Paramagnetic and Diamagnetic Susceptibility of Infinite Quantum Well

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Abstract. A material is said to be paramagnetic or diamagnetic depends on the sign of its magnetic susceptibility. When a material is exposed to an external magnetic field, magnetic susceptibility is defined as the ratio of the induced magnetization and the magnetic field. Theoretical study of paramagnetic susceptibility and diamagnetic susceptibility are well described by Pauli paramagnetism and Landau diamagnetism, respectively. Although paramagnetism and diamagnetism are among the simplest magnetic properties of material that are studied in basic physics, theoretical derivations of Pauli paramagnetic and Landau diamagnetic susceptibility require second quantization formalism of quantum mechanics. We aim to discuss the paramagnetic and diamagnetic susceptibilities for simplest case of quantum system using the simplest first quantization formalism of perturbation theory.

Keywords: Magnetic susceptibility, Pauli paramagnetism, Landau diamagnetism, quantum well, first quantization..

INTRODUCTION

Paramagnetism and diamagnetism are among the simplest magnetic properties of material that are studied in basic physics [1]. A material can be paramagnetic or diamagnetic depends on the sign of its magnetic susceptibility [2]. A paramagnetic material has magnetic susceptibility with positive sign. On the other hand, a diamagnetic material has magnetic susceptibility with negative sign. Magnetic susceptibility is defined as the ratio of its magnetization and the external magnetic field that induce its magnetization [3].

Theoretical study of paramagnetic susceptibility and diamagnetic susceptibility are well described by Pauli paramagnetism and Landau diamagnetism, respectively [4]. Theoretical derivations of these magnetic susceptibility use second quantization formalism of quantum mechanics[5]–[7]. The susceptibilities for a metal with Fermi energy E_F are determined by its density of state at Fermi energy $DOS(E_F)$ as follow.

$$\chi_{para} = \mu_B^2 DOS(E_F), \tag{1}$$

$$\chi_{dia} = -\frac{\mu_B^2}{3} DOS(E_F). \tag{2}$$

Where the total susceptibility indicates that a metal has a paramagnetic state.

$$\chi = \chi_{para} + \chi_{dia} = \frac{2}{3}\mu_B^2 DOS(E_F) > 0 \tag{3}$$

Theoretical research on paramagnetic susceptibility of conduction electrons lead to many useful effects for functional devices, such as interlayer coupling mediated by conduction spin (also known as Rudderman Kittel Kasuya Yosida (RKKY) interaction) [8]–[12], in magnetic nanostructures. Diamagnetic susceptibility of conduction electrons are theoretically studied as Landau - Peierls susceptibility [7], [13]–[16].

The simplest example of quantum system is infinite quantum well [17]. In the infinite quantum well, the movement of electrons are confined, and its energy is quantized. The main difference between wave function of electron in infinite quantum well and free electron model of conduction electron is that the former use vanishing wave function at the infinite potential wall while the later used a periodical boundary condition [17], [18]. Artificial confinement of electrons in nanostructure is an ongoing research [19], [20]. This article aims to theoretically determine the paramagnetic and diamagnetic susceptibilities for simple three-dimensional quantum well.

METHOD

To study the paramagnetic and diamagnetic susceptibility of the system, we need to introduce magnetic field magnetic field $\vec{B}$ and vector potential $\vec{A}$ into the Schrödinger equation. To be able to appropriately include magnetic field, we consider Pauli-Schrödinger equation that includes $\vec{A}$ and $\vec{B}$ [21], [22]. Pauli-Schrödinger equation is non-relativistic limit of Dirac equation [22], [23].

$$\hat{H}|\psi\rangle = \left(\frac{1}{2m_e}\left(\vec{p} + e\vec{A}(\vec{r})\right) \cdot \left(\vec{p} + e\vec{A}(\vec{r})\right) + \frac{e\hbar}{2m_e}\vec{\sigma} \cdot \vec{B}(\vec{r}) + V(\vec{r})\right)|\psi\rangle = E|\psi\rangle \tag{4}$$

Where $\vec{B} = \nabla \times \vec{A}$ and $|\psi\rangle$ is two component spinor wave function and $\vec{\sigma} = (\sigma_x,\ \sigma_y,\ \sigma_z)$ is Pauli matrices.

$$\vec{\sigma} = (\sigma_x,\ \sigma_y,\ \sigma_z) = \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right) \tag{5}$$

Infinite three-dimensional quantum well can be modeled by the following potential

$$V(x,y,z) = \begin{cases} 0, & 0 < x < L, 0 < y < L, 0 < z < L \\ \infty, & \text{elsewhere} \end{cases} \tag{6}$$

The solution of the time-independent Schrödinger equation and the boundary condition $|\psi\rangle(V = \infty) = 0$ dictates that the eigen wave function of the electron for zero magnetic field is [17]

$$\psi_{n_x,n_y,n_z}(\vec{r}) = \left(\frac{2}{L}\right)^{\frac{3}{2}} \sin\frac{n_x\pi x}{L}\sin\frac{n_y\pi x}{L}\sin\frac{n_z\pi x}{L} \tag{7}$$

Since $n_j = 1,2,3,\cdots, j = x,y,z$, the energy is quantized

$$E_{\vec{n}} = \frac{\hbar^2\pi^2}{2m_e L^2}\left(n_x^2 + n_y^2 + n_z^2\right) \tag{8}$$

In low temperature, the maximum energy is the Fermi energy E_F. To be able to analytically study the susceptibilities, we assume that L is very large. In that case, we can write n_x, n_y, n_z in term of a vector $\vec{k} = \frac{\pi}{L}(n_x, \quad n_y, \quad n_z)$ and the energy is similar to free electron.

$$E_{\vec{k}} = \frac{\hbar^2 k^2}{2m_e} \tag{9}$$

We can now define $E_F = \hbar^2 k_F^2/2m_e$ and any sum over n_x, n_y, n_z, can be approximated by integral over $\vec{k}$

$$\sum_{n_x,n_y,n_z} \cdots = \sum_{\vec{k}} \cdots \iiint \frac{d^3\vec{k}}{(\pi/L)^3} \cdots \tag{10}$$

Under small magnetic field, we can use perturbation theory to get the first order correction for $\vec{A}$ and $\vec{B}$ to

$$\widehat{H}_A = \frac{e}{2m_e}\left(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}\right) \tag{11}$$

$$\widehat{H}_B = \frac{e\hbar}{2m_e}\vec{\sigma}\cdot\vec{B} \tag{12}$$

respectively.

Here on, we use the following mathematical description of magnetic susceptibility that arise from Landau theory of free energy [24].

$$\chi = \left(\frac{\partial m}{\partial B}\right)_{B=0} \tag{13}$$

The paramagnetic magnetization is

$$M_{para} = -\frac{e\hbar}{2m_e L^3}\sum_{\vec{k}}\langle\vec{k}|\vec{\sigma}|\vec{k}\rangle_B \tag{14}$$

and the diamagnetic magnetization $\vec{M}_{dia}$ is defined by the following relation to diamagnetic current $\vec{J}_{dia}$

$$\nabla\times\vec{M}_{dia} = \vec{J}_{dia} = \frac{-e}{m_e L^3}\sum_{\vec{k}}\sum_{\vec{l}}\langle\vec{l}|(\vec{p} + eA)|\vec{k}\rangle_A \tag{15}$$

Since $\langle\vec{k}|\vec{\sigma}|\vec{k}\rangle$ is zero when number of spin up and down electrons are the same, we can see that the system is paramagnetic when there are unpaired electrons (see Figure 1).
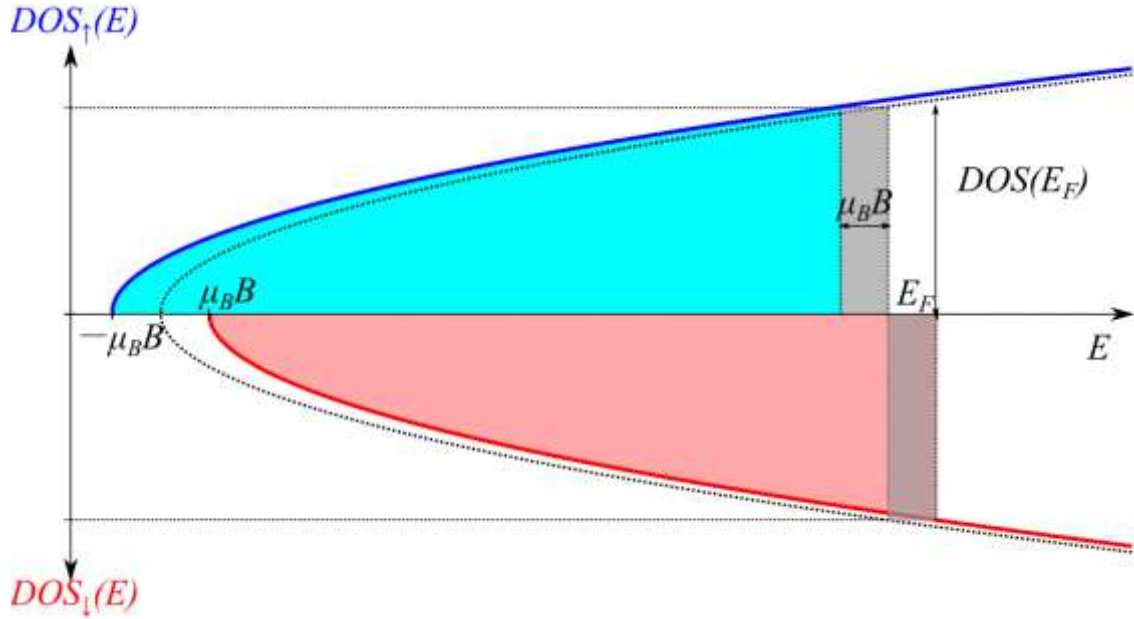
Figure 1. Spin-dependent Density of State (DOS). Perturbation by a static magnetic field B induces unpaired spin near the Fermi energi by shifting the Density of State of electrons with spin up (blue) and spin down (red). Here $\mu_B = -e\hbar/2m_e$ is Bohr magneton.

Here, subscripts A and B indicate that we take into account first order correction of the eigenstate due to $\hat{H}_A$ and $\hat{H}_B$.

$$|\vec{k}\rangle_{A,B} = \sum_{\vec{l}} \frac{\langle \vec{l}|\hat{H}_{A,B}|\vec{k}\rangle}{E_{\vec{k}} - E_{\vec{l}}}|\vec{l}\rangle \tag{16}$$

Paramagnetic susceptibility

To study the paramagnetic susceptibility, we will focus on $\hat{H}_B$ as the perturbation. The first order correction to magnetization due to electron spin as follows.

$$M_{para} = -\frac{e\hbar}{2m_e L^3} \sum_{\vec{k}} \langle \vec{k}|\vec{\sigma}|\vec{k}\rangle_B = -\frac{e\hbar}{2m_e L^3} \sum_{\vec{k}} \sum_{\vec{l}} \frac{\langle \vec{l}|\vec{\sigma}\cdot\vec{B}(\vec{r})|\vec{k}\rangle}{E_{\vec{k}} - E_l}\langle \vec{k}|\vec{\sigma}|\vec{l}\rangle \tag{17}$$

We note that this is the same as taking the following second order correction of the magnetic energy.

$$-M_{para}B^2 = \frac{1}{L^3}\sum_{\vec{k}}\sum_{\vec{l}} \frac{|\langle \vec{l}|\hat{H}_B|\vec{k}\rangle|^2}{E_{\vec{k}} - E_{\vec{l}}} = \left(\frac{e\hbar}{2m_e}\right)^2 \frac{1}{L^3}\sum_{\vec{k}}\sum_{\vec{l}} \frac{|\langle \vec{l}|\vec{\sigma}\cdot\vec{B}(\vec{r})|\vec{k}\rangle|^2}{E_{\vec{k}} - E_{\vec{l}}} \tag{18}$$

Although we focus on static magnetic field, we set $\vec{B}(x) = \hat{z}B\cos qx$ and take the limit $q \to 0$. Using the Pauli matrices identity $\sigma_a\sigma_b = 1\delta_{ab} + i\epsilon_{abc}\sigma_c$, we can simplify it as follows.

$$\chi_{para} = -\left(\frac{e\hbar}{2m_e}\right)^2 \frac{1}{L^3} \lim_{q\to 0} \sum_{\vec{k}}\sum_{\vec{l}} \frac{|\langle \vec{l}|\cos qx|\vec{k}\rangle|^2}{E_{\vec{k}} - E_{\vec{l}}} \tag{19}$$

$\langle \vec{l}|\cos qx|\vec{k}\rangle$ can be determined by examining the following integral

$$\langle \vec{l}|\cos qx|\vec{k}\rangle = (1 \quad 1)\binom{1}{1}\frac{2}{L}\int_0^L dx \sin l_x x \cos qx \sin k_x x = \delta_{l_x+q,k_x} + \delta_{l_x-q,k_x} \tag{20}$$

Therefore, integral expression for χ_{para} is as follows

$$\chi_{para} = -\left(\frac{e\hbar}{2m_e}\right)^2 \lim_{q\to 0} \iiint \frac{d^3\vec{k}}{\pi^3}\left(\frac{1}{E_{\vec{k}} - E_{\vec{k}-q\hat{x}}} + \frac{1}{E_{\vec{k}} - E_{\vec{k}+q\hat{x}}}\right) \tag{21}$$

Landau diamagnetism

To study the diamagnetic susceptibility, we first examine the magnetization that correspond with diamagnetic current

$$\vec{J}_{dia} = \nabla \times \vec{M}_{dia} = \frac{-e}{m_e L^3} \sum_{\vec{k}} \sum_{\vec{l}} \langle \vec{l} | (\vec{p} + eA) | \vec{k} \rangle_A. \tag{22}$$

To evaluate χ_{dia}, we substitute $\vec{M}_{dia} = \chi_{dia} \nabla \times \vec{A}$

$$-\chi_{dia} \nabla^2 \vec{A} = \frac{-e}{m_e L^3} \sum_{\vec{k}} \sum_{\vec{l}} \langle \vec{l} | \vec{p} | \vec{k} \rangle_A - \frac{e^2 \vec{A}}{m_e} N_e \tag{23}$$

Here $N_e = \frac{1}{L^3} \sum_{\vec{k}} \langle \vec{k} | \vec{k} \rangle$ is the total density of electrons. Similarly, we can assume $\vec{A} = \hat{y} A \cos qx$, therefore

$$\chi_{dia} \vec{A} = \lim_{q \to 0} \frac{1}{q^2} \frac{-e}{m_e L^3} \left(\sum_{\vec{k}} \sum_{\vec{l}} \langle \vec{l} | \vec{p} | \vec{k} \rangle_A + e \vec{A} N_e \right) \tag{24}$$

Using first order correction of the eigenstate.

$$| \vec{k} \rangle_A = \sum_{\vec{l}} \frac{\langle \vec{j} | \hat{H}_A | \vec{k} \rangle}{E_{\vec{k}} - E_{\vec{j}}} | \vec{j} \rangle \tag{25}$$

We can evaluate χ_{dia} as follows

$$\chi_{dia} = -\frac{e^2}{m_e L^3} \lim_{q \to 0} \frac{1}{q^2} \left(\sum_{\vec{k}} \sum_{\vec{l}} \frac{\langle \vec{l} | p^2 \cos qx | \vec{k} \rangle}{E_{\vec{k}} - E_{\vec{l}}} + e N_e \right) \tag{26}$$

$\langle \vec{l} | p^2 \cos qx | \vec{k} \rangle$ can be determined by examining the following integral

$$\langle \vec{l} | p^2 \cos qx | \vec{k} \rangle = 2 \left(\frac{2}{L} \right)^2 k_x \int_0^L dx \sin l_x x \cos qx \sin k_x x = k_x^2 \left(\delta_{l_x+q,k_x} + \delta_{l_x-q,k_x} \right) \tag{27}$$

Therefore, integral expression for χ_{dia} is as follows

$$\chi_{dia} = -\frac{e^2}{m_e} \lim_{q \to 0} \frac{1}{q^2} \left(e N_e + \iiint \frac{d^3 \vec{k} \, k_x^2}{\pi^3} \left(\frac{1}{E_{\vec{k}} - E_{\vec{k}-q\hat{x}}} + \frac{1}{E_{\vec{k}} - E_{\vec{k}+q\hat{x}}} \right) \right) \tag{28}$$

RESULT AND DISCUSSION

Carrying the integral over all $\vec{k}$ states that has the maximum energy is the Fermi energy E_F, we arrive at the following expression for paramagnetic and diamagnetic susceptibility

$$\chi_{para}(q) = \mu_B^2 DOS(E_F) \left(\frac{1}{2} + \frac{1 - \left(\frac{q}{2k_F} \right)^2}{\frac{2q}{k_F}} \ln \left| \frac{q + 2k_F}{q - 2k_F} \right| \right) \tag{29}$$

$$\chi_{dia}(q) = -\mu_B^2 \frac{DOS(E_F)}{8 \left(\frac{q}{2k_F} \right)^2} \left(1 + \left(\frac{q}{2k_F} \right)^2 - \frac{\left(1 - \left(\frac{q}{2k_F} \right)^2 \right)^2}{\frac{q}{k_F}} \ln \left| \frac{q + 2k_F}{q - 2k_F} \right| \right) \tag{30}$$

Our result is similar to those of Pauli paramagnetic and Landau-Peierls susceptibility. The limit for small $q \to 0$ is the same as Eq 1 and 2. Therefore, we can that the magnetic properties of electron in an infinite quantum well behave like those of conduction electron in a metal.

In a static magnetic field limit, the total susceptibility seems to indicate a paramagnetic state (see Figure 2).

$$\chi = \lim_{q \to 0} \left(\chi_{para}(q) + \chi_{dia}(q) \right) = \frac{2}{3} \mu_B^2 DOS(E_F) \tag{31}$$

However, in a more general system, collective movement of electrons that responsible for paramagnetism can have different effective mass than diamagnetism. Since $DOS(E_F)$ is proportional to the effective mass, if consider the different effective mass, the total magnetic susceptibility is as follows

$$\chi = \left(1 - \frac{1}{3} \frac{m_{dia}}{m_{para}} \right) \mu_B^2 DOS(E_F) \tag{32}$$

When $m_{dia} > 3m_{para}$ the system is diamagnetic.
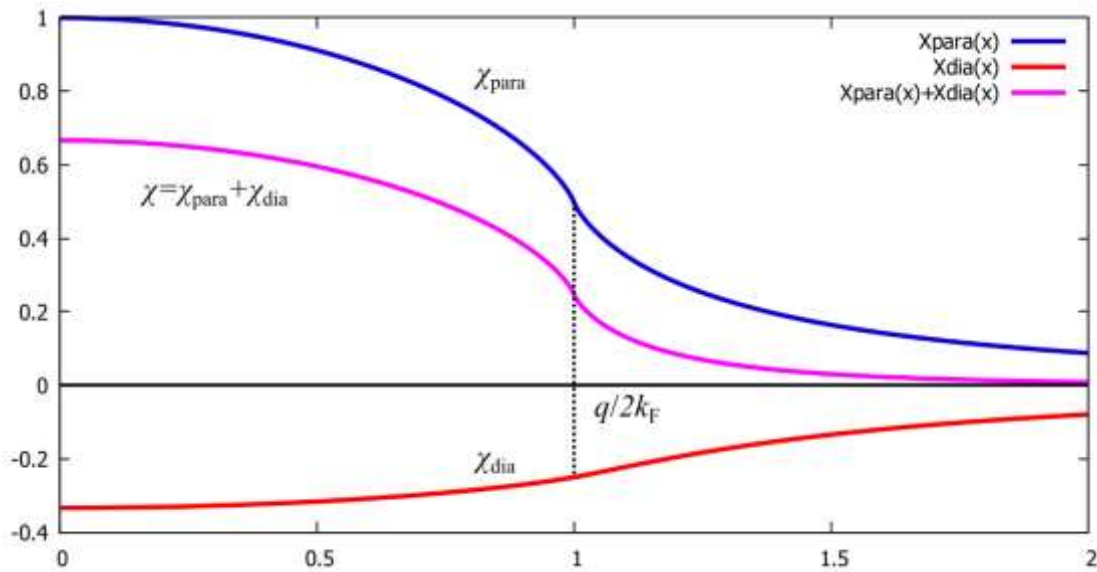
Figure 2. Paramagnetic susceptibility $\chi_{para}(q)$ and diamagnetic susceptibility $\chi_{dia}(q)$, $\chi_{para}(0)$ normalized to as a function of $q/2k_F$.

CONCLUSION

To summarize, we theoretically study the paramagnetic and diamagnetic susceptibility of a system with many electrons in infinite quantum well. While paramagnetism and diamagnetism are among the simplest magnetic properties of material that are studied in basic physics, theoretical derivations of magnetic susceptibilities require second quantization formalism of quantum mechanics, we can obtain the susceptibility using first quantization formalism.

The similar expression of our result with those of Pauli paramagnetic susceptibility and Landau-Peierls indicate that the magnetic properties of confined electron in an infinite quantum well behave like those of conduction electron in a metal. This is physically important because it show that electronic wave function in confined system with vanishing boundary condition behave similar to those with a periodic boundary condition.

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