Weyl Transform and the Magnetic Susceptibility of a Relativistic Dirac Electron Gas*

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(Received 25 September 1972; revised manuscript received 26 January 1973)

The Weyl transform in relativistic quantum dynamics is formulated in terms of the coordinate eigenfunction and momentum eigenfunction that correspond to the ordinary and magnetic Wannier function and ordinary and magnetic Bloch function, respectively, in solid-state theory. Using this method, a rigorous but fairly simple dynamical derivation of the magnetic susceptibility of a relativistic Dirac electron gas (which includes the effect of an anomalous magnetic moment) is given. The terms coming from the Landau-Peierls formula and Pauli spin paramagnetism are cancelled by the terms arising from the second-order effect of spin and by an unfamiliar dynamical effect due to the inherent spread of the electron (approximately equal to its Compton wavelength). The very simple result reduces to the sum of Landau orbital diamagnetism and Pauli spin paramagnetism in the nonrelativistic limit. It is suggested that different physical processes dominate in the very-low-electron-density limit as compared to that in the very-high-electron-density limit. Striking similarities with the magnetic properties of the electrons in bismuth crystal are pointed out.

I. INTRODUCTION

As is well known, nonclassical dynamical effects of quantum charged particles readily manifest themselves in physical phenomena involving the application of an external magnetic field. The inherent spin of the nonrelativistic electron is a typical example. The diamagnetism of Bloch electrons in solids has indeed come to be one of the difficult problems in solid-state theory[1] owing to the unfamiliar dynamical effects that give the most important contribution in some cases.[2] The dynamics of Bloch electrons in an external magnetic field are not yet completely understood.[1]

So far, our understanding of the quantum dynamical properties of the nonrelativistic (except for inclusion of spin) electron gas has guided the interpretation of the various physical properties of solids (simple metals in particular). The problem of a nonrelativistic electron gas in a magnetic field has been extensively studied in solid-state physics since the time of Landau[3,4] and these studies have been responsible for the significant progress in Fermi-surface studies and other magnetic phenomena in solids. For almost two decades great efforts have been made toward the understanding of diamagnetism of Bloch electrons in solids in terms of nonrelativistic free-electron properties, namely orbital diamagnetism and Pauli spin paramagnetism, or in terms of a one-band theory. As we shall see, this concept is quite limited and it is not surprising that it failed to explain the large diamagnetism of bismuth and other polyvalent nontransition metals.

A complete dynamical treatment of the response of a relativistic Dirac electron in an external magnetic field is not found in the literature. In principle, if one is just interested in numbers, there is little difficulty in calculating the magnetic susceptibility,[5] since the magnetic energy levels can easily be calculated. The purpose of this paper is to give a basic conceptual derivation, based on fundamental assumptions of quantum theory, of the low-field response of a noninteracting relativistic Dirac electron gas. Consideration is given to the effects of the electron anomalous magnetic moment. To the author's knowledge previous results did not include the anomalous magnetic moment.[5,6] The method of derivation is quite instructive and permits a clearer physical interpretation of the unfamiliar dynamical effects that emerge in the formalism. The formalism used yields some of the fundamental equations in solid-state theory.

An alternative formulation of quantum mechanics using ordinary functions in phase space for both states and physical quantities consists in introducing a Weyl transform instead of operators and a Wigner function instead of state vectors. This alternative description has proved to be very useful in making quantum corrections to classical formulas because it gives a systematic method for expanding physical quantities in powers of $\hbar$ and is extensively used in the theories of gaseous and liquid systems.[4] The use of the Weyl transform in nonrelativistic quantum dynamics has been clarified by Leaf[7] and the fundamental assumption is the existence of complete sets of position and momentum eigenfunctions. It was shown by Suttorp and de Groot[8] that a better understanding of the physical meaning of quantum-dynamical quantities can easily be obtained by looking at their Weyl transforms. In this sense the Weyl transform allows one to interpret classically purely quantum-mechanical quantities.

In this paper, a very useful application of the Weyl transform in relativistic quantum dynamics makes use of the fact that complete sets of position and momentum eigenfunctions, which are also labeled by a band index (± spin band for positive energy states and ± spin band for negative energy states), exist and form complete sets for each band even in the presence of a uniform magnetic field. They correspond to the ordinary and magnetic Wannier function and ordinary and magnetic Bloch function in the band theory of solids. Some of their properties are well known. This information is believed to be of great value in the formulation of relativistic quantum dynamics and in this paper this is used to calculate the magnetic susceptibility of a relativistic Dirac electron (with anomalous magnetic moment) gas in an elegant fashion.

The first part of this paper introduces the reader to the concept of Wannier function and Bloch function for a relativistic Dirac electron, both in the absence and presence of an externally applied uniform magnetic field. The second part derives the expression for the magnetic susceptibility based on these basis states using the elegant formalism of Leaf for taking the traces of products of operators. Finally the unfamiliar dynamical effects that contribute to the magnetic susceptibility are assigned definite physical meanings.

II. WANNIER FUNCTION AND BLOCH FUNCTION OF A RELATIVISTIC DIRAC ELECTRON

The Hamiltonian for a free relativisitic Dirac electron is of the form

$$\mathcal{H}=\beta\Delta+c\vec{\alpha}\cdot\vec{P}\ . \tag{1}$$

The equation for the eigenfunctions and eigenvalues is

$$\mathcal{H}b_\lambda(\vec{x},\vec{p})=E_\lambda(\vec{p})\,b_\lambda(\vec{x},\vec{p})\ , \tag{2}$$

where $E_\lambda(\vec{p})=\pm E(\vec{p})$ and λ labels the band index: plus and minus spin band for positive energy states, and plus and minus spin band for negative energy states. Throughout, quantum operators are written in capital letters and their eigenvalues in small letters.

In the absence of an external magnetic field we may define the Wannier function and the Bloch function[9] of a relativistic Dirac electron as

$$b_\lambda(\vec{x},\vec{p})=\frac{1}{(2\pi\hbar)^{3/2}}\,u_\lambda(\vec{p})\,e^{(i/\hbar)\vec{p}\cdot\vec{x}}\ , \tag{3}$$

$$a_\lambda(\vec{x}-\vec{q})=\frac{1}{(2\pi\hbar)^{3/2}}\int e^{-(i/\hbar)\vec{p}\cdot\vec{q}}\,b_\lambda(\vec{x},\vec{p})\,d\vec{p}\ , \tag{4}$$

where $b_\lambda(\vec{x},\vec{p})$ is the Bloch function, and $a_\lambda(\vec{x}-\vec{q})$ the corresponding Wannier function. Equation (4) is nothing but the Fourier transform of the eigenfunction $b_\lambda(\vec{x},\vec{p})$. $u_\lambda(\vec{p})$ is of course a four-component function in the usual Dirac basis. Moreover, the $u_\lambda(\vec{p})$'s are related to the $u_\lambda(0)$'s by a unitary transformation S which also transforms the Dirac Hamiltonian into an even form,[10] i.e., into a Hamiltonian which cannot couple the different bands. This transformation is equivalent to the transformation from the Kohn-Luttinger basis to Bloch functions in solid-state theory.[11,12] We have

$$S=(E+\beta\mathcal{H})/[2E(E+\Delta)]^{1/2}, \tag{5}$$

which can be written in matrix form as

$$S=\begin{pmatrix}[(E+\Delta)/2E]^{1/2} & c\{\vec{\sigma}\cdot\vec{p}\}^*/[2E(E+\Delta)]^{1/2}\\ -a\{\vec{\sigma}\cdot\vec{p}\}^*/[2E(E+\Delta)]^{1/2} & [(E+\Delta)/2E]^{1/2}\end{pmatrix}, \tag{6}$$

where the entries are 2×2 matrices, $\Delta=mc^2$, and all elements may be viewed as matrix elements of S between the $u_\lambda(0)$'s. We have taken the complex conjugate of the complex entries since their phase can be chosen arbitrarily by a mere change of the phases of $u_\lambda(0)$'s. Obviously $u_\lambda(0)$'s are the spin functions in Pauli representation.[12] The transformed Hamiltonian is

$$\mathcal{H}'=S\mathcal{H}S^\dagger=\beta E(\vec{P})\ . \tag{7}$$

The $a_\lambda(\vec{x}-\vec{q})$ is not a δ function because of the dependence of the $u_\lambda(\vec{p})$ on $\vec{p}$; it is spread out over a region of the order of the Compton wavelength of the electron, as pointed out by Foldy and Wouthuijsen and by Blount.[9]

The formalism to be used here, which is mainly based on the development by Leaf[7] of the correct Weyl correspondence between the classical function and the quantum-mechanical operator, revolves around the fundamental identities which, in our case, we write as follows:

$$\langle b_\lambda(\vec{x},\vec{p})|b_{\lambda'}(\vec{x},\vec{p}')\rangle = \delta(\vec{p}-\vec{p}')\delta_{\lambda\lambda'}, \quad (8a)$$

$$\langle a_\lambda(\vec{x}-\vec{q})|a_\lambda(\vec{x}-\vec{q}')\rangle = \delta(\vec{q}-\vec{q}')\delta_{\lambda\lambda'}, \quad 8(b)$$

$$\langle a_\lambda(\vec{x}-\vec{q})|b_\lambda(\vec{x},\vec{p})\rangle = e^{(i/\hbar)\vec{p}\cdot\vec{q}}/h^{3/2}, \quad 8(c)$$

$$\sum_\lambda \int d\vec{p}\, b^*_\lambda(\vec{x},\vec{p})\, b_\lambda(\vec{x},\vec{p}) = 1, \quad (8d)$$

$$\sum_\lambda \int d\vec{q}\, a^*_\lambda(\vec{x}-\vec{q})\, a_\lambda(\vec{x}-\vec{q}) = 1. \quad (8e)$$

The correct Weyl correspondence for the momentum and coordinate operator is then given by the prescription that the momentum operator $\vec{P}$ and coordinate operator $\vec{Q}$ be defined with the aid of the Wannier function and the Bloch function as

$$\vec{P}b_\lambda(\vec{x},\vec{p}) = \vec{p}b_\lambda(\vec{x},\vec{p}), \quad (9)$$

$$\vec{Q}a_\lambda(\vec{x}-\vec{q}) = \vec{q}a_\lambda(\vec{x}-\vec{q}), \quad (10)$$

and from this, the uncertainty relation[13]

$$[P_l, Q_m] = (\hbar/i)\,\delta_{lm} \quad (11)$$

follows in the formalism.

The above prescription is quite well known in solid-state theory.[14] Furthermore, any operator $A(\vec{P},\vec{Q})$ which is a function of $\vec{P}$ and $\vec{Q}$ can be written (generalized here for particles with spin)[8] as

$$A = \sum_{\lambda,\lambda'} \int d\vec{v}\, d\vec{u}\, \tilde{a}_{\lambda\lambda'}(\vec{u},\vec{v})\, e^{-(i/\hbar)(\vec{Q}\cdot\vec{u}+\vec{P}\cdot\vec{v})}\, \Omega_{\lambda\lambda'}, \quad (12)$$

where

$$\Omega_{\lambda\lambda'} = \int d\vec{p}\, b_\lambda(\vec{x},\vec{p})\, b^*_{\lambda'}(\vec{x},\vec{p}) = \int d\vec{q}\, a_\lambda(\vec{x}-\vec{q})\, a^*_{\lambda'}(\vec{x}-\vec{q}), \quad (13)$$

$$\tilde{a}_{\lambda\lambda'}(\vec{u},\vec{v}) = h^{-6}\int d\vec{p}\, d\vec{q}\, a_{\lambda\lambda'}(\vec{p},\vec{q})\, e^{(i/\hbar)(\vec{q}\cdot\vec{u}+\vec{p}\cdot\vec{v})}, \quad (14)$$

$$a_{\lambda\lambda'}(\vec{p},\vec{q}) = \int d\vec{v}\, e^{(i/\hbar)\vec{p}\cdot\vec{v}}\langle a_\lambda(\vec{x}-(\vec{q}-\tfrac{1}{2}\vec{v}))\, A\, a_{\lambda'}(\vec{x}-(\vec{q}+\tfrac{1}{2}\vec{v}))\rangle$$
$$= \int d\vec{u}\, e^{(i/\hbar)\vec{q}\cdot\vec{u}}\langle b_\lambda(\vec{x},\vec{p}+\tfrac{1}{2}\vec{u})A\, b_{\lambda'}(\vec{x},\vec{p}-\tfrac{1}{2}\vec{u})\rangle. \quad (15)$$

$a_{\lambda\lambda'}(\vec{p},\vec{q})$ is known as the Weyl transform of operator A. If we put $A = \mathcal{H}$ we find

$$h_{\lambda\lambda'}(\vec{p},\vec{q}) = E_{\lambda'}(\vec{p})\,\delta_{\lambda\lambda'}, \quad (16)$$

$$\tilde{h}_{\lambda\lambda'}(\vec{u},\vec{v}) = h^{-3}\,\delta(\vec{u})\,\delta_{\lambda\lambda'}\int d\vec{p}\, E_{\lambda'}(\vec{p})\, e^{(i/\hbar)\vec{p}\cdot\vec{v}}, \quad (17)$$

$$\mathcal{H} = \sum_\lambda E_\lambda(\vec{P})\,\Omega_{\lambda\lambda}. \quad (18)$$

The last line obtained using Eq. (12) is indeed a decomposition of the operator $\mathcal{H}$ into its invariant subspaces labeled by the band index λ. One can also easily see the effect of operating $\mathcal{H}$ on $a_\lambda(\vec{x}-\vec{q})$:

$$\mathcal{H}a_\lambda(\vec{x}-\vec{q}) = \int d\vec{q}'\, w_\lambda(\vec{q}-\vec{q}')\, a_\lambda(\vec{x}-\vec{q}'), \quad (19)$$

where

$$w_\lambda(\vec{v}) = \hbar^{-3}\int d\vec{p}\, E_\lambda(\vec{p})\, e^{-(i/\hbar)\vec{p}\cdot\vec{v}}$$

and only one band index is involved. Equation (19) is well known in solid-state theory.[14]

In the presence of a uniform magnetic field, magnetic Wannier Functions $A_\lambda(\vec{x},\vec{q})$ and magnetic Bloch functions $B_\lambda(\vec{x},\vec{p})$ exist.[14-16] This is proved by using symmetry arguments. The fundamental identities (a) to (e) in Eq. (8) also hold for these two basis states, which are related by the same unitary transformation of Eqs. (3) and (4). In general, these two basis functions are complete and span all the eigensolutions of the magnetic Hamiltonian belonging to a band index λ. Thus they are the most convenient set to use for magnetic problems since the Hamiltonian cannot couple magnetic Bloch functions and magnetic Wannier functions belonging to different bands.[14]

The even form of the Dirac Hamiltonian with magnetic field was first given by Case and later rederived by Erichsen.[10] We shall denote it here by $\mathcal{H}_B$:

$$\mathcal{H}_B = \beta\{m^2c^4 + [c\vec{P} - e\vec{A}(\vec{Q})]^2 - e\hbar c\vec{\sigma}\cdot\vec{B}\}^{1/2}, \quad (20)$$

where, as before,

$$\vec{P}B_\lambda(\vec{x},\vec{p}) = \vec{p}B_\lambda(\vec{x},\vec{p}), \quad (21)$$

$$\vec{Q}A_\lambda(\vec{x},\vec{q}) = \vec{q}A_\lambda(\vec{x},\vec{q}). \quad (22)$$

The result of the calculation using this Hamiltonian is not new. Therefore we will start with a Dirac Hamiltonian with the Pauli anomalous term.

The Dirac Hamiltonian which includes the coupling of the anomalous magnetic moment with the magnetic field is[8]

$$\mathcal{H} = \beta mc^2 + c\vec{\alpha}\cdot\vec{\Pi} - \beta\lambda'\mu_B\vec{\sigma}\cdot\vec{B}, \quad (23)$$

where $\vec{\Pi} = c\vec{P} - e\vec{A}(\vec{Q})$, $\lambda' = \frac{1}{2}(g-2)$, $\mu_B = e\hbar/2mc$, and the last (Pauli) term represents the coupling of the anomalous magnetic moment with the magnetic field. Equation (23) can easily be transformed into an even form by using the general expression for the canonical transformation, making the relativistic Hamiltonian by time-independent external fields even, given by Ericksen.[10] The result is

$$\mathcal{H}_B' = \beta(\mathcal{H}^2)^{1/2} = \beta[m^2c^4 + c^2\vec{\Pi}^2 - e\hbar c(1+\lambda')\vec{\sigma}\cdot\vec{B} + (e\hbar c\lambda'/mc^2)^2 B^2]^{1/2}. \quad (24)$$

The effect of operating the Hamiltonian on $A_\lambda(\vec{x},\vec{q})$ is very well known in solid-state theory.[14] This relationship may be written as

$$\mathcal{H}'_B A_\lambda(\vec{x},\vec{q}) = \int e^{(ie/\hbar c)\vec{A}(\vec{q})\cdot\vec{q}'}\, \tilde{E}_\lambda((\vec{q}-\vec{q}');B) \times A_\lambda(\vec{x},\vec{q}')\, d\vec{q}' \;, \tag{25}$$

where $\vec{A}(\vec{q}) = \frac{1}{2}\vec{B}\times\vec{q}$. The Weyl transform of the Hamiltonian operator is easily calculated using Eq. (25) and the first line of Eq. (15). The result is

$$h'_B(\vec{p},\vec{q})_{\lambda\lambda'} = \int d\vec{v} \exp\left[\frac{i}{\hbar}\left(\vec{p} - \frac{e}{c}\vec{A}(\vec{q})\right)\cdot\vec{v}\right]\tilde{E}_\lambda(\vec{v};B)\,\delta_{\lambda\lambda'}$$
$$\equiv E_\lambda(\vec{p} - (e/c)\vec{A}(\vec{q});B)\,\delta_{\lambda\lambda'} \tag{26}$$

where, as can be seen from the last line of Eq. (26), $\vec{p}$ and $\vec{q}$ enter in the canonical conjugate momentum only. Using Eq. (14) we obtain

$$h'_B(\vec{u},\vec{v})_{\lambda\lambda'} = \delta(\vec{u} - (e/c)\vec{A}(\vec{v}))\,\delta_{\lambda\lambda'} \times h^{-3}\int d\vec{K}\, e^{(i/\hbar)\vec{K}\cdot\vec{v}} E_\lambda(\vec{K};B)$$
$$= \delta(\vec{u} - (e/c)\vec{A}(\vec{v}))\,\delta_{\lambda\lambda'}\,\tilde{E}_\lambda(-\vec{v};B) \;, \tag{27}$$

and this is substituted in Eq. (12); the result is

$$\mathcal{H}'_B = h^{-3}\sum_\lambda \Omega_{\lambda\lambda}\int d\vec{K}d\vec{v} \times \exp\left\{-\frac{i}{\hbar}\left[\left(\vec{P} - \frac{e}{c}\vec{A}(\vec{Q})\right) - \vec{K}\right]\cdot\vec{v}\right\} E_\lambda(\vec{K};B) \;. \tag{28}$$

We note that the integral expression in Eq. (28) represents the one-band magnetic Hamiltonian and granting that the components of $\vec{\Pi}$ commute, this is equal to the replacement of $\vec{K}$ by $\vec{\Pi}$ in $E(\vec{K};B)$. If, moreover, $E(\vec{K};B)$ is made equal to the band-energy function in the absence of the field, i.e., $(m^2c^4 + c^2K^2)^{1/2}$, then we have the Hamiltonian that Onsager[17] first postulated for magnetic problems. As we will see later, besides the noncommutivity of the components of $\vec{\Pi}$, $E(\vec{K};B)$ has $(m^2c^4+c^2K^2)^{1/2}$ only as a zero-order term in its expansion in terms of B. It is very interesting to note, however, that the spectrum of the magnetic Hamiltonian in Eq. (28) [the same as in Eq. (24)] and the Onsager Hamiltonian look very identical except that the former is shifted from the latter with a field-dependent shift. This shift is very important in the theory of the total magnetic susceptibility. Equation (28) can be viewed as an exact mathematical prescription for the approximate and intuitive Onsager relation in solid-state theory.[17] One can easily verify Eq. (26) by inserting the expression for $\mathcal{H}'_B$ [in Eq. (28)] into the first line of Eq. (15) using Eq. (22) and the identity

$$e^{-(i/\hbar)\vec{P}\cdot\vec{v}}A_\lambda(\vec{x},\vec{q}+\tfrac{1}{2}\vec{V}) = A_\lambda(\vec{x},\vec{q}+\tfrac{1}{2}\vec{V}+\vec{v}) \;. \tag{29}$$

[The validity of this identity may be verified by multiplication with $B^*_\lambda(\vec{x},\vec{p})$ and the use of Eqs. (21) and (22) and the corresponding relation, Eq. (8c).]

III. DERIVATION OF THE SUSCEPTIBILITY χ

The low-field susceptibility is determined from the free energy by the relation

$$\chi = \lim_{B\to 0} -\frac{1}{V}\frac{\partial^2 F}{\partial B^2} \;, \tag{30}$$

where

$$F = N\mu + \mathrm{Tr}\, F(\mathcal{H}) \;, \tag{31}$$

$$F(\mathcal{H}) = -k_B T \ln\{1 + \exp[(\mu - \mathcal{H})/k_B T]\} \;. \tag{32}$$

As suggested by Blount,[18] a proper expansion of $F(\mathcal{H})$ in powers of $\mathcal{H}$ can be made by the use of the Laplace transform of $F(\mathcal{H})$. Thus

$$F(\mathcal{H}) = \int_{c-i\infty}^{c+i\infty} \varphi(s)\, e^{s\mathcal{H}} ds \;, \tag{33}$$

and the proper convergent expansion is

$$e^{s\mathcal{H}} = \sum_n \frac{s^n}{n!}\mathcal{H}^n \;. \tag{34}$$

Our problem is reduced to deriving the expression for $\mathrm{Tr}\mathcal{H}^n$. For this purpose we make use of the formula for the trace of the product of two operators given by Leaf,[7] which can easily be generalized for particles with spin[8]:

$$\mathrm{Tr}AB = h^{-3}\sum_{s,\lambda}\int d\vec{p}d\vec{q}\, a_{s\lambda}(\vec{p},\vec{q})\, b_{\lambda s}(\vec{p},\vec{q}) \;, \tag{35}$$

where

$$a_{s\lambda}(\vec{p},\vec{q}) = \int d\vec{v}\, e^{(i/\hbar)\vec{p}\cdot\vec{v}}\langle\vec{q} - \tfrac{1}{2}\vec{v}, s|A|\vec{q}+\tfrac{1}{2}\vec{v},\lambda\rangle \;.$$

The states $|\vec{q},s\rangle$ represent the magnetic Wannier function in the present case. We also need the following multiplication rule[8]: If $AB = C$, then

$$C_{s\lambda}(p,q) = \exp\left[\frac{\hbar}{2i}\left(\frac{\partial^{(a)}}{\partial\vec{p}}\cdot\frac{\partial^{(b)}}{\partial\vec{q}} - \frac{\partial^{(a)}}{\partial\vec{q}}\cdot\frac{\partial^{(b)}}{\partial\vec{p}}\right)\right]\sum_\sigma a_{s\sigma}(\vec{p},\vec{q})\, b_{\sigma\lambda}(\vec{p},\vec{q}) \;, \tag{36}$$

where the superscripts (*a*) and (*b*) indicate the quantity to be operated on the right. We can now evaluate the trace of any powers of A. This can easily be shown to be

$$\mathrm{Tr}A^n = h^{-3}\int d\vec{p}\,d\vec{q}\,\exp\left\{\frac{\hbar}{2i}\left[\sum_{\substack{j,k=1\\(j<k)}}^{n-1}\left(\frac{\partial^{(j)}}{\partial\vec{p}}\cdot\frac{\partial^{(k)}}{\partial\vec{q}}-\frac{\partial^{(j)}}{\partial\vec{q}}\cdot\frac{\partial^{(k)}}{\partial\vec{p}}\right)\right]\right\}\prod_{\substack{l=1\\(\sigma_{n+1}=\sigma_1)}}^{n} a^{(l)}_{\sigma_l,\sigma_{l+1}}(\vec{p},\vec{q}), \tag{37}$$

where the Einstein summation convention for band indices σ_l is understood. Putting $A=\mathcal{H}$, using Eq. (26) and since $\vec{p}$ and $\vec{q}$ occur in the canonical conjugate momentum only, differentiation with respect to $\vec{q}$ can be written in terms of differentiation with respect to components of $\vec{p}$. By changing the variable $\vec{p}$ to $\vec{\kappa}$ with Jacobian unity, we may write

$$\mathrm{Tr}\,\mathcal{H}^n = \sum_\lambda \int d\vec{\kappa}\,d\vec{q}\,\exp\left\{\frac{ie\hbar B}{2c}\left[\sum_{\substack{j,k=1\\(j<k)}}^{n-1}\left(\frac{\partial^{(j)}}{\partial\kappa_x}\frac{\partial^{(k)}}{\partial\kappa_y}-\frac{\partial^{(j)}}{\partial\kappa_y}\frac{\partial^{(k)}}{\partial\kappa_x}\right)\right]\right\}E^{(1)}_\lambda(\vec{\kappa};B)\,E^{(2)}_\lambda(\vec{\kappa};B)\cdots E^{(n)}_\lambda(\vec{\kappa},B), \tag{38}$$

where

$$\vec{\kappa}=\vec{p}-(e/c)\vec{A}(\vec{q}),\qquad \vec{A}(\vec{q})=\tfrac{1}{2}\vec{B}\times\vec{q},\qquad \vec{B}=\vec{B}(\vec{z}/|\vec{z}|).$$

Note that by using the magnetic Wannier function, matrix multiplication in front of the exponential is reduced to scalar multiplication. We are interested in the expression of $\mathrm{Tr}F(\mathcal{H})$ to second order in the magnetic field. We therefore expand the exponential operator in powers of B up to second order and obtain

$$\mathrm{Tr}\mathcal{H}^n=\sum_\lambda\int d\vec{\kappa}\,d\vec{q}\left[1-\frac{1}{8}\left(\frac{e\hbar B}{c}\right)^2\left(\sum_{\substack{j,k=1\\(j<k)}}^{n-1}\frac{\partial^{(j)}}{\partial\kappa_x}\frac{\partial^{(k)}}{\partial\kappa_y}-\frac{\partial^{(j)}}{\partial\kappa_y}\frac{\partial^{(k)}}{\partial\kappa_x}\right)^2\right]E^{(1)}_\lambda(\vec{\kappa},B)\,E^{(2)}_\lambda(\vec{\kappa},B)\cdots E^{(n)}_\lambda(\vec{\kappa},B), \tag{39}$$

where we have left out of the expansion terms of first order in B since they do not contribute to it. The square of the summation of the B^2 term may be simplified by writing it as

$$\sum_{\substack{j,k=1\\j',k'=1\\j<k,\,j'<k'}}^{n-1}\left(\frac{\partial^{(j)}}{\partial\kappa_x}\frac{\partial^{(k)}}{\partial\kappa_y}\frac{\partial^{(j')}}{\partial\kappa_x}\frac{\partial^{(k')}}{\partial\kappa_y}+\frac{\partial^{(j)}}{\partial\kappa_y}\frac{\partial^{(k)}}{\partial\kappa_x}\frac{\partial^{(j')}}{\partial\kappa_y}\frac{\partial^{(k')}}{\partial\kappa_x}\right)-\left(\frac{\partial^{(j)}}{\partial\kappa_x}\frac{\partial^{(k)}}{\partial\kappa_y}\frac{\partial^{(j')}}{\partial\kappa_y}\frac{\partial^{(k')}}{\partial\kappa_x}+\frac{\partial^{(j)}}{\partial\kappa_y}\frac{\partial^{(k)}}{\partial\kappa_x}\frac{\partial^{(j')}}{\partial\kappa_x}\frac{\partial^{(k')}}{\partial\kappa_y}\right). \tag{40}$$

Noting that $E^{(i)}_\lambda(\vec{\kappa};B)$ are equal for all i, the nonzero contributions come from terms of the following types:

Type		*Number of terms*
(i) (a)	$j=j',\ k\neq k'$,	$\frac{1}{6}(n-2)(n-1)(2n-3)-\frac{1}{2}(n-2)(n-1)$;
(b)	$k=k',\ j\neq j'$,	$\frac{1}{6}(n-2)(n-1)(2n-3)-\frac{1}{2}(n-2)(n-1)$;
(ii) (a)	$j=k',\ j'\neq k$,	$\frac{1}{6}(n-2)(n-2)n-\frac{1}{2}(n-2)(n-1)$;
(b)	$j'=k,\ j\neq k'$,	$\frac{1}{6}(n-1)(n-2)n-\frac{1}{2}(n-2)(n-1)$;
(iii)	$j=j',\ k=k'$,	$(n-1)(n-2)$.

By combining these terms we find type (ii) partially canceling type (i) and we end up with $\mathrm{Tr}\mathcal{H}^n$, up to second order in B in the exponential expansion, as

$$\begin{aligned}\mathrm{Tr}\mathcal{H}^n=h^{-3}\sum_\lambda\int d\vec{\kappa}\,d\vec{q}\,\Bigg\{&[E_\lambda(\kappa,B)]^n-\frac{1}{8}\left(\frac{e\hbar B}{c}\right)^2(n-1)(n-2)[E_\lambda(\kappa,B)]^{n-2}\left[\frac{\partial^2E_\lambda}{\partial\kappa_x^2}\frac{\partial^2E_\lambda}{\partial\kappa_y^2}-\left(\frac{\partial^2E_\lambda}{\partial\kappa_x\partial\kappa_y}\right)^2\right]\\&-\frac{1}{24}\left(\frac{e\hbar B}{c}\right)(n-1)(n-2)(n-3)[E_\lambda(\kappa,B)]^{n-3}\\&\times\left[\frac{\partial^2E_\lambda}{\partial\kappa_x^2}\left(\frac{\partial E_\lambda}{\partial\kappa_y}\right)^2+\frac{\partial^2E_\lambda}{\partial\kappa_y^2}\left(\frac{\partial E_\lambda}{\partial\kappa_x}\right)^2-2\frac{\partial^2E_\lambda}{\partial\kappa_x\partial\kappa_y}\frac{\partial E_\lambda}{\partial\kappa_y}\frac{\partial E_\lambda}{\partial\kappa_x}\right]\Bigg\}.\end{aligned} \tag{41}$$

Integration by parts in the $\vec{\kappa}$ integration permits the reduction of the last term to the form of the second term plus an integrated-out part which, however, upon substituting Eqs. (34) and (33) does not contribute to $\mathrm{Tr}F(\mathcal{H})$. This is obvious since the integrated part involved a very large value of the components of $\vec{\kappa}$. The final result for $\mathrm{Tr}\mathcal{H}^n$ is

$$\mathrm{Tr}\mathcal{H}^n=\frac{1}{(2\pi)^3}\sum\int d\vec{k}\,d\vec{q}\left\{[E_\lambda(k,B)]^n-\frac{1}{24}n(n-1)[E_\lambda(k,B)]^{n-2}\left(\frac{eB}{\hbar c}\right)^2\left[\frac{\partial^2E_\lambda}{\partial k_x{}^2}\,\frac{\partial^2E_\lambda}{\partial k_y{}^2}-\left(\frac{\partial E_\lambda}{\partial k_x\partial k_y}\right)^2\right]\right\}, \tag{42}$$

where we have changed from momentum variable $\vec{\kappa}$ to wave vector $\vec{k}$. This result is exactly the result of Wannier and Upadhyaya[19] for band electrons in solids. Compared with their derivation, we have here at no point in our derivation made use of any kind of periodicity in $\vec{k}$ space or $\vec{\kappa}$ space. Upon substituting in Eq. (33), we have

$$\mathrm{Tr}F(\mathcal{H})=\frac{1}{(2\pi)^3}\sum_\lambda\int d\vec{k}\,d\vec{q}\left\{F(E_\lambda(\vec{k},B))-\frac{1}{24}\left(\frac{eB}{\hbar c}\right)^2\frac{\partial^2F(E_\lambda(\vec{k},B))}{\partial E_\lambda^2}\left[\frac{\partial^2E_\lambda}{\partial k_x^2}\,\frac{\partial^2E_\lambda}{\partial k_y^2}-\left(\frac{\partial E_\lambda}{\partial k_x\partial k_y}\right)^2\right]\right\}. \tag{43}$$

Writing

$$E_\lambda(\vec{k},B)=E_\lambda(\vec{k},0)+BE_\lambda^{(1)}(\vec{k})+B^2E_\lambda^{(2)}(\vec{k})+\cdots, \tag{44}$$

and dropping the dependence of $E_\lambda(\vec{k};B)$ on B in the second term, the resulting expression for χ is

$$\chi=-\frac{1}{48\pi^3}\frac{e^2}{\hbar^2c^2}\sum_\lambda\int d\vec{k}\left\{\frac{\partial^2E_\lambda(\vec{k},0)}{\partial k_x^2}\,\frac{\partial^2E_\lambda(\vec{k},0)}{\partial k_y^2}-\left(\frac{\partial^2E_\lambda(\vec{k},0)}{\partial k_x\partial k_y}\right)^2\right\}\frac{\partial f(E_\lambda)}{\partial E_\lambda}$$
$$-\frac{1}{(2\pi)^3}\sum\int d\vec{k}[E_\lambda^{(1)}(\vec{k})]^2\frac{\partial f(E_\lambda)}{\partial E_\lambda}-\frac{1}{(2\pi)^3}\sum_\lambda\int d\vec{k}\,2E_\lambda^{(2)}(\vec{k})f(E_\lambda), \tag{45}$$

where $f(x)$ is the Fermi-Dirac distribution function. The first term is the well-known Landau-Peierls formula,[20] the second is the Pauli spin paramagnetism,[21] and the last, but quite important, term is due to the second-order effect of spin and, as we shall see, to the inherent spread of the electron.

IV. FUNCTION $E_\lambda(\vec{p}-(e/c)\vec{A}(\vec{q});B)$

The function $E_\lambda(\vec{p}-(e/c)\vec{A}(\vec{q});B)$ is the Weyl transform of $\beta(\mathcal{H}^2)^{1/2}$, where the matrix β served to designate the four bands. From Eqs. (44) and (45), in order to calculate χ we only need the knowledge of $E_\lambda(\vec{p}-(e/c)\vec{A}(\vec{q});B)$ in Eq. (45) as an expansion up to second order in the coupling constant e and after a change of variable in the manner used in deriving Eq. (42) from Eq. (37) [this is effected by setting $\vec{A}(\vec{q})=0$, $\vec{p}=\hbar\vec{k}$ in the expansion], we obtain the expression of Eq. (44) where the dependence in the field B is beyond the vector potential. The expansion is done in the Appendix and after setting $\vec{A}(\vec{q})=0$, $\vec{p}=\hbar\vec{k}$ the result is Eq. (44) in its explicit form,

$$E_\lambda(\vec{k},B)=\beta\left\{E(\vec{k})-\frac{e\hbar c}{2E(\vec{k})}(1+\lambda')\vec{\sigma}\cdot\vec{B}-\frac{[e\hbar c(1+\lambda')\vec{\sigma}\cdot\vec{B}]^2}{8E^3(\vec{k})}+\frac{(e\hbar c)^2}{8E^5(\vec{k})}\left[\epsilon^2+\lambda'^2\left(\frac{E^4(\vec{k})}{m^2c^4}\right)\right]B^2+\cdots\right\}, \tag{46}$$

where

$$\epsilon^2=m^2c^4+c^2\hbar^2k_z^2,\quad E(\vec{k})=(c^2\hbar^2\vec{k}^2+m^2c^4)^{1/2}.$$

We call $E_\lambda(\vec{k},B)$ the renormalized dispersion relation of a relativistic Dirac electron gas. The first term is the dispersion relation in the absence of B. The second term is due to the first-order effect of the spin and the anomalous magnetic moment, the third term to the second-order effect of the spin and the anomalous magnetic moment, and the last term to the combined effect of the spread of the electron associated with the normal spin and the spread associated with the anomalous magnetic moment. In Eq. (46) we shall see that, for the positive energy states, the first term gives the orbital diamagnetism, the second and third terms give the spin and the anomalous magnetic moment paramagnetism, and the last term gives an atomic type of diamagnetism due to the spread of the electron charge. For the case $\lambda'=0$ (Pauli anomalous term neglected) the last term can in fact be written in the form

$$-\frac{1}{4E}e^2\left[\hbar\frac{\partial}{\partial p_i}\left(\frac{cp_k}{E}\right)\right]\left[\hbar\frac{\partial}{\partial p_j}\left(\frac{cp_l}{E}\right)\right]\frac{\partial A_k}{\partial q_j}\frac{\partial A_l}{\partial q_i}, \quad (47)$$

and appear to arise from an induced magnetic moment due to the spread of the electron, similar to the standard atomic diamagnetism.[22] More will be said on the spread terms in Sec. V.

For the case $\lambda'=0$ the resulting Hamiltonian in Eq. (23) is equivalent to the $\vec{k}\cdot\vec{p}$ Hamiltonian near the L point of the Brillouin zone of bismuth. For the rest of this section we will consider the case $\lambda'=0$.

In solid-state physics one usually defines the cyclotron mass,[21] which is a property of an orbit in momentum space, as

$$m_c=\frac{1}{2\pi}\frac{\partial A}{\partial E_\lambda}, \quad (48)$$

where the A's are the cross-sectional areas, perpendicular to the magnetic field, of spheres in momentum space bounded by constant energy surfaces E_λ. Writing the magnetic moment due to the first-order effect of spin as

$$E_\lambda^1(\vec{k})=\beta(m/m_s)\mu_B=\tfrac{1}{2}mg_{\text{eff}}\,\mu_B, \quad (49)$$

where $\frac{1}{2}g_{\text{eff}}=1/m_s$ is the energy-dependent g factor of a relativistic Dirac electron,[23] then from Eqs. (44)–(46) one can easily show that $m_s=m_c$. This implies, for finite magnetic field, the equality between the energy-dependent spacing of the orbital energy levels and the spin energy splitting.[12] This situation is similar to that of the electrons at the L point of the Brillouin zone of bismuth.[24]

V. SPREAD OF THE ELECTRON

Until now the only known manifestation of the inherent spread of an electron is in the appearance of the Darwin term[25] in the nonrelativistic Hamiltonian obtained by successive unitary transformations. The spatial extension of this spread is well known and is about the Compton wavelength of the electron. For the case $\lambda'=0$ we shall show that the same amount of spread is responsible for the diamagnetic contribution to χ. Radiative corrections in quantum electrodynamics have shown that the electron behaves as if it had a charge distribution associated with the anomalous magnetic moment.[26] Our calculation of χ for the Dirac Hamiltonian with the Pauli anomalous term clearly shows the existence of a spread associated with the anomalous magnetic moment and its atomic diamagnetism type of contribution to χ.

The magnetic moment due to the spread of an electron from Eqs. (44)–(46) is

$$M=-\left[2E_\lambda^{(2)}(\vec{k})B\right]_{\text{sp}}=-\frac{(e\hbar c)^2}{4E_\lambda^5(\vec{k})}\left[\epsilon^2+\lambda'^2\left(\frac{E_\lambda^2(\vec{k})}{mc^2}\right)^2\right]B. \quad (50)$$

The induced magnetic moment due to a distribution of electric charge is[27]

$$M=-Be^2\langle r^2\rangle/4mc^2, \quad (51)$$

where $\langle r^2\rangle$ is the average of the square of the spatial spread of the distribution normal to the magnetic field. Equating Eqs. (50) with (51) we obtain

$$\langle r^2\rangle=\frac{mc^2(\hbar c)^2}{[E_\lambda(\vec{k})]^5}\left[\epsilon^2+\left(\frac{\lambda' E_\lambda^2(\vec{k})}{mc^2}\right)^2\right]. \quad (52)$$

For positive energy states $E_\lambda(\vec{k})=+(c^2\hbar^2k^2+m^2c^4)^{1/2}$ and in the nonrelativistic limit, Eq. (52) reduces to

$$\langle r^2\rangle=(1+\lambda'^2)(\hbar/mc)^2, \quad (53)$$

and thus the effective spread of the electron at rest and for $\lambda'=0$ is precisely equal to the Compton wavelength. Exactly the same expression for $\lambda'=0$ can be obtained by taking the nonrelativistic limit of Eq. (47) and comparing the result with the $\vec{A}^2$ term in the nonrelativistic Hamiltonian for an atom in external magnetic field. Equation (52) is the explicit expression of the effective spread perpendicular to the magnetic field of a moving electron. However, owing to the change of sign of $E_\lambda(\vec{k})$ for negative energy states, the above physical interpretation of the last term of Eq. (46) does not hold for the negative-energy-states electron, but can be applied to the holes or positrons in Dirac theory.

VI. EXPRESSION FOR χ

Let us rewrite Eq. (45) as a sum of terms

$$\chi=\chi_{LP}+\chi_P+\chi_{\text{sp}}+\chi_g, \quad (54)$$

where χ_{LP} and χ_P are the first and second terms of Eq. (45), the sum of χ_{sp} and χ_g is the last term of Eq. (45), χ_g is the term arising from the second-order effect of spin and the anomalous magnetic moment, and χ_{sp} is due to the spread of the electron charge. In performing the integration in Eq. (45) using the terms of the expansion in Eq. (46), we make a change of variables and write

$$(\hbar c)^3 \int d\vec{k} = \int_{-\infty}^{\infty} \int_0^{2\pi} \int_\epsilon^\infty d\eta\, d\phi\, E(\vec{k})\, dE(\vec{k}) , \quad (55)$$

where $\eta = \hbar c k_z$. We thus obtain for the positive energy states, after summing over band indices,

$$\chi_{LP} = \frac{1}{24\pi^2}\left(\frac{e^2}{\hbar c}\right)\int_{-\infty}^{\infty} d\eta \int_\epsilon^\infty \frac{\epsilon^2}{E^3}\frac{\partial f(E)}{\partial E}\, dE , \quad (56)$$

$$\chi_P = \frac{-(1+\lambda')^2}{8\pi^2}\left(\frac{e^2}{\hbar c}\right)\int_{-\infty}^{\infty} d\eta \int_\epsilon^\infty \frac{1}{E}\frac{\partial f(E)}{\partial E}\, dE , \quad (57)$$

$$\chi_{sp} = -\frac{1}{8\pi^2}\left(\frac{e^2}{\hbar c}\right)\int_{-\infty}^{\infty} d\eta \int_\epsilon^\infty \left[\frac{\epsilon^2}{E^4} + \left(\frac{\lambda'}{mc^2}\right)^2\right] f(E)\, dE , \quad (58)$$

$$\chi_g = \frac{(1+\lambda')^2}{8\pi^2}\left(\frac{e^2}{\hbar c}\right)\int_{-\infty}^{\infty} d\eta \int_\epsilon^\infty \frac{f(E)}{E^2}\, dE . \quad (59)$$

The sum of χ_{LP} and χ_{sp} and the sum of χ_P and χ_g give the diamagnetism and paramagnetism, respectively, of a relativistic Dirac electron gas. By using partial integration with respect to E, we obtain

$$\chi_{LP} + \chi_{sp} = -\frac{1}{(2\pi)^2}\left(\frac{e^2}{\hbar c}\right)\frac{1}{3}\int_0^\infty d\eta\, \frac{f(\epsilon)}{\epsilon} - \frac{1}{8\pi^2}\left(\frac{e^2}{\hbar c}\right)\left(\frac{\lambda'}{mc^2}\right)^2 \int_0^\infty d\eta\, G(\epsilon-\mu) , \quad (60)$$

where

$$G(\epsilon-\mu) = k_B T \ln\{1+\exp[-(\epsilon-\mu)/k_B T]\} = \int_\epsilon^\infty f(E)\, dE ;$$

$$\chi_P + \chi_g = \frac{(1+\lambda')^2}{(2\pi)^2}\left(\frac{e^2}{\hbar c}\right)\int_0^\infty d\eta\, \frac{f(\epsilon)}{\epsilon} ; \quad (61)$$

and therefore the total χ is

$$\chi = \left(\frac{1}{2\pi}\right)^2 \left(\frac{e^2}{\hbar c}\right)\left[(1+\lambda')^2 - \tfrac{1}{3}\right]\int_0^\infty d\eta\, \frac{f(\epsilon)}{\epsilon} - \frac{1}{8\pi^2}\left(\frac{e^2}{\hbar c}\right)\left(\frac{\lambda'}{mc^2}\right)^2 \int_0^\infty d\eta\, G(\epsilon-\mu) . \quad (62)$$

For the case $\lambda' = 0$, the above result reduces to that of Rukhadze and Silin[6] obtained by a different method. Also for this case we see in Eqs. (60) and (61) that the total diamagnetism is always $-\frac{1}{3}$ of the total paramagnetism for all energy ranges, whether relativistic or nonrelativistic.

For $T = 0$, Table I illustrates the relative importance of the four terms in Eq. (54) in the very-low and very-high-electron-density limits. We see that in a very-low-density limit $\chi \approx \chi_{LP} + \chi_P$; i.e., in this limit the diamagnetism is wholly orbital and the paramagnetism wholly due to the Pauli spin. This is, of course, very well known. On the other hand, in the very-high-density limit $\chi \approx \chi_{sp} + \chi_g$; i.e., in this limit the diamagnetism is almost wholly due to the smearing of the electron charge and the paramagnetism is almost wholly due to the second-order effect of spin. In this limit χ_{LP} and χ_P assume a constant value (at about $\eta_F/\Delta \approx 1$) whereas χ_{sp} and χ_g increase logarithmically with increasing electron density. The spread associated with the anomalous magnetic moment has a diamagnetic contribution that goes as a $\frac{2}{3}$ power of electron density. Thus it is concluded that the dominating physical processes involved in the two extreme limits are different.

Using partial integration with respect to E and using Eq. (55) in the counting of states, Eq. (62) yields the Curie-Langevin law for a classical gas at high temperatures and low density (nonrelativistic Boltzman electron gas)

$$\chi = \left[(1+\lambda')^2 - \tfrac{1}{3}\right](e\hbar/2mc)^2 (n/k_B T) , \quad (63)$$

where n is the electron density.

For $k_B T \gg mc^2$ we must take into account the formation of electron-positron pairs. The formalism we have used also enable us to calculate the magnetic susceptibility of the electron in the negative energy states. The result is Eq. (62) with opposite sign and with $f(\epsilon)$ and $G(\epsilon-\mu)$ replaced by $f(-\epsilon)$ and ∞, respectively. The physically meaningful contribution to the total susceptibility comes from the positrons or holes in the negative energy states (the contribution of the infinite sea of negative states of the electron is infinite and this we assume to be subtracted out). The contributions of the holes is obtained by replacement of $f(\epsilon)$ and $G(\epsilon-\mu)$ in Eq. (62) by $1-f(-\epsilon)$ and $G(\epsilon+\mu)$, respectively. Thus if electron-positron pairs are taken into account we have

$$\chi = \left(\frac{1}{2\pi}\right)^2\left(\frac{e^2}{\hbar c}\right)\left[(1+\lambda')^2 - \tfrac{1}{3}\right]\int_0^\infty d\eta\, \frac{f(\epsilon) + [1-f(-\epsilon)]}{\epsilon} - \left(\frac{\lambda'}{2\pi}\right)^2\left(\frac{e^2}{\hbar c}\right)\left(\frac{1}{mc^2}\right)^2\int_0^\infty d\eta\, [G(\epsilon-\mu) + G(\epsilon+\mu)] , \quad (64)$$

for the thermodynamic equilibrium state of the system.

VII. CONCLUDING REMARKS

We have given a fairly simple but rigorous derivation of the paramagnetic susceptibility of a relativistic Dirac electron gas. The derivation make use of an alternative formulation of quantum mechanics as a probabilistic theory in terms of the Weyl transform and the Wigner function. The use of the Weyl transform in nonrelativistic quantum dynamics has been clarified by Leaf.[7] In this paper we have formulated a very useful application of the Weyl transform in relativistic quantum dynamics in terms of a complete set of localized

TABLE I. Relative importance of the terms that make up χ, where n = electron density, $k_F=(3\pi^2 n)^{1/3}$, $\eta_F=\hbar c k_F$, $E_F=(\Delta^2+\eta_F^2)^{1/2}$.

$T=0$	Formula	Nonrelativistic	Ultrarelativistic
χ_{LP}	$-\frac{1}{12\pi^2}\left(\frac{e^2}{\hbar c}\right)\frac{1}{E_F^3}\left(\frac{\eta_F^3}{3}+\Delta^2\eta_F\right)$	$-\frac{1}{12\pi^2}\frac{e^2}{mc^2}k_F$	$-\frac{1}{12\pi^2}\left(\frac{e^2}{\hbar c}\right)\frac{1}{3}$
χ_P	$\frac{1}{4\pi^2}(1+\lambda')^2\left(\frac{e^2}{\hbar c}\right)\frac{\eta_F}{E_F}$	$\frac{1}{4\pi^2}(1+\lambda')^2\frac{e^2}{mc^2}k_F$	$\frac{1}{4\pi^2}(1+\lambda')^2\left(\frac{e^2}{\hbar c}\right)$
χ_{sp}	$-\frac{1}{12\pi^2}\left(\frac{e^2}{\hbar c}\right)\sinh^{-1}\frac{\eta_F}{\Delta}-\chi_{LP}$ $-\frac{\lambda'^2}{4\pi^2}\left(\frac{e^2}{\hbar c}\right)\left(\frac{\eta_F E_F}{2\Delta^2}-\frac{1}{2}\sinh^{-1}\frac{\eta_F}{\Delta}\right)$	~ 0	$-\frac{1}{12\pi^2}\left(\frac{e^2}{\hbar c}\right)\left(\ln\frac{2\eta_F}{\Delta}-\frac{1}{3}\right)$ $-\frac{\lambda'^2}{4\pi^2}\left(\frac{e^2}{\hbar c}\right)\left(\frac{\eta_F^2}{2\Delta^2}-\frac{1}{2}\ln\frac{2\eta_F}{\Delta}\right)$
χ_g	$\frac{(1+\lambda')^2}{4\pi^2}\left(\frac{e^2}{\hbar c}\right)\left(\sinh^{-1}\frac{\eta_F}{\Delta}-\frac{\eta_F}{E_F}\right)$	~ 0	$\frac{(1+\lambda')^2}{4\pi^2}\left(\frac{e^2}{\hbar c}\right)\left(\ln\frac{2\eta_F}{\Delta}-1\right)$

functions labeled by a band index λ that exist even in the presence of uniform magnetic fields. The first term in χ, which is the Landau-Peierls formula, is explicitly shown to arise from symmetry arguments (since symmetry arguments[15] for the existence of relativistic magnetic Wannier and Bloch functions labeled by a band index λ break down for space- and time-varying magnetic field, the first term in χ is really due to magnetostatics) and the exact form of the Hamiltonian is therefore not essential. Thus it is applicable in quasi-particle formulation of many-body problems.[28] The last three terms in Eq. (46) depend on our exact knowledge of the Dirac Hamiltonian with a magnetic field in even form.

Perhaps what can be claimed as a new result of this paper is our expression for χ for a relativistic Dirac electron gas which includes the effects of the anomalous magnetic moment. We have also given an explicit expression for χ that allows the formation of electron-positron pairs in a system at thermodynamic equilibrium. Moreover, we have shed light on the dynamical response of a relativistic Dirac electron gas in an external magnetic field and have shown evidence that different physical processes dominate in the very-low-density limit as compared to that in the very-high-electron-density limit.

A similar formula for χ, Eq. (45), holds in the band theory of solids. In the specialized situation encountered in bismuth, the same expression for χ, Eq. (62) with $\lambda'=0$, holds with only a change in scale factor.[29] The reason for this is that the $\vec{k}\cdot\vec{p}$ Hamiltonian based on the two-band model for the energy-band structure near the symmetry point L of the Brillouin zone of bismuth is equivalent to a Dirac Hamiltonian with a scaled canonical conjugate momentum.[7,29]

In bismuth, with the effective cyclotron mass substituted in Eq. (51) and using the appropriate expression corresponding to Eq. (50) with $\lambda'=0$, the Bloch-electron spread at the electron valley, between valence and conduction band, is about 1000 Å.[29] This agrees with the order of the estimate given by Blount[9] for the minimum spread of the wave packet for Bloch electrons in bismuth.

It is hoped that the result and the method of derivation presented here will shed more light on the complicated and sometimes heuristic formalism of the dynamics of Bloch electrons.[1,9,14] The formalism used here is similar to a unified version of Blount's mixed representation[9] and the Wannier formalism[14] of the dynamics of band electrons in solid-state theory. A unified Blount-Wannier representation has not been explicitly used in solid-state physics although Roth's[1] formalism and use of a multiplication rule is closer to it; Roth did not make use of the existence of the complete set of magnetic Wannier functions and magnetic Bloch functions as basis states in deriving the magnetic susceptibility of Bloch electrons. Wannier and Upadhyaya[1] made use of them on the same problem in a different method as compared to that of Roth. Thus a similar formalism to the one used in this paper is not quite realized in solid-state physics and the method used here is practically unknown in quantum electrodynamics. One of the results of the formalism used here is an exact prescription of the Onsager principle given by Eq. (28).

ACKNOWLEDGMENTS

The author is indebted to Dr. L. G. Suttorp for some valuable discussions and for pointing out the derivation presented in the Appendix. He would also like to thank Dr. U. N. Upadhyaya for some helpful discussions, Professor S. Lundqvist for his critical reading of the manuscript, and Professor Abdus Salam and Professor P. Budini, as well as the International Atomic Energy Agency and UNESCO, for hospitality at the International Centre for Theoretical Physics, Trieste. The work was done while the author served as a Senior Scientist in the science pool of the National Science Development Board, Republic of the Philippines.

APPENDIX: WEYL TRANSFORM OF THE HAMILTONIAN OF A DIRAC PARTICLE IN A HOMOGENEOUS MAGNETIC FIELD

The Dirac Hamiltonian for an electron in a magnetic field is

$$\mathcal{H}_{op} = \vec{\alpha}\cdot\vec{\Pi}_{op} + \beta mc^2 - \tfrac{1}{2}(g-2)\mu_B\beta\vec{\sigma}\cdot\vec{B}\,, \tag{A1}$$

where

$$\vec{\Pi}_{op} = c\vec{P}_{op} - e\vec{A}(\vec{Q}_{op}),\quad \mu_B = e\hbar/2mc\,, \tag{A2}$$

and the last (Pauli) term represents the coupling of the anomalous magnetic moment with the magnetic field. Then

$$(\mathcal{H}_{op})^2 = \vec{\Pi}^2_{op} + m^2c^4 - e\hbar c\,\vec{\sigma}\cdot\vec{B}(1+\lambda') + (e\hbar c\lambda'/mc^2)^2B^2\,, \tag{A3}$$

and its Weyl transform is

$$\vec{\Pi}^2_{op} + m^2c^4 - e\hbar c\,\vec{\sigma}\cdot\vec{B}(1+\lambda') + (e\hbar c\lambda'/mc^2)^2B^2$$

$$\rightleftharpoons \vec{\pi}^2 + m^2c^2 - e\hbar c\,\vec{\sigma}\cdot\vec{B}(1+\lambda') + (e\hbar c\lambda'/mc^2)^2B^2\,, \tag{A4}$$

$$\vec{\pi} = c\vec{p} - e\vec{A}(\vec{q})\,, \tag{A5}$$

where $\lambda' = \frac{1}{2}(g-2)$ and we have written the operator on the right and its Weyl transform on the left in (A4). The even form of the Hamiltonian operator (A1) is given in Eq. (24) and is

$$\mathcal{H}'_{op} = \beta[m^2c^4 + \vec{\Pi}^2_{op} - e\hbar c\vec{\sigma}\cdot\vec{B}(1+\lambda') + (e\hbar c\lambda'/mc^2)^2B^2]^{1/2}\,. \tag{A6}$$

We are interested in the Weyl transform of the square-root operator. The general form of the expansion of the square root with the same properties under rotation, space inversion, and time reversal reads, up to terms quadratic in e,

$$\begin{aligned}[\vec{\Pi}^2_{op} + m^2c^4 - e\hbar c\,\vec{\sigma}\cdot\vec{B}(1+\lambda') + (e\hbar c\lambda'/mc^2)^2B^2]^{1/2} \rightleftharpoons{}& E - (ec/E)\vec{p}\cdot\vec{A} - (e\hbar c\,\vec{\sigma}\cdot\vec{B}/2E)(1+\lambda') + eL_2(E)\vec{p}\cdot\vec{\sigma}\,\vec{p}\cdot\vec{B}\\ &+ e^2f_1(E)\vec{A}^2 + e^2f_2(E)(\vec{p}\cdot\vec{A})^2 + e^2f_3(E)\vec{p}\cdot\vec{A}\,\vec{\sigma}\cdot\vec{B}\\ &+ e^2f_4(E)\vec{p}\cdot\vec{B}\,\vec{\sigma}\cdot\vec{A} + e^2f_5(E)\vec{p}\cdot\vec{\sigma}\,\vec{A}\cdot\vec{B} + e^2f_6(E)\vec{p}\cdot\vec{A}\,\vec{p}\cdot\vec{B}\,\vec{p}\cdot\vec{\sigma}\\ &+ e^2f_7(E)(\vec{p}\cdot\vec{B})^2 + e^2f_8(E)B^2 + \cdots\,.\end{aligned} \tag{A7}$$

Taking the square of the operator and using the multiplication rule, we have

$$\{\Omega(\vec{P},\vec{Q})\}^2 \rightleftharpoons \exp\frac{\hbar}{2i}\left(\frac{\partial^{(a)}}{\partial\vec{p}}\cdot\frac{\partial^{(b)}}{\partial\vec{q}} - \frac{\partial^{(a)}}{\partial\vec{q}}\cdot\frac{\partial^{(b)}}{\partial\vec{p}}\right)\omega^{(a)}(\vec{p},\vec{q})\,\omega^{(b)}(\vec{p},\vec{q})\,. \tag{A8}$$

Since $\vec{A}(\vec{q})$ is linear in $\vec{q}$ we need the expansion of the exponential up to terms with second derivatives of $\omega(\vec{p},\vec{q})$, obtaining

$$[\Omega(\vec{P},\vec{Q})]^2 \rightleftharpoons [\omega(\vec{p},\vec{q})]^2 + \frac{i\hbar}{2}\left(\frac{\partial\omega}{\partial\vec{q}}\cdot\frac{\partial\omega}{\partial\vec{p}} - \frac{\partial\omega}{\partial\vec{q}}\cdot\frac{\partial\omega}{\partial\vec{p}}\right) + \frac{\hbar^2}{4}\frac{\partial^2\omega}{\partial\vec{p}\,\partial\vec{q}}:\frac{\partial^2\omega}{\partial\vec{p}\,\partial\vec{q}} - \frac{\hbar^2}{8}\frac{\partial^2\omega}{\partial\vec{p}\,\partial\vec{q}}:\frac{\partial^2\omega}{\partial\vec{q}\,\partial\vec{q}} - \frac{\hbar^2}{8}\frac{\partial^2\omega}{\partial\vec{q}\,\partial\vec{q}}:\frac{\partial^2\omega}{\partial\vec{p}\,\partial\vec{p}}\,, \tag{A9}$$

where the double dots indicate tensor contraction. Then one finds

$$\begin{aligned}\vec{\Pi}^2_{op} + m^2c^4 - e\hbar c\vec{\sigma}\cdot\vec{B}(1+\lambda') + \left(\frac{e\hbar c\lambda'}{mc^2}\right)^2B^2 \rightleftharpoons{}& [E^2 - 2ec\vec{p}\cdot\vec{A} - e\hbar c\,\vec{\sigma}\cdot\vec{B}(1+\lambda') + e^2\,2Ef_1(E)\vec{A}^2\\ &+ e^2\,2Ef_2(E)(\vec{p}\cdot\vec{A})^2 + e^2\,2Ef_3(E)\,\vec{p}\cdot\vec{A}\,\vec{\sigma}\cdot\vec{B} + e^2\,2Ef_4(E)\vec{p}\cdot\vec{B}\,\vec{\sigma}\cdot\vec{A}\\ &+ e^2\,2Ef_5(E)\vec{p}\cdot\vec{\sigma}\,\vec{A}\cdot\vec{B} + e^2\,2Ef_6(E)\vec{p}\cdot\vec{A}\,\vec{p}\cdot\vec{B}\,\vec{p}\cdot\vec{\sigma} + e^2\,2Ef_7(E)(\vec{p}\cdot\vec{B})^2\\ &+ e^2\,2Ef_8(E)B^2] + \left\{\frac{e^2c^2}{E^2}(\vec{p}\cdot\vec{A})^2 + \frac{e^2\hbar c^2}{E^2}\vec{p}\cdot\vec{A}\,\vec{\sigma}\cdot\vec{B} + \frac{e^2\hbar^2c^2}{4E^2}B^2(1+\lambda')^2\right\}\\ &+ \frac{\hbar^2e^2c^2}{4}\left[\frac{\partial}{\partial p_i}\left(\frac{p_k}{E}\right)\frac{\partial}{\partial p_j}\left(\frac{p_l}{E}\right)\frac{\partial A_k}{\partial q_j}\frac{\partial A_l}{\partial q_i}\right]\\ &- \frac{e^2\hbar^2}{4}\frac{\partial^2 E}{\partial\vec{p}\,\partial\vec{p}}:\frac{\partial^2}{\partial\vec{q}\,\partial\vec{q}}\left[f_1(E)\vec{A}^2 + f_2(E)(\vec{p}\cdot\vec{A})^2\right] + O(e^3)\end{aligned} \tag{A10}$$

(summation convention). The $L_2(E)$ terms are omitted since $L_2(E)$ can easily be shown to be zero:

$$\frac{e^2c^2\hbar^2}{4}\left[\frac{\partial}{\partial p_i}\left(\frac{p_k}{E}\right)\frac{\partial}{\partial p_j}\left(\frac{p_l}{E}\right)\frac{\partial A_k}{\partial p_j}\frac{\partial A_l}{\partial q_i}\right]=\frac{e^2c^2}{4}\left(\delta_{ik}-c^2\frac{p_ip_k}{E^2}\right)\left(\delta_{jl}-c^2\frac{p_jp_l}{E^2}\right)\tfrac{1}{4}e_{kmj}B_m e_{lni}B_n$$

$$=\frac{\hbar^2e^2c^2}{16E^2}\left(e_{imj}e_{jni}B_mB_n-e_{imj}c^2\frac{p_jp_l}{E^2}e_{lni}B_mB_n-e_{kmj}e_{jni}c^2\frac{p_ip_k}{E^2}B_mB_n\right)$$

$$=(\hbar^2e^2c^2/16E^2)\{-2B^2-(2c^2/E^2)[(\vec{p}\cdot\vec{B})^2-p^2B^2]\}$$

$$=(e^2c^2\hbar^2/8E^4)[m^2c^4B^2+c^2(\vec{p}\cdot\vec{B})^2]\,. \tag{A11}$$

The last term is

$$-\frac{e^2\hbar^2}{4E}\left(\overleftrightarrow{u}-c^2\frac{\vec{p}\vec{p}}{E^2}\right):\frac{\partial^2}{\partial\vec{q}\,\partial\vec{q}}\,[f_1(E)\vec{A}^2+f_2(\vec{p}\cdot\vec{A})^2]$$

$$=\frac{e^2\hbar^2}{4E}\left(\overleftrightarrow{u}-c^2\frac{\vec{p}\vec{p}}{E^2}\right):[\tfrac{1}{2}f_1(E)(B^2\overleftrightarrow{u}-\vec{B}\vec{B})+\tfrac{1}{2}f_2(E)(\vec{p}\times\vec{B})\cdot(\vec{p}\times\vec{B})]$$

$$=\frac{-\hbar^2e^2}{8E}f_1(E)\left[3B^2-c^2\frac{\vec{p}^2\vec{B}^2}{E^2}-B^2+c^2\frac{(\vec{p}\cdot\vec{B})^2}{E^2}\right]-\frac{\hbar^2e^2}{8E}f_2(E)c^l[\vec{p}^2\cdot\vec{B}^2-(\vec{p}\cdot\vec{B})^2]$$

$$=e^2\hbar^2B^2\left[\left(-\frac{1}{4E}+c^2\frac{\vec{p}^2}{8E^3}\right)f_1(E)-\frac{\vec{p}^2c^l}{8E}f_2(E)\right]+(\vec{p}\cdot\vec{B})^2\left[-\frac{1}{8E^3}f_1(E)+\frac{1}{8E}f_2(E)\right](e\hbar c)^2\,, \tag{A12}$$

where $\overleftrightarrow{u}$ is a unit dyadic and the double dot indicates tensor contraction. Comparing (A4) and (A10) [with (A11) and (A12) inserted] we find for the form factors

$$f_1(E)=1/2E\,, \tag{A13}$$

$$f_2(E)=-1/2E^3\,, \tag{A14}$$

$$f_3(E)=(-\hbar c^2/2E^3)(1+\lambda')\,, \tag{A15}$$

$$f_4(E)=f_5(E)=f_6(E)=0\,, \tag{A16}$$

$$f_7(E)=\hbar^2c^2/8E^5\,, \tag{A17}$$

$$f_8(E)=\left(-\frac{(1+\lambda')^2}{8E^3}+\frac{m^2c^4}{8E^5}\right)\hbar^2c^2+\left(\frac{\hbar c\lambda'}{mc^2}\right)^2\frac{1}{8E}\,. \tag{A18}$$

Thus

$$\mathcal{H}'_{\rm op}\doteq\beta\left[E-\frac{ec}{E}\vec{p}\cdot\vec{A}-\frac{e\hbar c\vec{\sigma}\cdot\vec{B}}{2E}(1+\lambda')+\frac{e^2\vec{A}^2}{2E}-\frac{e^2c^2}{2E^3}(\vec{p}\cdot\vec{A})^2-\frac{e^2\hbar^2c^2}{2E^3}(1+\lambda')\vec{p}\cdot\vec{A}\,\vec{\sigma}\cdot\vec{B}\right.$$

$$\left.+\frac{(e\hbar c)^2}{8E^5}(\vec{p}\cdot\vec{B})^2+(e\hbar c)^2B^2\left(-\frac{(1+\lambda')^2}{8E^3}+\frac{m^2c^4}{8E^5}\right)+\left(\frac{e\hbar c\lambda'}{mc^2}\right)^2\frac{B^2}{8E}+O(e^3)\right]. \tag{A19}$$

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*An early version of this work appeared as International Centre for Theoretical Physics Report No. IC/72/68 (unpublished).

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