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GENERALIZED CANONICAL DENSITY MATRIX

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Abstract: In the present paper we give approximative expressions of the generalized density matrix of Bloch, which can be calculated exactly for the case of free electrons in a uniform magnetic field, while for the case of lattice electrons it can be expressed by the help of the Wannier functions. For the case of high temperatures the generalized density matrix coincides to the Green-function.

1. Introduction

As it is known[1] the generalized canonical density matrix of Bloch $D(\vec{r}', \vec{r}, b, J)$ contains another factor of occupation, the so-called Fermi-Dirac occupation factor.

The generalized density matrix can be defined by the same way as the ordinary density matrix[2] by the help of the eigenfunctions and eigenvalues of the Hamiltonian operator, according to the relation

$$D(\vec{r}', \vec{r}, b, J\} = \sum_i \psi_i^*(\vec{r}_i')\,\psi(\vec{r})\,\{1 + e^{b(E_i - J)}\}^{-1}, \tag{1.1}$$

where $b = \frac{1}{kT}$ (k the Boltzmann constant and T the absolute temperature), J the Fermi energy and also hold the following Schrödinger equation

$$H\psi_i(\vec{r}) = E_i\psi_i(\vec{r}). \tag{1.2}$$

The diagonal elements $D(\vec{r}', \vec{r}, b, J)$ give the total density $\eta(\vec{r})$ which corresponds to a potential energy $V(\vec{r})$ for an electronic cloud of any degree of degeneracy.

The above so defined generalized density matrix is used today for the solution of many problems in solid state physics and especially for the calculation of the dielectric function of a degenerate electronic cloud and the optical transitions in a high-doped semiconductor[3].

It has been proved that the generalized density matrix $D(\vec{r}', \vec{r}, b, J)$ fulfills a differential equation analogous to the one of Bloch, which for the present case will be of the form

$$(H - J)\frac{\partial D}{\partial J} + b\frac{\partial D}{\partial b} = 0, \tag{1.3}$$

with the initial condition

$$\lim_{b\to 0}\lim_{J\to -\infty} e^{-bJ} D(\vec{r}', \vec{r}, b, J) = \delta(\vec{r}' - \vec{r}), \tag{1.4}$$

or the corresponding one

$$\lim_{b\to 0} D(\vec{r}', \vec{r}, b, J) = \frac{1}{2}\delta(\vec{r}' - \vec{r}), \tag{1.5}$$

which results at once from (1.1).

Equ. (1.3) for the case of free-electrons $V(\vec{r}) = 0$, can be easily solved and its solution is referred in[1] and is of the form

$$D(\vec{r}', \vec{r}, b, J) = 2\left(\frac{m}{2\pi h^2 b}\right)^{3/2} \sum_{n=0}^{\infty} \frac{1}{n!}\left\{-\frac{m}{2bh^2}(\vec{r}' - \vec{r})^2\right\}^n F_{n+\frac{1}{2}}(bJ), \tag{1.6}$$

where the function $F_{n+\frac{1}{2}}(x)$ represents the Fermi integral (Ref.[4])*)

$$F_n(x) = \frac{1}{\Gamma(n+1)}\int_0^\infty \frac{y^n\, dy}{1 + e^{x-y}}. \tag{1.7}$$

In what follows we shall try to find approximative expressions for the generalized density matrix $D(\vec{r}', \vec{r}, b, J)$ and to calculate it exactly for the case of a free-electron in a uniform magnetic field. For the case of lattice electrons we shall express it by the help of the Wannier functions[5].

*) The Fermi-integral is here defined without the F-function.

2. *Approximative expression of* $D(\vec{r}', \vec{r}, b, J)$

Between the generalized density matrix $D(\vec{r}', \vec{r}, b, J)$ and the ordinary Bloch one $\psi(\vec{r}', \vec{r}, b)$ exist the following integral transformations[2)]

$$D(\vec{r}', \vec{r}, b, J) = \int_0^\infty \gamma(\vec{r}', \vec{r}, E) \frac{\partial}{\partial E}\left(\frac{1}{1 + e^{b(E-J)}}\right) dE, \tag{2.1}$$

$$\gamma(\vec{r}', \vec{r}, E) = \frac{1}{2\pi i} \int_{\sigma+i\infty}^{\sigma+i\infty} e^{bE} \frac{1}{b} \psi(\vec{r}', \vec{r}, b)\, db. \tag{2.2}$$

In the case in which for the ordinary Bloch density matrix $\psi(\vec{r}', \vec{r}, b)$ has been used the method of iterations e. g. up to the second class, then by the help of the expressions (2.1) and (2.2) we can calculate the generalized density matrix $D(\vec{r}', \vec{r}\, b, J,)$ in an analogous way c. g.; if $\psi_0(\vec{r}', \vec{r}, b)$ is the Bloch density matrix of a non-perturbed problem and $H_1(\vec{r})$ the perturbing potential, then as it is known[2)], the ordinary matrix of Bloch, up to the second order approximation is given by the relation

$$\psi(\vec{r}', \vec{r}, b) = \psi_0(\vec{r}', \vec{r}, b) + \psi_1(\vec{r}', \vec{r}, b) + \psi_2(\vec{r}', \vec{r}, b) + \ldots =$$

$$= \psi_0(\vec{r}', \vec{r}, b) + \iint_0^b d\vec{r}_1\, db_1\, \psi_0(\vec{r}', \vec{r}_1, b - b_1)\, H_1(\vec{r}_1)\, \psi_0(\vec{r}_1, \vec{r}, b_1) +$$

$$+ \iiint_0^b \int_0^{b_1} d\vec{r}_1\, d\vec{r}_2\, db_1\, db_2\, \psi_0(\vec{r}', \vec{r}_1, b - b_1)\, H_1(\vec{r}_1)\, \psi_0(\vec{r}_1, \vec{r}_2, b_1 - b_2) \cdot$$

$$\cdot H_1(\vec{r}_2)\, \psi_0(\vec{r}_2, \vec{r}, b_2). \tag{2.3}$$

Introducing (2.3) in (2.2) and then into (2.1) we get finally the aproximative calculation of the generalized density matrix

$$D(\vec{r}', \vec{r}, b, J) = D_0(\vec{r}', \vec{r}, b, J) + D_1(\vec{r}', \vec{r}, b, J) + D_2(\vec{r}', \vec{r}, b, J). \tag{2.4}$$

An expression similar to (2.4) has been used by Eisenberg and Unger[3)] up to the first class, departing from the case of free-electrons.

Another approximative expression for the generalized density matrix $D(r', r, b, J)$ results directly from the definition (1.1) for the case $b(E - J) \gg 1$. If the eigenvalues of the energy are positive, then for $J < 0$ we will have

$$D(\vec{r}', \vec{r}, b, J) = \sum_{n=0}^\infty (-1)^n e^{(n+1)Jb} \sum_i \psi_i^*(\vec{r}')\, \psi_i(\vec{r})\, e^{-(n+1)bE_J} =$$

$$= \sum_{n=0}^\infty (-1)^n e^{(n+1)Jb}\, \psi\,[\vec{r}', \vec{r}, (n+1)\, b]. \tag{2.5}$$

For the total density per unit volume, we obtain easily

$$\eta(b, J) = \int D(\vec{r}', \vec{r}, b, J)\, d\vec{r} = \sum_{n=0}^{\infty} (-1)^n e^{(n+1)Jb} Z[(n+1)b], \quad (2.6)$$

where $Z[(n+1)b]$ represents the Boltzmann partition function.

Also from the definition (1.1) after integration in respect to the diagonal elements we get the total density, namely

$$\eta(b, J) = \sum_j \frac{1}{1 + e^{b(E_j - J)}}. \quad (2.7)$$

The above formula for the case of the freeelectrons becomes

$$\eta(b, J) \sim \iiint_{-\infty}^{\infty} \frac{dk_x\, dk_y\, dk_z}{1 + e^{-bJ} \cdot e^{\frac{bh^2}{2m} k^2}} \quad (2.8)$$

and after integration in spherical coordinates we get the result

$$\eta(b, J) = 2 \left(\frac{m}{2\pi b h^2}\right)^{3/2} F_{1/2}(Jb), \quad (2.9)$$

which concides to the result of (1.6) for $\vec{r}' = \vec{r}$.

3. *Calculation of $D(\vec{r}', \vec{r}, b, J)$ for free electrons in a uniform magnetic field*

For the calculation of the function $D(\vec{r}', \vec{r}, b, J)$ for an electron which moves in a uniform magnetic field, we shall use the Schraubenfunctions[6)]. Then the function $D(\vec{r}', \vec{r}, b, J)$ is given by the relation

$$D(\vec{r}', \vec{r}, b, J) \sim \sum_n \iiint_{-\infty}^{\infty} \frac{\psi^{*}_{\vec{k},n}(\vec{r}')\, \psi_{\vec{k},n}(\vec{r})\, dk_x\, dk_y\, dk_z}{1 + e^{b\left\{\mu H(2n+1) + \frac{h^2 k_z^2}{2m} - J\right\}}}, \quad (3.1)$$

where n is the Landau quantum number, $\mu = \dfrac{eh}{2mc}$ the Bohr magneton and $\psi_{\vec{k},n}(\vec{r})$ the Schraubenfunctions, which are of the form

$$\psi_{\vec{k},n}(\vec{r}) = \left(\frac{B}{2\pi}\left(\frac{2}{B}\right)^n \frac{1}{n!}\right)^{1/2} e^{-\frac{1}{B}\{K_x^2 + K_y^2\} + i\vec{k}\cdot\vec{r}} (-K - iK_x)^n, \quad (3.2)$$

$$B = \frac{eH}{hc} \text{ and } \vec{K} = \vec{k} - \frac{e}{hc}\vec{A}(\vec{r}), \tag{3.3}$$

with the symmetric vector potential $A = \left(-\frac{1}{2}Hy, \frac{1}{2}Hx, 0\right)$.

Introducing the function (3.2) into (3.1) and after the integrations in respect to k_x, k_y we get

$$D(\vec{r}', \vec{r}, b, J) \sim \sum_{n=0}^{\infty} e^{-\frac{B}{4}\{(x-x')^2 + (y-y')^2 - 2i(x'y - y'x)\}} L_n\left\{\frac{B}{2}((x-x')^2 + (y-y)^2\right\} \cdot$$
$$\cdot I_n(z - z'), \tag{3.4}$$

where L_n are the Laguerre polynomials and the function $I_n(z - z')$ is given by the integral.

$$I_n(z - z') = 2\int_0^{\infty} \frac{\cos k_z(z - z')\, dk_z}{1 + e^{b\left\{\mu H(2n+1) + \frac{h^2 k_z^2}{2m} - J\right\}}}. \tag{3.5}$$

Consequently the generalized density per unit volume is given by the relation

$$\eta(b, J) \sim 2\sum_n \int_0^{\infty} \frac{dk_z}{1 + e^{-b\{J - \mu H(2n-1)\}\frac{bh^2}{e2m}k_z^2}} = \frac{2m}{bh^2}\sum_n \int_0^{\infty} \frac{du \cdot u^{-1/2}}{1 + e^{u - b\{J - \mu H(2n+1)\}}}. \tag{3.6}$$

Finally, after the integration we get

$$\eta(b, J) \sim 2\frac{m\pi}{h^2 b}\sum_n F_{-1/2}\{b[J - \mu H(2n + 1)]\}. \tag{3.7}$$

4. The case of the Bloch electron

The calculation of the generalized density matrix for the Bloch electron with the help of the Wannier function[5] will be of the form

$$D(\vec{r}', \vec{r}, b, J) = \sum_{\vec{r}_g, \vec{r}_q} \sum_{m,n} a_m(\vec{r}' - \vec{r}_q)\, a_n(\vec{r} - \vec{r}_g)\frac{\Omega}{2\pi}\int \frac{e^{i\vec{k}(\vec{r}_g - \vec{r}_q)} d^3k}{1 + e^{b\{E_n(\vec{k}) - J\}}}, \tag{4.1}$$

where Ω is the volume of the main district.

From the above relation for $\vec{r}' = \vec{r}$ and by the integration in respect to $\vec{r}$, and if also we consider the properties of the Wannier functions, we obtain for the generalized density the following expression

$$\eta(b, J) \sim \sum_n \frac{\Omega}{(2\pi)^3} \int \frac{d^3k}{1 + e^{b\{E_n(\vec{k}) - J\}}}. \tag{4.2}$$

Integrals of the above form for several forms of the functions $E_n(\vec{k})$ are of interest and we shall consider them in a future paper.

In the case in which we have high temperatures, then by developing the exponential function $e^{b\{E_n(\vec{k}) - J\}}$ up to the linear term, namely

$$e^{b\{E_n(\vec{k}) - J\}} \approx 1 + \frac{b}{1!} E_n(\vec{k}) - J\} \tag{4.3}$$

the generalized density matrix (4.1) takes the form

$$D(\vec{r}', \vec{r}, b, J) \approx \frac{1}{b} G\left(\vec{r}', \vec{r}, J - \frac{2}{b}\right), \tag{4.4}$$

where $G\left(\vec{r}', \vec{r}, J - \frac{2}{b}\right)$ is the corresponding Green-function of the lattice electron[7] — formula (13) — with the energy $E = j - \frac{2}{b} = J - 2kT$.

Equ. (4.4) for high temperatures holds not only for the lattice electron, but also in general and it results easily from the definition (1.1) of the generalized density matrix and also from the definition of the Green-function.

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