{(D_1(K)-\Delta_{K-2\pi/a})}{(E''-D_1(K))} - \frac{(D_2(K)-\Delta_{K-2\pi/a})}{(E'' - D_2(K))}\right]\ . \quad (21)$$

where one uses $E'' = E - \frac{1}{2}\, g_s\ {}_B H_o$.

By using a procedure that is by now very familiar (only several mentioned here$^{(2,3,4,5)}$ one may obtain the pertinent correlation functions to be (using the definitions for E' and E'')

$$<a^+_{K,\uparrow}\ a_{K,\uparrow}> \quad =$$

$$\frac{1}{D_1(K)-D_2(K)}\ \left\{\frac{D_1(K) - \Delta_{K\ -\ 2\pi/a}}{\exp[\beta(D_1(K)-1/2 g_s\mu_B H_o]+1} - \frac{D_2(K) - \Delta_{K\ -\ 2\pi/a}}{\exp[\beta(D_2(K)-1/2\ g_s\mu_B H_o)]+1}\right\}$$

(22)

and

$$\langle a^{+}_{K,\downarrow}\, a_{K,\downarrow}\rangle = \qquad (23)$$

$$\frac{1}{D_1(K)-D_2(K)} \left\{ \frac{D_1(K) - \Delta_{K - 2\pi/a}}{\exp[\beta(D_1(K)+1/2\ g_s\mu_B H_o]+1} - \frac{D_2(K) - \Delta_{K - 2\pi/a}}{\exp[\beta(D_2(K)+1/2\ g_s\mu_B H_o)]+1} \right\}$$

The magnetization per unit length, <M>, is

$$\langle M\rangle = \frac{(1/2)g_s\mu_B}{L} \left\{ \begin{array}{l} \text{(Total number of particles having spin up)} \\ -\text{(Total number of particles having spin down)} \end{array} \right\} .$$

Therefore, one has the magnetization per unit length to be, using Eqs. (22) and (23),

$$\langle M\rangle = \frac{g_s\mu_B}{2L}\ 2 \sum_{K>0} (\langle a^{+}_{K,\uparrow} a_{K,\uparrow}\rangle - \langle a^{+}_{K,\downarrow} a_{K,\downarrow}\rangle)$$

$$= \frac{g_s\mu_B}{L} \left\{ \sum_{K>0} \frac{1}{D_1(K)-D_2(K)} \left[\frac{D_1(K) - \Delta_{K - 2\pi/a}}{\exp[\beta(D_1(K)-1/2g_s\mu_B H_o)]+1} - \frac{D_2(K) - \Delta_{K - 2\pi/a}}{\exp[\beta(D_2(K)-1/2g_s\mu_B H_o)]+1} \right.\right.$$

$$\left.\left. - \frac{D_1(K) - \Delta_{K - 2\pi/a}}{\exp[\beta(D_1(K)+1/2g_s\mu_B H_o)]+1} + \frac{D_2(K) - \Delta_{K - 2\pi/a}}{\exp[\beta(D_2(K)+1/2g_s\mu_B H_o)]+1} \right] \right\} . \qquad (24)$$

As in the previous paper, one can summarize that for U not very large $H_o \rightarrow 0$, μ for $T = 0$ would be of the order of

$$\mu \simeq \hbar^2 K^2_f/2m - U/2 \quad , \qquad (25)$$

K_f being the Fermi momentum. The chemical potential is equal to the Fermi energy for $U = 0$ (free particle), or,

$$E_f = \mu = \hbar^2 K^2{}_f / 2m \quad . \tag{26}$$

By assuming that at $T = 0$ the first Brillouin zone (first band) is filled, one may write that Ne, the number of electrons, is

$$Ne = 4 \sum_{K>0}^{k_f} = 4 \ (L/2\ ) \int_0^{K_f} dK = 2L/\pi \ K_f ,$$

such that one has

$$K_f = (\pi/2) \ (Ne/L) \quad . \tag{27}$$

Since one has for this problem that Ne is twice the number of lattice points (one atom per lattice point, two electrons contributed per atom), one may write

$$Ne = 2N, \ L = Na, \ K_f = \pi/a \ ,$$

where $\pm \frac{\pi}{2}$ are the limits of the first Billouin zone. Now, going back to Eq. (24) and by replacing the sum by an integral, one can write

$$\langle M \rangle = (g_s \mu_B / 2\pi) \left\{ \int_0^{2K_f} dk \, \frac{1}{D_1(K) - D_2(K)} \right. .$$

$$\cdot \left[\frac{D_1(K) - \Delta_{K-2\pi/a}}{\exp[\beta(D_1(K) - 1/2 \ g_s \mu_B H_o)] + 1} - \frac{D_2(K) - \Delta_{K-2\pi/a}}{\exp[\beta(D_2(K) - 1/2 \ g_s \mu_B H_o)] + 1} \right.$$

$$- \frac{D_1(K) - \Delta_{K - 2\pi/a}}{\exp[\beta(D_1(K) + 1/2\ g_s\mu_B H_o)]+1} - \frac{D_2(K) - \Delta_{K - 2\pi/a}}{\exp[\beta(D_2(K) + 1/2\ g_s\mu_B H_o)]+1} \Bigg]\Bigg\} ,$$

$$\langle M\rangle = (g_s\mu_B/2\pi) \int_0^{2K_f} dK \frac{1}{D_1(K) - D_2(K)} \cdot$$

$$\cdot \Bigg\{ (D_1(K) - \Delta_{K-2\pi/a}) \Bigg(\frac{1}{\exp[\beta(D_1(K)-1/2\ g_s\mu_B H_o)]+1} - \frac{1}{\exp[\beta(D_1(K)-1/2\ g_s\mu_B H_o]+1} \Bigg)$$

$$- (D_2(K) - \Delta_{K-2\pi/a}) \Bigg(\frac{1}{\exp[\beta(D_2(K)-1/2\ g_s\mu_B H_o)]+1} - \frac{1}{\exp[\beta(D_2(K)+1/2\ g_s\mu_B H_o)+1} \Bigg) \Bigg\} . \tag{28}$$

The susceptibility, χ, is given by

$$\chi = - (\partial \langle M\rangle/\partial H_o) | H_o \to 0 \quad ,$$

$$\chi = \frac{(g_s\mu_B)^2 \beta}{\pi} \Bigg\{ \int_0^{2K_f} dK \frac{1}{(D_1(k) - D_2(K))} \cdot$$

$$\cdot \Bigg[\frac{(D_1(K) - \Delta_{K-2Kf})e^{\beta D_1(K)}}{(e^{\beta D_1(K)} + 1)^2} - \frac{(D_2(K) - \Delta_{K-2Kf})e^{\beta D_2(K)}}{(e^{\beta D_2(K)} + 1)^2} \Bigg] \Bigg\} . \tag{29}$$

From Eqs. (5), (25) and (26), one may write

$$\Delta_K = E_f[(K/K_f)^2 - 1] \quad ,$$

$$\Delta_{K-2Kf} = E_f [(K/K_f - 2)^2 - 1] \quad ,$$

$$D_1(K) = E_f(1 - K/K_f)^2 + \sqrt{4E_f{}^2|(1 - K/Kf)|^2 + (U/4)^2} ,$$

$$D_2(K) = E_f(1 - K/K_f)^2 - \sqrt{4E_f{}^2|(1 - K/K_f)|^2 + (U/4)^2} . \qquad (30)$$

By making a change of variables such that one has

$$x = 1 - K/K_f \quad ,$$

one may write the Eqs. (30) in terms of x as

$$\Delta_K = \Delta_x = E_f \, x \, (x-2) \quad ,$$

$$\Delta_{K-2K_f} = \Delta_{-x} = E_f \, x \, (x+2) \quad ,$$

$$D_1(K) = D_1(x) = E_f x^2 + \sqrt{4E_f^2|x|^2 + (U/4)^2} \quad ,$$

$$D_2(K) = D_2(x) = E_f x^2 - \sqrt{4E_f^2|x|^2 + (U/4)^2} \; . \qquad (31)$$

With the indicated change of variables, Eq. (29) becomes,

$$\chi = \frac{(g_s\mu_B)^2\beta}{\pi} \times K_f \left\{ \int_{-1}^{1} dx \, \frac{1}{D_1(x) - D_2(x)} \times \right.$$

$$\left. \left[\frac{(D_1(x) - \Delta_{-x})e^{\beta D_1(x)}}{(e^{\beta D_1(x)} + 1)^2} - \frac{(D_2(x) - \Delta_{-x})e^{\beta D_2(x)}}{(e^{\beta D_2(x)} + 1)^2} \right] \right\} . \qquad (32)$$

Making use of the parity of the functions involved, one has

$$\chi = \frac{2(g_s\mu_B)^2\ \beta K_f}{\pi} \left\{ \int_0^1 \frac{dx}{D_1(x) - D_2(x)} \right.$$

$$\left. \left[\frac{(D_1(x) - E_f x^2)e^{\beta D_1(x)}}{(E^{\beta D_1(x)} + 1)^2} - \frac{(D_2(x) - E_f x^2)e^{\beta D\ 2(x)}}{(e^{\beta D_2(x)} + 1)^2} \right] \right\} . \qquad (33)$$

But from Eqs. (31), one has

$$E_f x^2 = \frac{D_1(x) + D_2(x)}{2}$$

Hence, the susceptibility is finally written as

$$\chi = \frac{(g_s\mu_\beta)^2 \beta K_f}{\pi} \left\{ \int_0^1 dx \left[\frac{e^{-\beta D_1(x)}}{(1+e^{-\beta D_1(x)})^2} + \frac{e^{\beta D_2(x)}}{(e^{\beta D_2(x)+1})^2} \right] \right\} . \qquad (34)$$

Equation (34) is solved by the aid of an electronic computer and Simpson's rule for various values of $K_B T$ and well depth U. The results are shown in the figures that follow.

5. RESULTS AND DISCUSSION

In Figs. 1-3, the paramagnetic susceptibility is shown as a function of $1/K_B T$ for various values of well depth, U, for the situation in which the first band is completely filled, second band empty, at T = 0. Very large temperature values (small $1/K_B T$) values) are unrealistic for a solid, but such plots are given to examine the behavior of the analytical function.

Figure 1 shows the paramagnetic susceptibility as a function of $1/K_B T$ for the free electron model (U = 0.0 ev). The variation of the susceptibility is as expected$^{(6,7,8)}$ in that one has metallic behavior in the high temperature range (the typical 1/T dependence of susceptibility) and a "flat" susceptibility curve for low temperatures.

In Figure 2, for a small well depth of $U = 9.40 \times 10^{-3}$ ev, metallic behavior seems to be evident for $0 \leqslant \beta \leqslant 10.7\ (\mathrm{ev})^{-1}$ ($K_B T \geqslant 0.93 \times 10^{-1}$ ev, $T \geqslant 1.05 \times 10^3$ k). For $\beta > 10.7\ (\mathrm{ev})^{-1}$ ($K_B T \leqslant 0.931 \times 10^{-1}$ ev) semiconductor behavior becomes evident; the susceptibility decreases due to the attraction between the electrons and the ion cores.

In Figure 3 for a well depth of $U = 0.40 \times 10^{-2}$ ev (10 times more than in Fig. 2), the susceptibility starts deviating from the metallic behavior at around $\beta \simeq 1.1\ (\mathrm{ev})^{-1}$, $K_B T \simeq 0.98$ ev, $T \simeq 10^4$ k. One should note that as the temperature increases beyond that which gives $K_B T \geqslant U/2$, the band gap ($T \simeq 2 \times 10^5$ k, $\beta \simeq 0.05\ (\mathrm{ev})^{-1}$), one observes a gradual change towards metallic behavior giving a typical Curie plot at higher temperatures. One might explain this the following way: the thermal energy of electrons becomes so high that the assumed sinusoidal potential has minimal effect on them, and they behave as if thew were free electrons.

The results for the model for the first band completely filled and second empty at T = 0 are as predicted$^{(8)}$, *i.e.*, semiconductor or insulator behavior is predicted when the first band is completely filled or when there is as even number of electrons per lattice site available for conduction.

It should be stated that susceptibility calculations were made by one of the present authors (A.T.)* for the situation in which the first band is half-filled and the second band is empty at T = 0 (one electron per atom available for conduction). For such a calculation, the Fermi temperature is $T_F = 5.0 \times 10^4$ k, which is half the Fermi temperature for when the first band is completely filled at T = 0. For all well depths, the suceptibility as a function of $1/K_B T$ is approximately the same. The deviation from metallic behavior is not as pronounced as in

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* Much of the present work is from A.T.'s Masters' Thesis presented to the University of Texas at El Paso for partial fulfillment of M.S. degree requirements, July, 1982.

the presented figures and the results for the susceptibility are nearly the same as for the free electron model. Such should be the case when there are odd numbers of electrons per lattice site available for conduction.

The above calculations have been made without including the realistic electron-electron interactions. If such interactions had been included in our calculations, however, in addition to the obvious added mathematical manipulations, one should see an upward shift in the susceptibility, especially in the low temperature region. In the low temperature region, this shift would also be nearly temperature independent. Such will be the case because in an electron's energy there will be a shift due to a change in the distribution of electrons with which a given electron interacts. What proves to be significant is the negative exchange energy term. The overall qualitative features for the susceptibility calculations should be the same, however.

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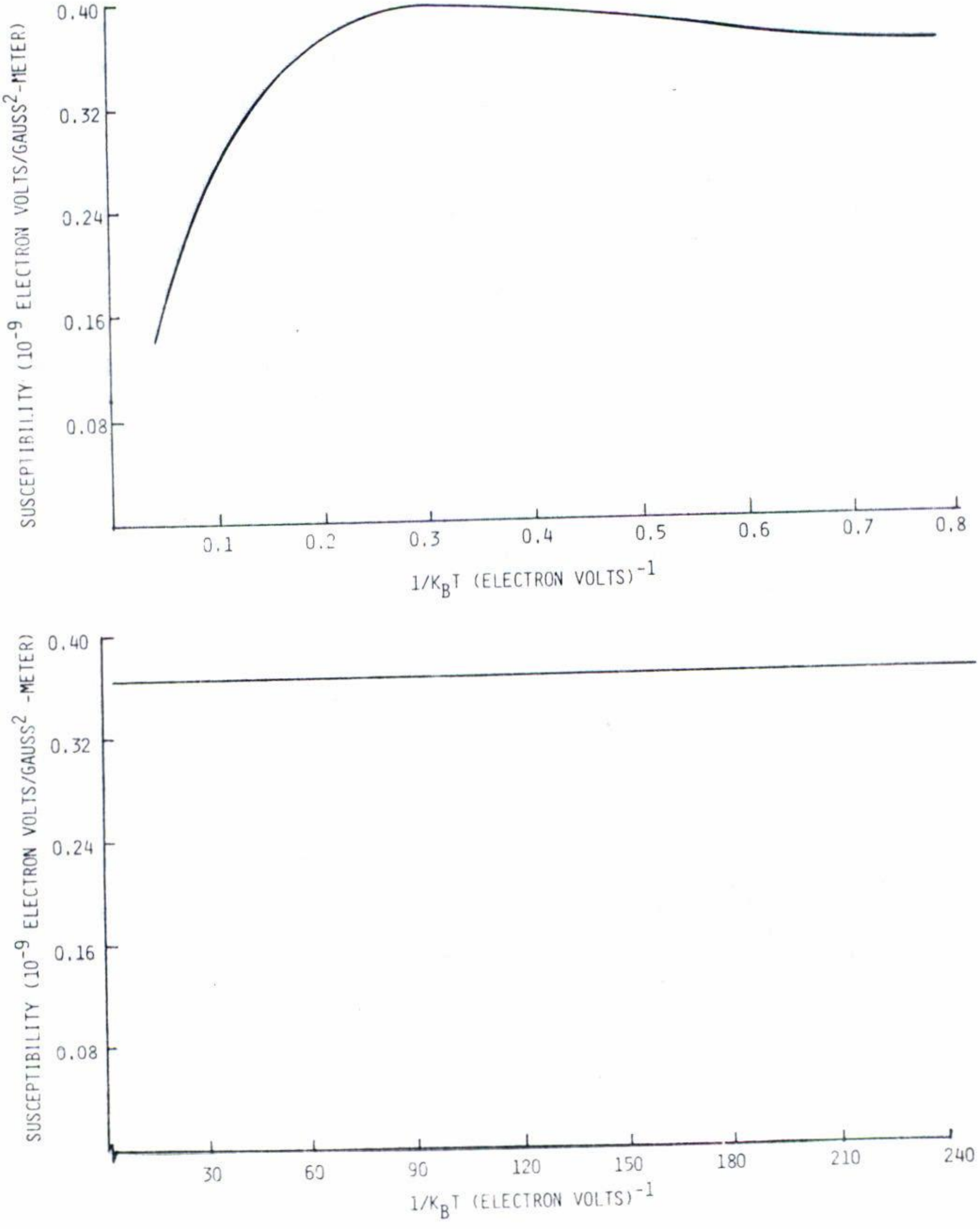

Fig. 1A, 1B. Temperature dependence of the paramagnetic susceptibility for U = 0.0 ev (free electron model).

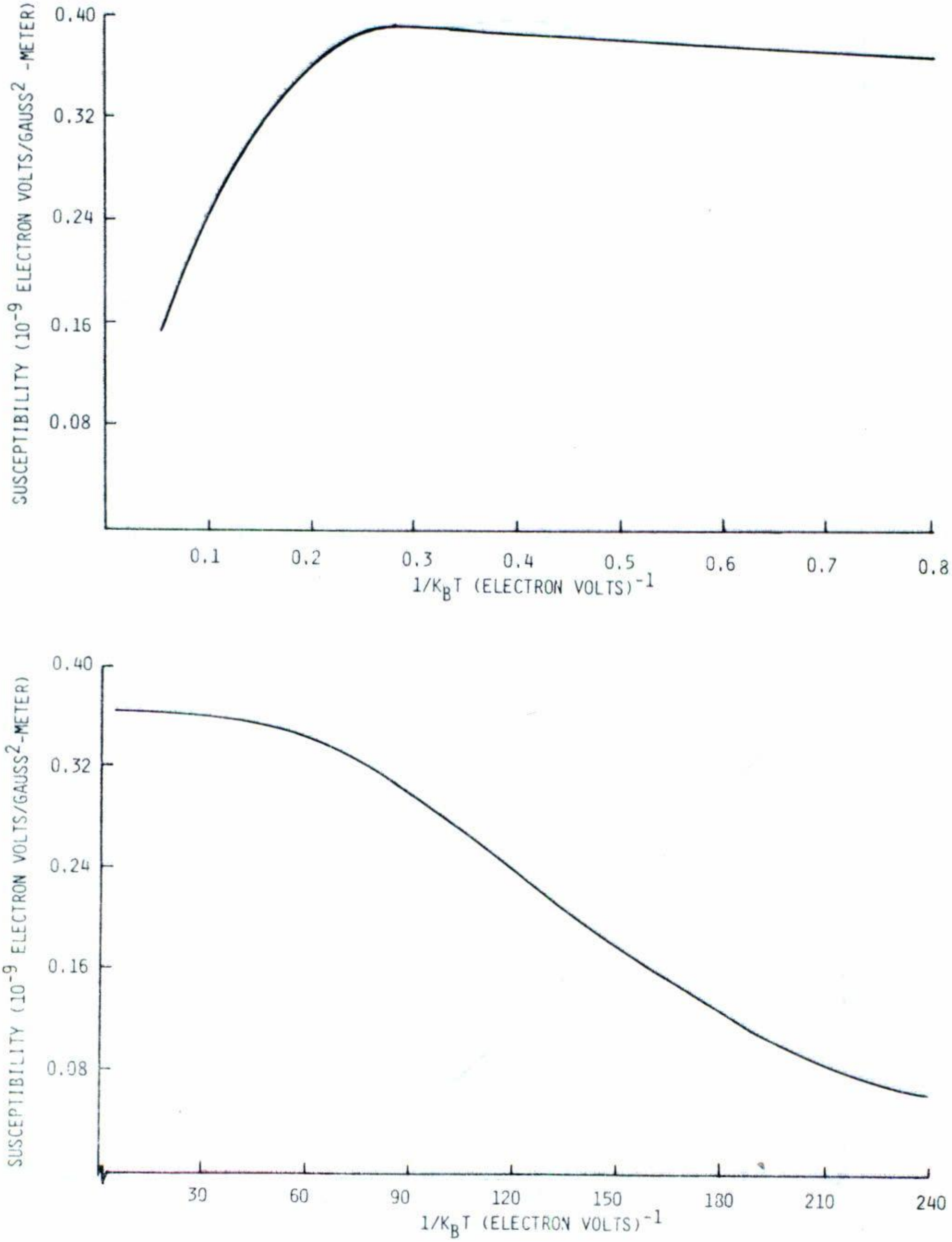

Fig. 2A, 2B. Temperature dependence of the paramagnetic susceptilibity for $U = 9.4 \times 10^{-3}$ electron volts.

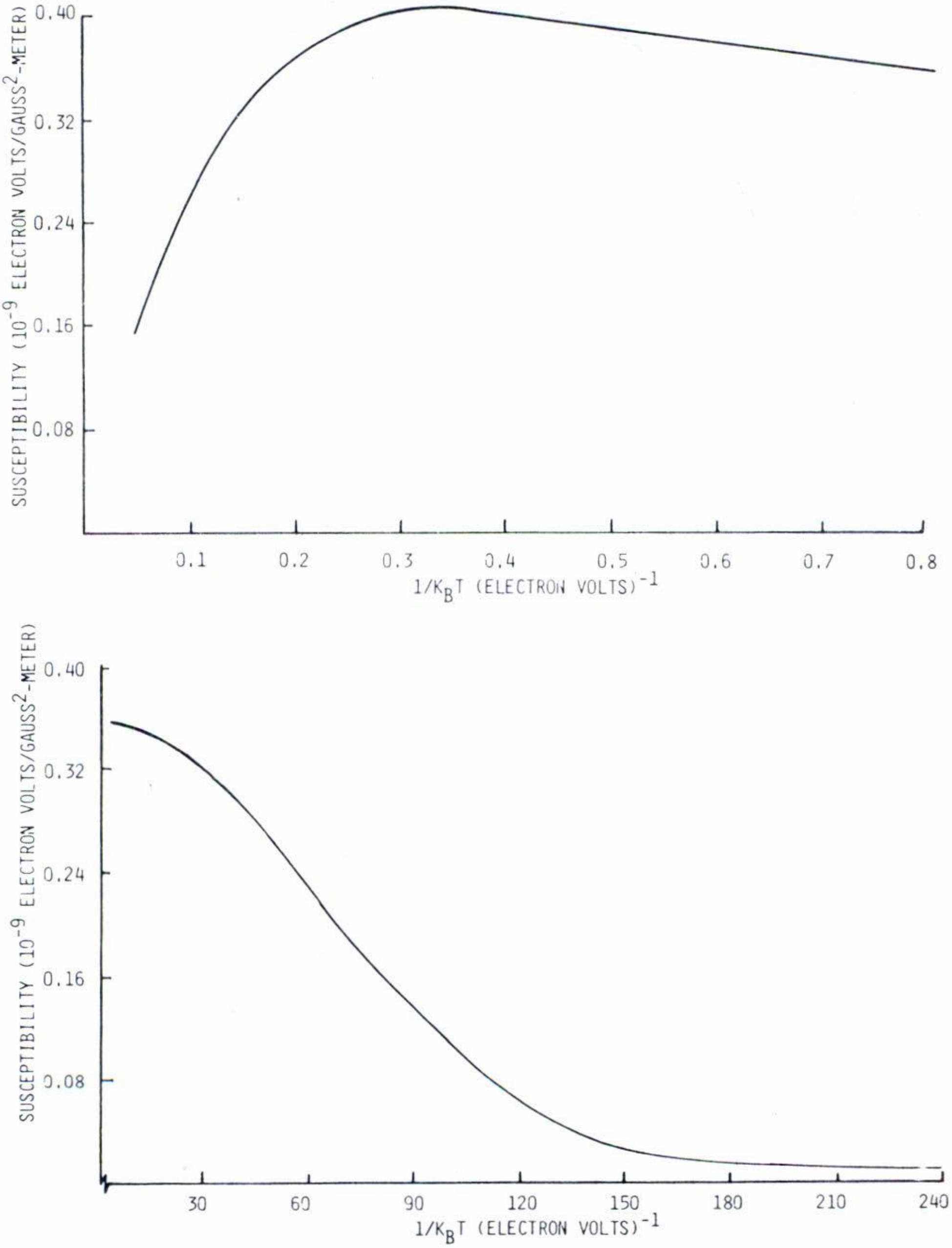

Fig. 3A, 3B. Temperature dependence of the paramagnetic susceptibility for $U = 9.4 \times 10^{-2}$ electron volts.