Pauli Spin Paramagnetism and Electronic Specific Heat in generalised $d$-dimensions

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Abstract: The temperature variations of pauli spin paramagnetic susceptibility and the electronic specific heat of solids, are calculated as functions of temperature following the free electron approximation, in generalised $d$-dimensions. The results are compared and become consistent with that obtained in three dimensions. Interestingly, the Pauli spin paramagnetic susceptibility becomes independent of temperature only in two dimensions.

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Introduction:

As a consequence of having the intrinsic spin, the electrons bear magnetic dipole moment. Pauli spin paramagnetism results entirely from the spin magnetic moments of electrons. In three dimensions, using free electron approximation, the temperature dependent susceptibility is calculated by Stoner [1] and in the low temperature regime, it is quadratic in the temperature. Following the same type of calculations, the electronic specific heat becomes linear in temperature. These results are well known and documented in the standard textbooks [2, 3, 4, 5].

However, no such derivations are observed in the standard literature, in any generalised $d$-dimensions. Although, in reality, we are mainly concerned with the systems in three dimensions, one may extend these calculations in generalised $d$-dimensions just for pure pedagogical or mathematical interest.

In this paper, the Pauli spin paramagnetic susceptibility and the electronic specific heat are calculated in free electron approximation as a function of temperature in generalised $d$-dimensions.

Calculations in $d$-dimensions:

1. Pauli spin paramagnetism:

In a generalised $d$-dimensions, if we consider a system (unit volume) of electron gas, each electron will contribute $-\mu_B$ ($\mu_B$ is Bohr magneton) to the magnetisation density if its spin is parallel to the applied magnetic field $H$, and $\mu_B$, if antiparallel. Hence, if $N_\pm$ is the number of electrons per unit volume with spin parallel(+) or antiparallel(-) to $H$, the magnetisation density will be [6]

$$M = -\mu_B(N_+ - N_-).$$

(1)

When the interactions of the electrons with the magnetic field will be considered, then the only effect of the field is to shift the energy of each electronic level by $\pm\mu_B H$, according to whether the spin is parallel or antiparallel to $H$. This may be expressed in terms of the density of electronic states for a given spin. If $g_\pm(E)dE$ is the number of electrons in the specified spin per
unit volume in the energy range $E$ and $E + dE$, one may write

$$g_{\pm}(E) = g(E)/2,$$  
(for $H = 0$) \hfill (2)

where $g(E)$ is the ordinary density of states. In the application of external magnetic field $H$, the density of parallel and antiparallel spin states are

$$g_{+}(E) = \frac{1}{2} g(E - \mu_B H)$$
$$g_{-}(E) = \frac{1}{2} g(E + \mu_B H).$$ \hfill (3)

So, for each spin species, the number of electrons will be,

$$N_{\pm} = \int g_{\pm}(E) F(E) dE,$$ \hfill (4)

where $F(E)$ is the Fermi-Dirac distribution function\(^4\)

$$F(E) = \frac{1}{e^{\beta(E-\mu)} + 1},$$ \hfill (5)

where, $\mu$ is in general temperature dependent chemical potential.

For small field $H$, one may write

$$g_{\pm}(E) = \frac{1}{2} g(E \pm \mu_B H) \simeq \frac{1}{2} g(E) \pm \frac{1}{2} \mu_B H g'(E)$$ \hfill (6)

and consequently,

$$N_{\pm} = \frac{1}{2} \int_0^{\infty} g(E) F(E) dE \mp \frac{1}{2} \mu_B H \int g'(E) F(E) dE. \hfill (7)$$

Hence, the magnetisation density becomes,

$$M = \mu_B^2 H \int_0^{\infty} g'(E) F(E) dE.$$ \hfill (8)

Now, the primary task is to evaluate the following integral \([4]\)

$$I = \int_0^{\infty} g'(E) F(E) dE$$ \hfill (9)

where, the derivative $g'(E)$ has to be calculated for the electronic density of states $g(E)$ in a generalised $d$-dimensions. This type of integral was evaluated
in general in [4] (page-393). So,

\[ I = \int_0^\infty g'(E)F(E)dE \]
\[ = \sum_{m=0}^{\infty} I_m \frac{(kT)^m}{m!} \left[ \frac{d^m g(E)}{dE^m} \right] \mu \]
\[ = \int_0^\mu g'(E)dE + \frac{\pi^2 k^2 T^2}{6} g''(\mu) + \sum_{m=4}^{\infty} I_m \frac{(kT)^m}{m!} \left[ \frac{d^m g(E)}{dE^m} \right] \mu \]  \hspace{1cm} (10)

where, \( m = 0, 2, 4, 6 \ldots \) etc and \( I_m = \int_0^\infty \frac{x^m e^x}{(e^x+1)^2} dx \). \( g''(\mu) \) is second derivative of \( g(E) \) evaluated at \( E = \mu \). It may be noted here that only the even-derivatives (i.e., \( \frac{d^2 g(E)}{dE^2}, \frac{d^4 g(E)}{dE^4}, \frac{d^6 g(E)}{dE^6} \) etc.) of \( g(E) \) are present in \( I \). Here, \( \mu \) is in general temperature dependent chemical potential. The quantity \( I \) may be written as,

\[ I = \int_0^{\mu_0} g'(E)dE + \int_{\mu_0}^\mu g'(E)dE + \frac{\pi^2 k^2 T^2}{6} g''(\mu) + \sum_{m=4}^{\infty} I_m \frac{(kT)^m}{m!} \left[ \frac{d^m g(E)}{dE^m} \right] \mu \]
\[ \simeq g(\mu_0) + g'(\mu_0)(\mu - \mu_0) + \frac{\pi^2 k^2 T^2}{6} g''(\mu), + \sum_{m=4}^{\infty} I_m \frac{(kT)^m}{m!} \left[ \frac{d^m g(E)}{dE^m} \right] \mu \]  \hspace{1cm} (11)

where the second integral term is approximately equal to \( g'(\mu_0)(\mu - \mu_0) \). Here, \( \mu_0 \) denotes the Fermi energy \((T = 0)\) of the electron gas. Now, the task is to evaluate \((\mu - \mu_0)\). It is well known [4] that

\[ \mu - \mu_0 = - \frac{\pi^2 k^2 T^2 g'(\mu_0)}{6g(\mu_0)} \]  \hspace{1cm} (12)

if calculated using quadratic (upto \( T^2 \) term) approximation.

After simplification (from above two equations), one may write

\[ I = g(\mu_0)[1 - \frac{\pi^2 k^2 T^2 g'(\mu_0)^2}{6 \ g(\mu_0)^2} + \frac{\pi^2 k^2 T^2 g''(\mu_0)}{6 \ g(\mu_0)}] + \sum_{m=4}^{\infty} I_m \frac{(kT)^m}{m!} \left[ \frac{d^m g(E)}{dE^m} \right] \mu \]  \hspace{1cm} (13)

Now, to calculate \( I \), one has to calculate, \( g(\mu_0), g'(\mu_0) \) and \( g''(\mu_0) \) in generalised-\( d \)-dimensions. The density of electronic states \( g(E) \), in \( d \)-dimensions, has been calculated very recently [8]. In \( d \)-dimensions, \( g(E) = C E^{d/2} \), where \( C \) is a mass dependent constant. Thus, \( g(\mu_0) = C \mu_0^{\frac{d-2}{2}}, g'(\mu_0) = C(\mu_0^{\frac{d-4}{2}}), \) and \( g''(\mu_0) = C(\frac{d-2}{2})(\frac{d-4}{2}) \mu_0^{\frac{d-6}{2}} \). Considering, \( N = \int_{\mu_0}^\mu g(E)dE \), the total
number of electrons, in $d$-dimensions, $g(\mu_0) = dN/(2\mu_0)$. Using these, $I$ becomes

$$I = \frac{dN}{2\mu_0}[1-(\frac{\pi^2kT^2}{24\mu_0^2})((d-2)^2-(d-2)(d-4))] + \sum_{m=4}^{\infty} I_m \frac{(kT)^m}{m!} \left[ \frac{d^m g(E)}{dE^m} \right]_\mu$$

It should be noted here that, in the summation of the expression of $I$ in above equation due to the presence of all even-derivatives of $g(E)$, all terms include a factor $(d-2)$ (since $g(E) = CE^{\frac{d-2}{2}}$). The magnetisation density $M = \mu_r^2 H I$. Hence, the pauli paramagnetic susceptibility $\chi = M/H = \mu_r^2 I$ is calculated here in generalised $d$-dimensions. This general (in $d$- dimensions) calculation is not yet done and it is not found in the literature of quantum statistical physics [2, 3, 4, 5].

The Pauli spin paramagnetic susceptibility is independent of the temperature for two-dimensional electronic systems when the higher order terms are included. However, this is based on the factor that the chemical potential is calculated using quadratic approximation in eqn (12). Actually, the temperature-independent feature of Pauli spin paramagnetic susceptibility for $d = 2$ is very general. See eqn (8), for $d = 2$, the derivative of density of state equals zero. Hence, the temperature dependent part of the magnetization and then the Pauli spin paramagnetic susceptibility vanish completely.

Reader may easily check that in three dimensions (putting $d = 3$ in the general expression of $I$), $\chi$ becomes (in quadratic approximation),

$$\frac{3N\mu_r^2}{2\mu_0}[1 - \frac{\pi^2kT^2}{12\mu_0^2}]$$

which was obtained by Stoner [1, 7].

Here, it may be noted that, in two dimensions only, (putting $d = 2$ in the general expression), the susceptibility becomes independent of temperature. This was not predicted by Stoner [1]. This is an interesting result and not yet available in standard literature. This is a very general result also. Even if one calculate the susceptibility using all terms in the summation (in equation 14), due to the presence of a common factor of $(d-2)$ (in all $T$ dependent terms), the Pauli spin susceptibility will become temperature independent in two dimensions.

2. Electronic Specific heat:
Here, the total energy $\bar{E}$ is calculated as [4]

$$\bar{E} = E_0 + \frac{\pi^2 k^2 T^2}{3} g(\mu_0),$$

(16)

$E_0$ is the electronic energy at $T = 0$. In $d$-dimensions $g(\mu_0) = dN/(2\mu_0)$. Using this form of $g(\mu_0)$ the electronic specific heat in $d$-dimensions, becomes

$$C_v = \frac{\pi^2 k^2 N d}{6\mu_0} T.$$  

(17)

The above result will yield well known result [4, 7] of electronic specific heat ($C_v = (\pi^2 k^2 N T)/(2\mu_0)$) in three dimensions, if one puts $d = 3$ in the general expression of $C_v$ written above.

**Concluding remarks:**

In this paper, the pauli spin paramagnetic susceptibility and electronic specific heat are calculated in generalised $d$-dimensions. The results are compared with that obtained in three dimensions. The susceptibility and the specific heat are calculated as functions of dimensionality $d$. The well known results in three dimensions are restored just by putting $d = 3$ in the respective general expressions. *Interestingly*, the Pauli spin paramagnetic susceptibility becomes independent of temperature *only* in two dimensions, which was not predicted by Stoner[1]. These general calculations are not available in the standard literatures of quantum statistical mechanics. Although, $d$-dimensions is not a realistic concept, this study is pedagogically interesting and this result has a significance in modern technology. If any electronic device requires the temperature independent spin-magnetism, one may think it to prepare in two dimensions.

It may be noted here that the Pauli spin susceptibility becomes independent of temperature in two dimensions but the electronic specific heat does not. A possible explanation may be stated as follows: the spin dependent magnetism and hence the susceptibility has a nontrivial dependence on the topological arrangement of the electrons. As a result the planar arrangement (in two dimensions) of electrons does not produce any temperature dependent susceptibility. However, the temperature dependence of the electronic kinetic energy has a trivial dependence on the dimensionality. Hence, the temperature dependence of electronic specific heat is always linear in any dimensions.
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