Physica **107A** (1981) 587–597 *North-Holland Publishing Co.*

WIGNER REPRESENTATION OF BLOCH ELECTRONS IN UNIFORM FIELDS

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Received 14 November 1980

In this paper we calculate the Wigner distribution function and the partition function of Bloch electrons in uniform electric and magnetic fields with the help of the effective hamiltonian. We also calculate the magnetic and the electric susceptibilities. Using standard techniques of operator ordering, the above quantities are calculated in a manner which shows the exact contribution of the electric field.

1. Introduction

The application of the Wigner representation gave for the known problems the same results and succeeded sufficiently in many new ones. Wigner representation, which Wigner originally introduced[1]) in Statistical Mechanics, has been later founded by Bopp[2]) and Kubo[3]). Especially Kubo used this formulation in various applications to electrons in a uniform magnetic field. Many other applications of this formulation can be found in some papers of Agarwal and Wolf[4]), Buot[5]), Tenreiro and Hakim[6]), Jannussis et al.[7,8]), and in their references. For the elegance of the Wigner representation, which simplifies many problems, we calculate here the Wigner distribution function of Bloch electrons in uniform electric and magnetic fields, using the effective hamiltonian.

According to Kubo the Wigner distribution function satisfies the Bloch equation

$$\frac{\partial f}{\partial b} = -\tfrac{1}{2}[H(\hat{p}, \hat{q}) + H(\hat{p}^*, \hat{q}^*)]f, \tag{1.1}$$

and can be written as

$$f(p, q, b) = \exp\{-\tfrac{1}{2}b[H(\hat{p}, \hat{q}) + H(\hat{p}^*, \hat{q}^*)]\}1, \tag{1.2}$$

where $H(\hat{p}, \hat{q})$ is the hamilton operator and

$$\hat{p} = p - \frac{i\hbar}{2}\frac{\partial}{\partial q}, \qquad \hat{q} = q + \frac{i\hbar}{2}\frac{\partial}{\partial p}, \tag{1.3}$$

are the so-called Bopp–Wigner operators.

The above operators satisfy the standard commutation relations

$$[\hat{p}, \hat{q}] = -i\hbar, \quad [\hat{p}^*, \hat{q}^*] = i\hbar, \quad [\hat{p}, \hat{p}^*] = [\hat{q}, \hat{q}^*] = 0. \tag{1.4}$$

For the case of Bloch electrons the effective hamilton operator of an energy band[9,10]) is given by $\mathscr{E}(\boldsymbol{K})$, which is a periodic function with periodicity the reciprocal lattice vector, that is

$$\mathscr{E}(\boldsymbol{K}) = \sum_{r_l} \mathscr{E}(\boldsymbol{r}_l) e^{i\boldsymbol{K}\boldsymbol{r}_l}, \tag{1.5}$$

where $\mathscr{E}(\boldsymbol{r}_l)$ are the Fourier coefficients of Bloch energy.

2. Bloch electrons in electromagnetic fields

Let us consider a Bloch electron in a magnetic field which results from a vector potential $\boldsymbol{A}(\boldsymbol{q}) = (-\frac{1}{2}Hq_2, \frac{1}{2}Hq_1, 0)$ and in a uniform electric field $\boldsymbol{E}(E_1, E_2, E_3)$. The effective Hamiltonian is given by the relation

$$H(\boldsymbol{K}, \boldsymbol{q}) = \mathscr{E}(\boldsymbol{K}) - e\boldsymbol{E}\boldsymbol{q}, \tag{2.1}$$

where

$$\boldsymbol{K} = \boldsymbol{k} - \frac{e}{\hbar c} \mathbf{A}(\boldsymbol{q}), \tag{2.2}$$

and its components K_1, K_2 satisfy the following commutation relations

$$[\hat{K}_1, \hat{K}_2] = iB, \qquad B = (eH/\hbar c). \tag{2.3}$$

In Wigner representation we obtain as Bopp–Wigner operators, the operators

$$\hat{\boldsymbol{K}} = \boldsymbol{k} - \frac{e}{\hbar c}\mathbf{A}(i\nabla_k) - \frac{i}{2}\nabla_q, \qquad \hat{\boldsymbol{q}} = \boldsymbol{q} + \frac{i}{2}\nabla_k,$$

$$\hat{\boldsymbol{K}}^* = \boldsymbol{k} + \frac{e}{\hbar c}\mathbf{A}(i\nabla_k) + \frac{i}{2}\nabla_q, \qquad \hat{\boldsymbol{q}}^* = \boldsymbol{q} - \frac{i}{2}\nabla_k. \tag{2.4}$$

The above operators satisfy the commutation relations

$$[\hat{K}_1, \hat{K}_2] = iB, \qquad [\hat{K}_i, \hat{q}_j] = -i\delta_{ij}. \tag{2.5}$$

Inserting operators (2.4) in eq. (1.2) we obtain as the Wigner distribution the following expression

$$f(\boldsymbol{k}, \boldsymbol{q}, b) = \exp\left\{\frac{b}{2}\left[\mathscr{E}\left(k_1 - \frac{i}{2}\frac{\partial}{\partial q_1} + i\frac{B}{2}\frac{\partial}{\partial k_2}, k_2 - \frac{i}{2}\frac{\partial}{\partial q_2} - i\frac{B}{2}\frac{\partial}{\partial k_1}, k_3 - \frac{i}{2}\frac{\partial}{\partial q_3}\right)\right.\right.$$
$$\left.\left. + \mathscr{E}\left(k_1 + \frac{i}{2}\frac{\partial}{\partial q_1} - i\frac{B}{2}\frac{\partial}{\partial k_2}, k_2 + \frac{i}{2}\frac{\partial}{\partial q_2} + i\frac{B}{2}\frac{\partial}{\partial k_1}, k_3 + \frac{i}{2}\frac{\partial}{\partial q_3}\right) - 2e\boldsymbol{E}\boldsymbol{q}\right]\right\} 1. \tag{2.6}$$

The operator function $\mathscr{E}(\hat{K}_1, \hat{K}_2, \hat{K}_3)$ in the exponential can be expanded in powers of B as follows:

$$\mathscr{E}(\hat{K}_1, \hat{K}_2, \hat{K}_3) = \exp\left(-\frac{i}{2}\nabla_k\nabla_q\right)\left[\mathscr{E}(\boldsymbol{k}) + i\frac{B}{2}\left(\frac{\partial\mathscr{E}(\boldsymbol{k})}{\partial k_1}\frac{\partial}{\partial k_2} - \frac{\partial\mathscr{E}(\boldsymbol{k})}{\partial k_2}\frac{\partial}{\partial k_1}\right)\right.$$
$$+\frac{B^2}{8}\left(\frac{\partial^2\mathscr{E}(\boldsymbol{k})}{\partial k_1^2}\frac{\partial^2}{\partial k_2^2} - 2\frac{\partial^2\mathscr{E}(\boldsymbol{k})}{\partial k_1\partial k_2}\frac{\partial^2}{\partial k_1\partial k_2}\right.$$
$$\left.\left.+\frac{\partial^2\mathscr{E}(\boldsymbol{k})}{\partial k_2^2}\frac{\partial^2}{\partial k_1^2}\right)\right]\exp\left(\frac{i}{2}\nabla_k\nabla_q\right) + O(B^3). \tag{2.7}$$

If we insert the above expansion in eq. (2.6) we obtain

$$f(\boldsymbol{k}, \boldsymbol{q}, b) = \exp\left\{-b\left\{[\cos(\tfrac{1}{2}\nabla_k\nabla_q)\mathscr{E}(\boldsymbol{k})] - e\boldsymbol{E}\boldsymbol{q}\right.\right.$$
$$+\frac{B}{2}\left[\sin(\tfrac{1}{2}\nabla_k\nabla_q)\left(\frac{\partial\mathscr{E}}{\partial k_1}\frac{\partial}{\partial k_2} - \frac{\partial\mathscr{E}}{\partial k_2}\frac{\partial}{\partial k_1}\right)\right]$$
$$\left.\left.-\frac{B^2}{8}\left[\cos(\tfrac{1}{2}\nabla_k\nabla_q)\left(\frac{\partial^2\mathscr{E}}{\partial k_1^2}\frac{\partial^2}{\partial k_2^2} - 2\frac{\partial^2\mathscr{E}}{\partial k_1\partial k_2}\frac{\partial^2}{\partial k_1\partial k_2} + \frac{\partial^2\mathscr{E}}{\partial k_2^2}\frac{\partial^2}{\partial k_1^2}\right)\right]\right\}\right\}1, \tag{2.8}$$

where the action of the operators $\cos(\frac{1}{2}\nabla_k\nabla_q)$ and $\sin(\frac{1}{2}\nabla_k\nabla_q)$ is limited in the corresponding brackets.

In the following we expand the exponent operator of (2.8), up to the B^2 term. Setting

$$H_0 = \cos(\tfrac{1}{2}\nabla_k\nabla_q)\mathscr{E}(\boldsymbol{k}) - e\boldsymbol{E}\boldsymbol{q},$$
$$H_1 = \sin(\tfrac{1}{2}\nabla_k\nabla_q)\left(\frac{\partial\mathscr{E}}{\partial k_1}\frac{\partial}{\partial k_2} - \frac{\partial\mathscr{E}}{\partial k_2}\frac{\partial}{\partial k_1}\right), \tag{2.9}$$
$$H_2 = \cos(\tfrac{1}{2}\nabla_k\nabla_q)\left(\frac{\partial^2\mathscr{E}}{\partial k_1^2}\frac{\partial^2}{\partial k_2^2} - 2\frac{\partial^2\mathscr{E}}{\partial k_1\partial k_2}\frac{\partial^2}{\partial k_1\partial k_2} + \frac{\partial^2\mathscr{E}}{\partial k_2^2}\frac{\partial^2}{\partial k_1^2}\right),$$

we have

$$f(\boldsymbol{k}, \boldsymbol{q}, b) = e^{-bH_0}\left\{1 - \frac{B}{2}\int_0^b e^{b'H_0}H_1\, e^{-b'H_0}\,db' + \frac{B^2}{8}\int_0^b e^{b'H_0}H_2\, e^{-b'H_0}\,db'\right.$$
$$\left.+\frac{B^2}{4}\int_0^b e^{b'H_0}H_1\, e^{-b'H_0}\,db'\int_0^{b'} e^{b''H_0}H_1\, e^{-b''H_0}\,db''\right\}1. \tag{2.10}$$

Finally, by the help of the identity, which has been proved in the appendix,

$$e^{-bH_0} = \exp(-b[\tfrac{1}{2}\mathscr{E}(\hat{\boldsymbol{K}}) + \tfrac{1}{2}\mathscr{E}(\hat{\boldsymbol{K}}^*) - e\boldsymbol{E}\hat{\boldsymbol{q}}])$$
$$= e^{be\boldsymbol{E}\hat{\boldsymbol{q}}}\exp\left(-\tfrac{1}{2}\int_0^b\left[\mathscr{E}\left(\hat{\boldsymbol{K}} - \frac{ie\boldsymbol{E}}{2}u\right) + \mathscr{E}\left(\hat{\boldsymbol{K}}^* + \frac{ie\boldsymbol{E}}{2}u\right)\right]du\right),$$

and after a simple calculation, we find

$$f(\boldsymbol{k}, \boldsymbol{q}, b) = \mathrm{e}^{be\boldsymbol{E}\boldsymbol{q}}\, \mathrm{e}^{-\Lambda(b)\mathscr{E}(\boldsymbol{k})}\Big\{1 + \frac{B}{2}\int_0^b \Big[\Big(\sin\frac{b'e}{2}\boldsymbol{E}\nabla_k \cdot \frac{\partial\mathscr{E}}{\partial k_1}\Big)\Big(\Lambda(b')\frac{\partial\mathscr{E}}{\partial k_2}\Big)$$
$$- \Big(\sin\frac{b'e}{2}\boldsymbol{E}\nabla_k \cdot \frac{\partial\mathscr{E}}{\partial k_2}\Big)\Big(\Lambda(b')\frac{\partial\mathscr{E}}{\partial k_1}\Big)\Big]\mathrm{d}b'$$
$$+ \frac{B^2}{4}\int_0^b \Big[\Big(\sin\frac{b'e}{2}\boldsymbol{E}\nabla_k \cdot \frac{\partial\mathscr{E}}{\partial k_1}\Big)(\Lambda(b') - \Lambda(b))\frac{\partial\mathscr{E}}{\partial k_2}$$
$$- \Big(\sin\frac{b'e}{2}\boldsymbol{E}\nabla_k \cdot \frac{\partial\mathscr{E}}{\partial k_2}\Big)(\Lambda(b') - \Lambda(b))\frac{\partial\mathscr{E}}{\partial k_1}\Big]\mathrm{d}b'$$
$$+ \int_0^{b'} \Big[\Big(\sin\frac{b''e}{2}\boldsymbol{E}\nabla_k \cdot \frac{\partial\mathscr{E}}{\partial k_1}\Big)\Big(\Lambda(b'')\frac{\partial\mathscr{E}}{\partial k_2}\Big)$$
$$- \Big(\sin\frac{b''e}{2}\boldsymbol{E}\nabla_k \cdot \frac{\partial\mathscr{E}}{\partial k_2}\Big)\Big(\Lambda(b'')\frac{\partial\mathscr{E}}{\partial k_1}\Big)\Big]\mathrm{d}b''$$
$$+ \frac{B^2}{8}\int_0^b \Big[\Big(\cos\frac{b'e}{2}\boldsymbol{E}\nabla_k \cdot \frac{\partial^2\mathscr{E}}{\partial k_1^2}\Big)\Big(\Big(\Lambda(b')\frac{\partial\mathscr{E}}{\partial k_2}\Big)^2$$
$$- \Lambda(b')\frac{\partial^2\mathscr{E}}{\partial k_1^2}\Big) - 2\Big(\cos\frac{b'e}{2}\boldsymbol{E}\nabla_k \cdot \frac{\partial^2\mathscr{E}}{\partial k_1 \partial k_2}\Big)$$
$$\times\Big(\Big(\Lambda(b')\frac{\partial\mathscr{E}}{\partial k_1}\Big)\Big(\Lambda(b')\frac{\partial\mathscr{E}}{\partial k_2}\Big) - \Lambda(b')\frac{\partial^2\mathscr{E}}{\partial k_1 \partial k_2}\Big) + \Big(\cos\frac{b'e}{2}\boldsymbol{E}\nabla_k \cdot \frac{\partial^2\mathscr{E}}{\partial k_2^2}\Big)$$
$$\times\Big(\Big(\Lambda(b')\frac{\partial\mathscr{E}}{\partial k_1}\Big)^2 - \Lambda(b')\frac{\partial\mathscr{E}}{\partial k_1^2}\Big)\Big]\mathrm{d}b'\Big\}, \tag{2.11}$$

where

$$\Lambda(b) = \frac{\sin(\frac{1}{2}be\boldsymbol{E}\nabla_k)}{\frac{1}{2}e\boldsymbol{E}\nabla_k}.$$

This formula contains the full contribution of the electric field to the considered approximations. Integration of (2.11) with respect to $\boldsymbol{k}$ and $\boldsymbol{q}$ gives the partition function, namely

$$Z(b) = \frac{1}{(2\pi)^3}\int f(\boldsymbol{k}, \boldsymbol{q}, b)\mathrm{d}\boldsymbol{k}\, \mathrm{d}\boldsymbol{q}^*. \tag{2.12}$$

Because of the term $\exp(be\boldsymbol{E} \cdot \boldsymbol{q})$ which represents the centribution of the electric field to the Wigner distribution function it is necessary to assume that

*The limits of integration with respect to $\boldsymbol{k}$ depend on the structure form of $\mathscr{E}(\boldsymbol{k})$.

the particle is enclosed in a box of edge-length L_i, where L_i are the lattice dimensions. Periodic boundary conditions have now to be taken into account, so the limits of integration are restricted in the interval $[-\frac{1}{2}L_i, \frac{1}{2}L_i]$.

To avoid the divergence of this distribution function we have to work in an inertial frame of reference S' which moves with constant velocity $\boldsymbol{v} = 2c(\boldsymbol{E}\times\boldsymbol{H})/(H^2)$. In this frame the observer understands only the rotational motion of the particle and consequently only the magnetic field seems to influence the motion[11]). The scalar potential becomes zero:

$$\varphi' = \varphi - \frac{1}{c}\boldsymbol{v}\cdot\mathbf{A} = 0. \tag{2.13}$$

In order to obtain in the S' system the new hamiltonian, namely

$$H' = \mathscr{E}(\boldsymbol{K}) + e\varphi', \qquad \boldsymbol{K} = \boldsymbol{k} - \frac{e}{\hbar c}\mathbf{A}'(\boldsymbol{q}, t) \tag{2.14}$$

we perform the following gauge transformation:

$$\mathbf{A}' = \mathbf{A} + \nabla\Phi, \qquad \varphi' = \varphi - \frac{1}{c}\frac{\partial}{\partial t}\Phi, \tag{2.15}$$

where

$$\Phi(\boldsymbol{q}, t) = -ct\boldsymbol{E}\cdot\boldsymbol{q}.$$

We now consider the primed hamiltonian

$$H' = \mathscr{E}(\boldsymbol{K} - \frac{e}{\hbar c}\mathbf{A}'(\boldsymbol{q}, -\mathrm{i}\hbar b)) + e\varphi'(\boldsymbol{q}, -\mathrm{i}\hbar b), \tag{2.16}$$

where

$$\mathbf{A}' = \tfrac{1}{2}\boldsymbol{H}\times\boldsymbol{q} + i\hbar cb\boldsymbol{E}, \qquad \varphi' = 0.$$

The effective hamiltonian (2.16) has been studied in ref. 12. It is easily seen that if $f(\boldsymbol{p}, \boldsymbol{q}, t)$ is a solution of the Bloch equation (1.1) then the distribution function

$$\begin{aligned} f'(\boldsymbol{p}, \boldsymbol{q}, b) &= \exp(\mathrm{i}\frac{e}{\hbar c}\Phi(\boldsymbol{q}, -\mathrm{i}\hbar b)f(\boldsymbol{p}, \boldsymbol{q}, b) \\ &= \exp(-eb\boldsymbol{E}\cdot\boldsymbol{q})f(\boldsymbol{p}, \boldsymbol{q}, b) \end{aligned} \tag{2.17}$$

is a solution of the primed Bloch equation

$$\frac{\partial f}{\partial b} = -\tfrac{1}{2}[H'(\hat{p}, \hat{q}) + H'(\hat{p}^*, \hat{q}^*)]f. \tag{2.18}$$

It is clear that the chosen gauge eliminates the divergent part of the distribution function which now becomes independent of $\boldsymbol{q}$.

As an example we calculate the partition function in the case of the free electron, that is

$$\mathscr{E}(\boldsymbol{K}) = \frac{\hbar^2}{2m}(k_1^2 + k_2^2 + k_3^2).$$

A straightforward calculation yields

$$Z(b) = \left(\frac{m}{2\pi b\hbar^2}\right)^{3/2} \exp\left(\frac{b^2 e^2 \hbar^2}{24m} E^2\right)\left\{1 - \frac{B^2 b^2}{24}\left[\frac{\hbar^4}{m^2} + \frac{b^3 e^2 \hbar^6}{60 m^3}(E_1^2 + E_2^2)\right]\right\}. \quad (2.19)$$

Since we know $Z(b)$, we can easily obtain the magnetic susceptibility by means of the relation

$$\chi = \frac{1}{bH}\frac{\partial}{\partial H}\log Z(b), \quad (2.20)$$

we have

$$\chi = -\frac{1}{3KT}\mu^2\left(1 + \frac{\hbar^2 e^2 (E_1^2 + E_2^2)}{60 m (kT)^3}\right), \qquad \mu = \frac{e\hbar}{2mc}, \quad (2.21)$$

which is already known and has been found at first by Janussis[13]). Notice that the resulting increase depends on the crossed component $E^2 = E_1^2 + E_2^2$ of the electric field.

3. Bloch electrons in uniform electric field

The Wigner distribution function of Bloch electrons in a uniform electric field can be derived from eq (2.11), setting $B = 0$ we find

$$f(\boldsymbol{k}, \boldsymbol{q}, b) = \exp\left\{\frac{\sin(\frac{1}{2}be\boldsymbol{E}\nabla_k)}{\frac{1}{2}e\boldsymbol{E}\nabla_k}\mathscr{E}(\boldsymbol{k})\right\}, \quad (3.1)$$

which is the exact one. It must be pointed out, however, that it holds only for states within a band when external fields are not too large, since interband transitions do not occur in this case. Integration of (3.1) with respect to $\boldsymbol{k}$ and $\boldsymbol{q}$ gives the partition function

$$Z(b) = \frac{1}{(2\pi)^3}\int \exp\left\{-\frac{\sin(\frac{1}{2}be\boldsymbol{E}\nabla_k)}{\frac{1}{2}e\boldsymbol{E}\nabla_k}\mathscr{E}(\boldsymbol{k})\right\}\mathrm{d}\boldsymbol{k}. \quad (3.2)$$

The operator on the exponential acts as follows:

$$\frac{\sin(\frac{1}{2}be\boldsymbol{E}\nabla_k)}{\frac{1}{2}e\boldsymbol{E}\nabla_k}\mathscr{E}(\boldsymbol{k}) = \tfrac{1}{2}\int_0^b \left[\mathscr{E}\left(\boldsymbol{k} - \mathrm{i}\frac{\tau e}{2}\boldsymbol{E}\right) + \mathscr{E}\left(\boldsymbol{k} + \mathrm{i}\frac{\tau e}{2}\boldsymbol{E}\right)\right]\mathrm{d}\tau.$$

The partition function (3.2) can be calculated exactly in some interesting cases. We consider the simple cubic lattice with the following dispersion law

$$\mathscr{E}(k) = \epsilon(\cos \alpha_1 k_1 + \cos \alpha_2 k_2 + \cos \alpha_3 k_3). \tag{3.3}$$

Substituting (3.3) in (3.2) we find

$$Z(b) = \prod_{i=1}^{3} I_0\left(\epsilon \frac{\sinh(\frac{1}{2}beE_i\alpha_i)}{\frac{1}{2}eE_i\alpha_i}\right), \tag{3.4}$$

where I_0 is the modified zeroth-order Bessel function.

In the sequel we find the electric susceptibility using the known, Laplace transform method. An approximation of (3.2) up to E^2 term yields

$$Z(b) = \frac{1}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k}\ \mathrm{e}^{-b\mathscr{E}(\boldsymbol{k})}\left\{1 + \frac{e^2 b^3}{24}(\boldsymbol{E}\nabla_k)^2 \mathscr{E}(\boldsymbol{k})\right\}. \tag{3.5}$$

We consider the integrals of (3.5) over b and E involved in the computation of the free energy. Omitting constant terms with respect to E_i we have[14])

$$\frac{1}{2\pi \mathrm{i}}\int_0^\infty \mathrm{d}\epsilon \int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty} \mathrm{d}b \left\{\frac{e^2 b}{24}(\boldsymbol{E}\nabla_k)^2 \mathscr{E}(\boldsymbol{k})\right\} \mathrm{e}^{b(\epsilon-\mathscr{E}(\boldsymbol{k}))}\frac{\partial f}{\partial \epsilon}$$

$$= -\frac{e^2}{24}(\boldsymbol{E}\nabla_k)^2 \mathscr{E}(\boldsymbol{k})\frac{\partial^2 f}{\partial \epsilon^2}.$$

So the free energy is as follows:

$$F - \eta\zeta = F_0 - \frac{1}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k}\left\{\frac{e^2}{24}(\boldsymbol{E}\nabla_k)^2 \mathscr{E}(\boldsymbol{k})\right\}\frac{\partial^2 f}{\partial \epsilon^2}, \tag{3.6}$$

where F_0 is independent of $\boldsymbol{E}$.

We can find the electric susceptibility[15]) through the relation

$$\eta = -\frac{1}{|\boldsymbol{E}|}\frac{\partial F}{\partial |\boldsymbol{E}|}. \tag{3.7}$$

We find

$$\eta = \frac{e^2}{48\pi^2}\int \mathrm{d}k \left\{\sum_{i,j} \frac{\hbar^2}{m_{ij}}\frac{\partial^2 f}{\partial \epsilon^2}\right\}, \tag{3.8}$$

where

$$\frac{1}{m_{ij}} = \frac{1}{\hbar^2}\frac{\partial^2 \mathscr{E}(\boldsymbol{k})}{\partial k_i \partial k_j}$$

is the effective mass tensor.

4. Magnetic susceptibility

To find the magnetic susceptibility of Bloch electrons in an electro-magnetic field we consider an approximation of (2.11) up to E^2 terms. After integration by parts in $\boldsymbol{k}$ integration we find

$$Z(b)=\frac{1}{(2\pi)^3}\int \mathrm{d}\boldsymbol{k}\ \mathrm{e}^{-b\mathscr{E}(\boldsymbol{k})}\Big\{1+\frac{b^3e^2}{24}(\boldsymbol{E}\nabla_k)^2\mathscr{E}(\boldsymbol{k}) - \frac{B^2}{24}[b^2\alpha(\boldsymbol{k})+b^4\beta(\boldsymbol{k})+b^5\gamma(\boldsymbol{k})]\Big\}, \tag{4.1}$$

where

$$\alpha(\boldsymbol{k})=\frac{\partial^2\mathscr{E}}{\partial k_1^2}\frac{\partial^2\mathscr{E}}{\partial k_2^2}-\left(\frac{\partial^2\mathscr{E}}{\partial k_1\partial k_2}\right)^2,$$

$$\beta(\boldsymbol{k})=-\frac{e^2}{3}\left[\frac{\partial^2\mathscr{E}}{\partial k_1^2}(\boldsymbol{E}\nabla_k)^2\frac{\partial^2\mathscr{E}}{\partial k_2^2}+\frac{\partial^2\mathscr{E}}{\partial k_2^2}(\boldsymbol{E}\nabla_k)^2\frac{\partial^2\mathscr{E}}{\partial k_1^2}-2\frac{\partial^2\mathscr{E}}{\partial k_1\partial k_2}(\boldsymbol{E}\nabla_k)^2\frac{\partial^2\mathscr{E}}{\partial k_1\partial k_2}\right]$$
$$-\frac{e^2}{30}\left[\left(\boldsymbol{E}\nabla_k\frac{\partial^2\mathscr{E}}{\partial k_1^2}\right)\left(\boldsymbol{E}\nabla_k\frac{\partial\mathscr{E}}{\partial k_2^2}\right)-\left(\boldsymbol{E}\nabla_k\frac{\partial^2\mathscr{E}}{\partial k_1\partial k_2}\right)^2\right],$$

$$\gamma(\boldsymbol{k})=\frac{e}{24}(\boldsymbol{E}\nabla_k)^2\mathscr{E}(\boldsymbol{k})\left[\frac{\partial^2\mathscr{E}}{\partial k_1^2}\frac{\partial^2\mathscr{E}}{\partial k_2^2}-\left(\frac{\partial^2\mathscr{E}}{\partial k_1\partial k_2}\right)^2\right]$$
$$+\frac{e^2}{60}\left[\left(\boldsymbol{E}\nabla_k\frac{\partial\mathscr{E}}{\partial k_1}\right)^2\frac{\partial^2\mathscr{E}}{\partial k_2^2}+\left(\boldsymbol{E}\nabla_k\frac{\partial\mathscr{E}}{\partial k_2}\right)^2\frac{\partial^2\mathscr{E}}{\partial k_1^2}\right.$$
$$\left.-2\left(\boldsymbol{E}\nabla_k\frac{\partial\mathscr{E}}{\partial k_1}\right)\left(\boldsymbol{E}\nabla_k\frac{\partial\mathscr{E}}{\partial k_2}\right)\frac{\partial^2\mathscr{E}}{\partial k_1\partial k_2}\right].$$

We consider the integration over b and E involved in the computation of the free energy. We find, with the help of the delta function,

$$-2\frac{B^2}{24}\frac{1}{2\pi\mathrm{i}}\int_0^\infty \mathrm{d}\epsilon\int_{c-\mathrm{i}\infty}^{c+\mathrm{i}\infty}\mathrm{d}b\ \mathrm{e}^{b(\epsilon-\mathscr{E}(\boldsymbol{k}))}[\alpha(\boldsymbol{k})+b^2\beta(\boldsymbol{k})+b^3\gamma(\boldsymbol{k})]\frac{\partial f}{\partial\epsilon}$$
$$=-\frac{B^2}{12}\left[\alpha(\boldsymbol{k})\frac{\partial f}{\partial\epsilon}+\beta(\boldsymbol{k})\frac{\partial^3 f}{\partial\epsilon^3}-\gamma(\boldsymbol{k})\frac{\partial^4 f}{\partial\epsilon^4}\right].$$

Thus the magnetic susceptibility is as follows:

$$\chi=\frac{e^2}{48\hbar^2c^2\pi^3}\int\mathrm{d}\boldsymbol{k}\left\{\alpha(\boldsymbol{k})\frac{\partial f}{\partial\epsilon}+\beta(\boldsymbol{k})\frac{\partial^3 f}{\partial\epsilon^3}-\gamma(\boldsymbol{k})\frac{\partial^4 f}{\partial\epsilon^4}\right\}. \tag{4.2}$$

For $E=0$, formula (4.2) reduces to

$$\chi=\frac{e^2}{48\hbar^2c^2\pi^3}\int\mathrm{d}\boldsymbol{k}\left[\frac{\partial^2\mathscr{E}}{\partial k_1^2}\frac{\partial^2\mathscr{E}}{\partial k_2^2}-\left(\frac{\partial^2\mathscr{E}}{\partial k_1\partial k_2}\right)^2\right]\frac{\partial f}{\partial\epsilon}, \tag{4.3}$$

which coincides with the known formula of Landau–Peierls susceptibility.

For free electrons with an effective mass m^* (4.2) can be written as

$$\chi = \frac{e^2}{6\hbar^2 c^2 \pi^2} \int_0^\infty \epsilon^{1/2}\,\mathrm{d}\epsilon \left\{ \frac{\partial f}{\partial \epsilon} - \left(\frac{e^2\hbar^2 \boldsymbol{E}^2}{24m^*} + \frac{e^2\hbar^2(E_1^2 + E_2^2)}{60m^*} \right) \frac{\partial^4 f}{\partial \epsilon^4} \right\}. \tag{4.4}$$

With the notation of ref. 17, the calculation of (4.4) for arbitrary temperatures yields

$$\chi = -\frac{nm^2\mu_0^2}{3m^{*2}kT} \left\{ \frac{F_{1/2}^{(1)}(\xi)}{F_{1/2}(\xi)} + \frac{e^2\hbar^2}{12m^*(kT)^3} \left(\frac{\boldsymbol{E}^2}{2} + \frac{E_1^2 + E_2^2}{5} \right) \frac{F_{1/2}^{(4)}(\xi)}{F_{1/2}(\xi)} \right\}, \tag{4.5}$$

where $\xi = (\zeta/kT)$ and

$$F_n(\xi) = \int_0^\infty \frac{x^n\,\mathrm{d}x}{\mathrm{e}^{x-\xi} + 1}, \qquad n > -1.$$

Expression (4.5) can alternatively be written as

$$\chi = \chi_0 \left\{ 1 + \frac{e^2\hbar^2}{60m^*(kT)^3} \left(E_1^2 + E_2^2 + \frac{5}{2}\boldsymbol{E}^2 \right) \frac{F_{1/2}^{(4)}(\xi)}{F_{1/2}(\xi)} \right\}, \tag{4.6}$$

where

$$\chi_0 = -\frac{nm^2\mu_0^2}{3m^{*2}kT} \frac{F_{1/2}^{(1)}(\xi)}{F_{1/2}(\xi)}$$

is the well-known[17]) zero magnetic field susceptibility for free electrons with an effective mass m^*.

5. Conclusion

The Kubo formulation, using the Wigner distribution function, seems to give elegant and simplified results in many quantum-mechanical problems. In this paper, as an application, the exact contribution of the uniform electric field to the magnetic susceptibility of Bloch electrons in uniform fields has been calculated with the help of the effective hamiltonian.

The resulting expression easily reduces to the Landau–Peierls susceptibility when the electric field vanishes. For free electrons the resulting increase is proportional to the square of the crossed component of the electric field. This term comes from the interaction of the two fields, while for the case of Fermi–Dirac statistics, another term due to the electric field only and depending on the resultant of the electric field has to be added. Within the fremework of the validity of the effective hamiltonian method the exact partition function of Bloch electrons in a uniform electric field has also been calculated. The calculations proceed easily in some interesting cases as, for instance, the cubic lattices. Finally an expression for the steady electric susceptibility has been found, involving the effective mass tensor.

The use of Wigner representation is today one of the best methods for the calculation of the partition function in many physical problems with external fields as well as in plasma physics. In this connection we mention the papers of Fukuyama and Jashioka[18]) and Alastuey and Jancovici[19]).

The Wigner representation is also applied by the Brussels School[20]).

Appendix

To prove the identity

$$\exp\{-b[\tfrac{1}{2}\mathscr{E}(\boldsymbol{k})+\tfrac{1}{2}\mathscr{E}(\hat{\boldsymbol{k}}^*)-e\boldsymbol{E}\hat{\boldsymbol{q}}]\}$$
$$= \mathrm{e}^{be\boldsymbol{E}\hat{\boldsymbol{q}}}\exp\left\{-\frac{1}{2}\int_0^b\left[\mathscr{E}\left(\hat{\boldsymbol{k}}-\frac{\mathrm{i}e\boldsymbol{E}}{2}u\right)+\mathscr{E}\left(\hat{\boldsymbol{k}}^*+\frac{\mathrm{i}e\boldsymbol{E}}{2}u\right)\right]\mathrm{d}u\right\}, \qquad \text{(A.1)}$$

where

$$[\hat{k},\hat{q}]=-\tfrac{1}{2}\mathrm{i}, \qquad [\hat{k}^*,\hat{q}]=\tfrac{1}{2}\mathrm{i},$$

we use the method of parametric differentiation[16]). Differentiating eq. (A.1) with respect to b and multiplying the resulting formula by the inverse of (A.1) we find

$$-\tfrac{1}{2}\mathscr{E}(\hat{\boldsymbol{k}})-\tfrac{1}{2}\mathscr{E}(\hat{\boldsymbol{k}}^*)+e\boldsymbol{E}\hat{\boldsymbol{q}} = e\boldsymbol{E}\exp\left\{\frac{1}{2}\int_0^b\left[\mathscr{E}\left(\hat{\boldsymbol{k}}-\frac{\mathrm{i}e\boldsymbol{E}}{2}u\right)+\mathscr{E}\left(\hat{\boldsymbol{k}}^*+\frac{\mathrm{i}e\boldsymbol{E}}{2}u\right)\right]\mathrm{d}u\right\}$$
$$\times\, \boldsymbol{q}\exp\left\{-\frac{1}{2}\int_0^b\left[\mathscr{E}\left(\hat{\boldsymbol{k}}-\frac{\mathrm{i}e\boldsymbol{E}}{2}u\right)+\mathscr{E}\left(\hat{\boldsymbol{k}}^*+\frac{\mathrm{i}e\boldsymbol{E}}{2}u\right)\right]\mathrm{d}u\right\}$$
$$-\frac{1}{2}\frac{\partial}{\partial b}\int_0^b\left[\mathscr{E}\left(\hat{\boldsymbol{k}}-\frac{\mathrm{i}e\boldsymbol{E}}{2}u\right)+\mathscr{E}\left(\hat{\boldsymbol{k}}^*+\frac{\mathrm{i}e\boldsymbol{E}}{2}u\right)\right]\mathrm{d}u. \qquad \text{(A.2)}$$

Using the identity

$$\mathrm{e}^{\varphi(\hat{A})}f(\hat{\boldsymbol{B}})\,\mathrm{e}^{-\varphi(\hat{A})}=f\left(\hat{\boldsymbol{B}}+c\frac{\partial\varphi}{\partial A}\right), \quad [\hat{A},\hat{\boldsymbol{B}}]=c, \qquad \text{(A.3)}$$

eq. (A.2) becomes

$$-\tfrac{1}{2}\mathscr{E}(\hat{k})-\tfrac{1}{2}\mathscr{E}(\hat{k}^*)+e\boldsymbol{E}\hat{q}=e\boldsymbol{E}\Big[\hat{q}-\frac{\mathrm{i}}{4}\nabla_k\int_0^b\mathscr{E}\Big(\hat{k}-\frac{\mathrm{i}e\boldsymbol{E}}{2}u\Big)\mathrm{d}u$$

$$-\frac{\mathrm{i}}{4}\nabla_k\cdot\int_0^b\mathscr{E}\Big(\hat{k}^*+\frac{\mathrm{i}e\boldsymbol{E}}{2}u\Big)\mathrm{d}u\Big]-\frac{1}{2}\frac{\partial}{\partial b}\int_0^b\Big[\mathscr{E}\Big(\hat{k}-\frac{\mathrm{i}e\boldsymbol{E}}{2}u\Big)+\mathscr{E}\Big(\hat{k}^*+\frac{\mathrm{i}e\boldsymbol{E}}{2}u\Big)\Big]\mathrm{d}u, \tag{A.4}$$

which easily implies the desired identity.

References

1) E.P. Wigner, Phys. Rev. **40** (1932) 749.
2) F. Bopp, Wer. Heisenberg und die Physik unserer Zeit (Vieweg, Braunschweig, 1961) p. 128.
3) R. Kubo, J. Phys. Soc. Japan **19** (1964) 2127.
4) G. Agarwal and E. Wolf, Phys. Rev. **2** (1970) 2167.
5) F.A. Buot, Phys. Rev. **A8** (1973) 1570; **B10** (1974) 3700. **B14** (1976) 977.
6) D. Tenreiro and R. Hakim, Phys. Rev. **D15** (1977) 1435.
7) A. Jannussis, A. Streklas, D. Sourlas and K. Vlachos, Lett. Nuovo Cimento **18** (1977) 349.
8) A. Jannusis and N. Patargias, Phys. Lett. **A53** (1975) 357.
9) R. Peierls, Z. Physik **80** (1933) 763, **81** (1933) 186.
10) W. Kohn, Phys. Rev. **115** (1959) 1460.
11) Kyu-Myung Chung und B. Mrowka, Z. Physik **259** (1973) 157–176.
12) A. Jannussis, V. Papatheou, G. Brodimas and G. Goudaroulis, Phys. Lett. **61**A (1977) 347.
13) A. Jannussis, Phys. Stat. Sol. **36** K17 (1969).
14) J. Callaway, Energy Band Theory (Academic Press, New York, London, 1964) p. 269.
15) J. Van Vleck, The Theory of Electric and Magnetic Susceptibilities (Oxford Univ. Press, Oxford, 1932).
16) R. Wilcox, J. Math. Phys. **8** (1967) 962.
17) A.H. Wilson, The Theory of Metals (Cambridge Univ. Press, London, 1965) section 6.42.
18) H. Fukuyama and D. Yoshioka, J. Phys. Soc. Japan **48** (1980) 1853.
H. Fukuyama, J. Phys. Soc. Japan 48 (1980) 1841.
19) A. Alastuey and B. Jancovici, Physica **97**A (1979) 349, 102A (1980) 327.
B. Jancovici, Physica **101A** (1980) 324.
20) C. George and I. Prigogine, Physica **99A** (1979) 369, and references therein.