PHYSICAL REVIEW B VOLUME 14, NUMBER 8 15 OCTOBER 1976

Magnetic susceptibility of interacting free and Bloch electrons*

F. A. Buot

Department of Physics, St. Francis Xavier University, Antigonish, Nova Scotia, Canada

(Received 2 July 1975)

The form of the magnetic-susceptibility formula given by Roth and by Wannier and Upadhyaya for noninteracting Bloch electrons is generalized to include all many-body effects. The arguments used do not involve any approximations and are entirely based on the translational-symmetry property of the system. Spin and orbital susceptibility of some well-known cases, Fermi liquid and strongly correlated electrons in a narrow band, are shown to follow from the most general formula for the magnetic susceptibility of interacting free and Bloch (with or without spin-orbit coupling) electrons derived in this paper.

I. INTRODUCTION

For over three decades[1] several studies of the many-body effects on the magnetic susceptibility χ of free and Bloch electrons have been made. Using a field-theoretical Green's-function technique, but neglecting the current vertex corrections, Fukuyama[2] has recently given a formula for χ of interacting Bloch electrons. Philippas and McClure,[3] among other things, have established the validity of the Sampson-Seitz[1] prescription applied to the Landau-Peierls formula. In their work it was an essential assumption that the self-energy function does not depend on the energy variable. Consequently, Fukuyama and McClure[4] investigated the orbital χ of an interacting free-electron gas, taking into account the exact functional form of the self-energy. Their results yield a generalized form of the Landau-Peierls formula.

Thus far, it appears that all studies made involve some kind of approximation, either in obtaining the self-energy part, current vertex function, or in the band model considered. It would certainly be more revealing if a straightforward and a most general type of analysis to the problem could be employed enabling us to see, and perhaps, understand the exact form that the total χ takes for interacting Fermi systems possessing translational symmetry. It has been the author's belief that an analysis, entirely based on the translational symmetry property of the system,[5] should provide the most general considerations appropriate to the problem. Indeed, the generalized form of the Landau-Peierls formula obtained by Fukuyama and McClure[4] already supports this view. We shall see that symmetry arguments enable us to generalize, in a unified manner, the derivation of χ for noninteracting to that of interacting Fermi systems possessing translational symmetry.

The purpose of this paper is twofold. First, we present a more rigorous formulation of the description of the dynamics of a Fermi system, possessing translational symmetry, in $\vec{p}$-$\vec{q}$ space labeled by a band index λ, where $\vec{p}$ is the crystal momentum $\hbar k$ (limited to the first Brillouin zone) and $\vec{q}$ is the lattice-point coordinate. Second, we give a derivation of the exact expression for χ of interacting Fermi system possessing translational symmetry by use of symmetry arguments.

Section II discusses the effective one-particle Schrödinger equation for many-body systems possessing translational symmetry in terms of crystal-momentum and lattice-position operators. The transformation to these canonically conjugate operators appropriate for solid-state problems[5] is carried out by means of the lattice Weyl transform.[6,7] The effective Hamiltonian is then diagonalized with respect to the band indices defining a new set of Bloch functions and Wannier functions which are, in general, energy dependent and biorthogonal.[8,9] In the absence of the magnetic field, the transformation that diagonalizes the effective one-particle Hamiltonian operator is just the transformation from the Bloch function and Wannier function (in the absence of interaction) to the Bloch function and Wannier function (in the presence of interaction) which are, in general, biorthogonal and energy dependent. In the presence of a uniform external magnetic field, the diagonalized effective-Hamiltonian operator determines a set of magnetic Wannier functions and magnetic Bloch functions (in general, both energy dependent and biorthogonal). Using these biorthogonal basis states, the free energy is then calculated up to second order in the magnetic field strength, using the temperature Green's-function formalism of Luttinger and Ward, for obtaining the susceptibility χ. The most general expression for χ is then applied to the calculation of spin and orbital susceptibility of some well-known cases: Fermi liquids and highly correlated electrons in a narrow band represented by the Hubbard model. Further discussion on the general formula for χ, regarding the presence of spin indices which are suppressed in the developments of Secs. III and IV, is given in Sec. VI.

II. EFFECTIVE SCHRÖDINGER EQUATION FOR MANY-BODY SYSTEMS: TRANSFORMATION TO CRYSTAL-MOMENTUM AND LATTICE-POSITION OPERATORS FOR SYSTEMS POSSESSING TRANSLATIONAL SYMMETRY

In this section, we will set up an eigenvalue problem whose solution for a zero-field case determines the transformation from the Wannier functions and Bloch functions of the noninteracting case to the Wannier functions and Bloch functions of the interacting case which are, in general, energy dependent and biorthogonal. The solution to the eigenvalue problem, in the presence of an externally applied uniform magnetic field, determines the transformation which diagonalizes the effective Hamiltonian with respect to the band indices and, thus, also determines the transformation from the magnetic Wannier functions and magnetic Bloch functions[5-7] of the noninteracting case to the eigensolutions of the effective Hamiltonian labeled by the band index λ. The corresponding "diagonal" effective-Hamiltonian operator, in turn, determines new sets of magnetic Wannier functions and magnetic Bloch functions of the interacting Bloch electrons in a uniform magnetic field. These new basis states are used in calculating the free energy, exact up to order $\hbar^2$, in Sec. IV.

The effective one-particle Schrödinger equation in the presence of a uniform magnetic field is defined by[8,9]

$$[\mathcal{H}_0+\Sigma(z)]\phi(z)=E(z)\,\phi(z), \qquad (2.1)$$

where $\Sigma(z)$ is the nonlocal energy-dependent (z is the energy variable) complex quantity called the self-energy operator. $\mathcal{H}_0$ is given by

$$\mathcal{H}_0=\frac{1}{2m}\left(\frac{\hbar}{i}\nabla_{\vec{r}}-\frac{e}{c}\vec{A}(\vec{r})\right)^2+V(\vec{r})-g\mu_B s_z B, \qquad (2.2)$$

$\vec{A}(\vec{r})$ is the vector potential [symmetric gauge, $\vec{A}(\vec{r})=\frac{1}{2}\vec{B}\times\vec{r}$, will be used], B is the magnetic field strength (directed along positive z axis), and $V(\vec{r})$ is the average periodic local potential. $V+\Sigma(z)$ represents the effective potential which is a non-Hermitian operator leading to the use of biorthogonal eigenfunctions, with the dual sets obtained from the eigenfunctions of $\mathcal{H}_0+\Sigma(z)$ and its adjoint.[8,9]

We will transform the effective-Hamiltonian operator $\mathcal{H}=\mathcal{H}_0+\Sigma(z)$ to an effective Hamiltonian expressed in terms of the crystal-momentum operator and the lattice-position operator.[5] This is conveniently done by the use of the lattice Weyl transform[6] (lattice Weyl transform and Weyl transform will be used interchangeably) and is clarified in Appendix A. We obtain

$$\mathcal{H}_{\text{eff}}(\vec{P},\vec{Q},z)=(N\hbar^3)^{-2}\sum_{\substack{\vec{p},\vec{q},\lambda,\lambda'\\ \vec{u},\vec{v}}} H_{\lambda\lambda'}\left(\vec{p}-\frac{e}{c}\vec{A}(\vec{q});B,z\right)\exp\left(\frac{2i}{\hbar}(\vec{p}-\vec{P})\cdot\vec{v}\right)\times\exp\left(\frac{2i}{\hbar}(\vec{q}-\vec{v}-\vec{Q})\cdot\vec{u}\right)\Omega_{\lambda\lambda'}, \qquad (2.3)$$

where the lattice Weyl transform of $\mathcal{H}$ is defined by

$$H_{\lambda\lambda'}\left(\vec{p}-\frac{e}{c}\vec{A}(\vec{q}),B,z\right)=\sum_{\vec{v}}e^{(2i/\hbar)\vec{p}\cdot\vec{v}}\langle\vec{q}-\vec{v},\lambda|\mathcal{H}_0+\Sigma(z)|\vec{q}+\vec{v},\lambda'\rangle, \qquad (2.4)$$

$$\Omega_{\lambda\lambda'}=\sum_{\vec{q}}|\vec{q},\lambda\rangle\langle\vec{q},\lambda'|=\sum_{\vec{p}}|\vec{p},\lambda\rangle\langle\vec{p},\lambda'|. \qquad (2.5)$$

The summation over $\vec{p}=\hbar\vec{k}$ and $\vec{u}$ is limited to the first Brillouin zone and the summation over $\vec{q}$ and $\vec{v}$ is over all lattice points. $\vec{P}$ and $\vec{Q}$ are, respectively, the crystal-momentum operator and lattice-position operator. $|\vec{p},\lambda\rangle$ is an eigenfunction of $\vec{P}$ with eigenvalue $\vec{p}$ and $|\vec{q},\lambda\rangle$ is an eigenfunction of $\vec{Q}$ with eigenvalue $\vec{q}$, where $|\vec{p},\lambda\rangle$ and $|\vec{q},\lambda\rangle$ are the Bloch function and Wannier function, respectively, both without or with an externally applied uniform magnetic field (often referred to as magnetic Bloch function and magnetic Wannier function in the presence of magnetic field), of the noninteracting Bloch electrons represented by $\mathcal{H}_0$.[6,7] If we expand the eigensolutions of (2.3) in terms of the complete set of magnetic Wannier functions or of magnetic Bloch functions[5]

$$\phi(\vec{r},z)=\sum_{\vec{p},\lambda}f_\lambda(\vec{p},z)|\vec{p},\lambda\rangle, \qquad (2.6)$$

$$\phi(\vec{r},z)=\sum_{\vec{q},\lambda}f_\lambda(\vec{q},z)|\vec{q},\lambda\rangle, \qquad (2.7)$$

an equivalent eigenvalue problem is obtained. In $\vec{q}$ space we have

$$\sum_{\lambda'}W_{\lambda\lambda'}(\vec{\pi};B,z)f_{\lambda'}(\vec{q},z)=E(z)f_\lambda(\vec{q},z), \qquad (2.8)$$

and the corresponding eigenvalue equation in $\vec{p}$

space is

$$\sum_{\lambda'} W_{\lambda\lambda'}(\vec{\pi};B,z)f_{\lambda'}(\vec{p},z)=E(z)f_\lambda(\vec{p},z), \quad (2.9)$$

where

$$W_{\lambda\lambda'}(\vec{\pi};B,z)=(N\hbar^3)^{-1}\sum_{\vec{p}',\vec{v}} H_{\lambda\lambda'}(\vec{p}';B,z) \times\exp\left(\frac{2i}{\hbar}(\vec{p}'-\vec{\pi})\cdot\vec{v}\right), \quad (2.10)$$

$$\vec{\pi}=\begin{cases}(\hbar/i)\nabla_{\vec{q}}-(e/c)\vec{A}(\vec{q}) & \text{in } \vec{q} \text{ space}, \quad (2.11)\\ \vec{p}+(e/c)\vec{A}[(\hbar/i)\nabla_{\vec{p}}] & \text{in } \vec{p} \text{ space}. \quad (2.12)\end{cases}$$

Since $W_{\lambda\lambda'}(\vec{\pi};B,z)$ is a non-Hermitian operator, one also needs to solve the adjoint problem,[9] either in $\vec{q}$ space or $\vec{p}$ space,

$$\sum_{\lambda'} W^*_{\lambda'\lambda}(\vec{\pi};B,z)e_{\lambda'}(\vec{q},z)=E^*(z)e_\lambda(\vec{q},z), \quad (2.13)$$

$$\sum_{\lambda'} W^*_{\lambda'\lambda}(\vec{\pi};B,z)e_{\lambda'}(\vec{p},z)=E^*(z)e_\lambda(\vec{p},z). \quad (2.14)$$

We have indeed transformed the original integro-differential eigenvalue equation,[8] Eq. (2.1), into a diagonalization of a matrix operator whose elements are themselves complex functions of a Hermitian operator $\vec{\pi}$. $W(\vec{\pi};B,z)$ may be viewed as a generalized Hamiltonian of the Dirac type[7] occurring in the relativistic quantum theory of electrons. Since we are using magnetic Wannier functions and magnetic Bloch functions of the noninteracting Bloch electrons in a uniform magnetic field as basis states, $\mathcal{H}_0$ is diagonal in band indices and we may write

$$W_{\lambda\lambda'}(\vec{\pi};B,z)=W_0(\vec{\pi};B)_\lambda\delta_{\lambda\lambda'}+\Sigma(\vec{\pi};B,z)_{\lambda\lambda'}, \quad (2.15)$$

where $W_0(\vec{\pi};B)_\lambda$ is the effective magnetic Hamiltonian, belonging to the band λ, of noninteracting Bloch electrons in a uniform magnetic field.

Let us first discuss the solution of our eigenvalue problem for the zero-field case. The functional form of $W_{\lambda\lambda'}$, which we denote by $H^0_{\lambda\lambda'}$, is then given by the lattice Weyl transform of $\mathcal{H}_0+\Sigma(z)$ using Wannier functions or Bloch functions of noninteracting Bloch electrons. The eigenvalue equation becomes a pure matrix problem in $\vec{p}$ space, as well as in $\vec{q}$ space if one writes $f(\vec{q},z)=f(\vec{p},z)e^{i\vec{p}\cdot\vec{q}/\hbar}$. The matrix $H^0_{\lambda\lambda'}$ can in general be diagonalized if all the eigenvalues are different; therefore we make the assumption that all the bands are nondegenerate (i.e., band index λ is a good quantum number). The eigenfunctions $f(\vec{p},z)$ of $H^0_{\lambda\lambda'}$ and those of its adjoint define a similarity transformation which diagonalizes $H^0_{\lambda\lambda'}$. We have

$$U^{-1}H^0U=\tilde{H}^0_\lambda\delta_{\lambda\lambda'}, \quad (2.16)$$

where the matrix of U is given by f_{ij}, where f_{ij} denotes the ith component of an eigenvector belonging to the jth eigenvalue of the matrix $H^0_{\lambda\lambda'}$. The matrix of U^{-1} is the matrix formed by e^*_{ji}, where e_{ji} is the ith component of the jth eigenvector of the adjoint matrix. U and U^{-1} also determine the transformation from the Wannier function and Bloch function of noninteracting Bloch electrons to the Wannier function and Bloch function of interacting Bloch electrons, which are, in general, energy dependent and biorthogonal. Denoting these by $|\vec{q},\lambda,z\rangle$ and $|\vec{p},\lambda,z\rangle$, we have

$$|\vec{p},\lambda,z\rangle=\sum_i f_{i\lambda}(\vec{p},z)|\vec{p},i\rangle, \quad (2.17)$$

$$\langle\vec{p},\lambda,z|=\sum_i e^*_{\lambda i}(\vec{p},z)\langle\vec{p},i|, \quad (2.18)$$

$$|\vec{q},\lambda,z\rangle=(N\hbar^3)^{-1/2}\sum_{\vec{q}} e^{(i/\hbar)\vec{p}\cdot\vec{q}}|\vec{p},\lambda,z\rangle, \quad (2.19)$$

$$\langle\vec{q},\lambda,z|=(N\hbar^3)^{-1/2}\sum_{\vec{p}} e^{(i/\hbar)\vec{p}\cdot\vec{q}}\langle\vec{p},\lambda,z|. \quad (2.20)$$

In terms of these basis states, $\tilde{H}^0_\lambda(\vec{p},z)\delta_{\lambda\lambda'}$ is given by

$$\tilde{H}^0_\lambda(\vec{p},z)=\sum_{\vec{v}} e^{(2i/\hbar)\vec{p}\cdot\vec{v}} \times\langle\vec{q}-\vec{v},\lambda,z|\mathcal{H}_0+\Sigma(z)|\vec{q}+\vec{v},\lambda,z\rangle, \quad (2.21)$$

or equivalently by

$$\tilde{H}^0_\lambda(\vec{p},z)=\sum_{\vec{u}} e^{(2i/\hbar)\vec{q}\cdot\vec{u}} \times\langle\vec{p}+\vec{u},\lambda,z|\mathcal{H}_0+\Sigma(z)|\vec{p}-\vec{u},\lambda,z\rangle. \quad (2.22)$$

$\tilde{H}^0_\lambda(\vec{p},z)$ may be interpreted as an energy-dependent band function. The one-particle energy z_λ belonging to the band index λ is, in the quasiparticle picture,[9] given as usual by the solution of

$$z_\lambda-\tilde{H}^0_\lambda(\vec{p},z_\lambda)=0. \quad (2.23)$$

III. REMOVAL OF INTERBAND TERMS IN EFFECTIVE HAMILTONIAN

The problem of diagonalizing the effective-Hamiltonian operator of interacting Bloch electrons in a magnetic field can proceed in either of the two equivalent routes. The basic idea[10,11] is that instead of diagonalizing the operator $W_{\lambda\lambda'}(\vec{\pi};B,z)$ directly, one tries to diagonalize the lattice Weyl transform[6] of $\mathcal{H}$ [Eqs. (2.4) and (2.5)]. The power and advantage of this approach lies in being able to deal with ordinary c numbers instead of quantum-mechanical operators. Since the operator and its Weyl transform are related one to one through Eq. (2.3), to diagonalize the operator $W_{\lambda\lambda'}(\vec{\pi};B,z)$ we seek a transformation S_{op} such that

$$S_{op}^{-1}\mathcal{H}_{eff}S_{op} \rightleftharpoons \tilde{H}(\vec{p}-(e/c)\vec{A}(\vec{q});B,z)_\lambda \delta_{\lambda\lambda'}, \qquad (3.1)$$

where we have used $\rightleftharpoons$ to denote the one-to-one Weyl correspondence between operator and its Weyl transform. Using the diagonalized Weyl transform the transformed effective Hamiltonian $\tilde{W}_\lambda(\vec{\pi},B,z)$ for each band index λ is thus given, in place of Eq. (2.10), as

$$\tilde{W}_\lambda(\vec{\pi};B,z)=(N\hbar^3)^{-1}\sum_{\vec{p}',\vec{v}}\tilde{H}_\lambda(\vec{p}';B,z)\times\exp\left(\frac{2i}{\hbar}(\vec{p}'-\vec{\pi})\cdot\vec{v}\right). \qquad (3.2)$$

The general expression for the Weyl transform of a product of three operators[6,7] applied to the left-hand side of Eq. (3.1) gives

$$S_{op}^{-1}\mathcal{H}_{eff}S_{op} \rightleftharpoons \exp\left[\frac{i\hbar eB}{2c}\left(\frac{\partial^{(a)}}{\partial\vec{k}_x}\frac{\partial^{(b)}}{\partial\vec{k}_y}-\frac{\partial^{(a)}}{\partial\vec{k}_y}\frac{\partial^{(b)}}{\partial\vec{k}_x}+\frac{\partial^{(a)}}{\partial\vec{k}_x}\frac{\partial^{(c)}}{\partial\vec{k}_y}-\frac{\partial^{(a)}}{\partial\vec{k}_y}\frac{\partial^{(c)}}{\partial\vec{k}_x}+\frac{\partial^{(b)}}{\partial\vec{k}_x}\frac{\partial^{(c)}}{\partial\vec{k}_y}-\frac{\partial^{(b)}}{\partial\vec{k}_y}\frac{\partial^{(c)}}{\partial\vec{k}_x}\right)\right]\times S^{-1(a)}(\vec{k},B,z)H^{(b)}(\vec{k},B,z)S^{(c)}(\vec{k},B,z), \qquad (3.3)$$

where we have changed variables, $\vec{p}-(e/c)\vec{A}(\vec{q})\to\hbar\vec{k}$; $S_{op}^{-1}\rightleftharpoons S^{-1}(\vec{k},B,z)$, $\mathcal{H}_{eff}\rightleftharpoons H(\vec{k},B,z)$, and $S_{op}\rightleftharpoons S(\vec{k},B,z)$. The procedure is to diagonalize the effective-Hamiltonian operator, and hence the lattice Weyl transform of $\mathcal{H}$, by means of successive similarity transformations

$$S_{op}=\prod_{i=1}^{\infty}S_{op}^{0}e^{G_{op}^{(i)}}. \qquad (3.4)$$

Once S_{op}^0 can be found, $G_{op}^{(i)}$ can easily be determined. To find S_{op}^0 we expand $H(\vec{k};B,z)$ in powers of B

$$H(\vec{k},B,z)=H^0(\vec{k},z)+BH^{(1)}(\vec{k},z)+\cdots, \qquad (3.5)$$

and require that the zero-order term on the right-hand side of Eq. (3.3) be diagonal. Denoting the matrix which diagonalizes $H^0(\vec{k},z)$ by $U(\vec{k},z)$ we have

$$U^{-1}(\vec{k},z)H^0(\vec{k},z)U(\vec{k},z)=\tilde{H}_\lambda^0(\vec{k},z)\delta_{\lambda\lambda'}. \qquad (3.6)$$

Equation (3.6) is a pure matrix diagonalization problem and was already solved in Sec. II for the zero-field case. There, we have assumed that the eigenvalues of $H^0(\vec{k},z)$ are nondegenerate; the resulting eigenvectors of $H^0(\vec{k},z)$ and those of its adjoint define a similarity transformation from Wannier function and Bloch function for $\Sigma=0$ to the Wannier function and Bloch function for $\Sigma\neq0$, which are, in general, energy dependent and biorthogonal.[9] The operator corresponding to $U(\vec{k},z)$, Eq. (3.6), is, however, a similarity transformation only for the zero-field case; thus writing $U_{op}^{-1}\rightleftharpoons U^{-1}(\vec{k},z)$, $U_{op}\rightleftharpoons U(\vec{k},z)$, and setting $H_{eff}=1$ in Eq. (3.3), we have

$$\{U_{op}^{-1}U_{op}\}\rightleftharpoons\exp\left[\frac{ie\hbar B}{2c}\left(\frac{\partial^{(a)}}{\partial\vec{k}_x}\frac{\partial^{(b)}}{\partial\vec{k}_y}-\frac{\partial^{(a)}}{\partial\vec{k}_y}\frac{\partial^{(b)}}{\partial\vec{k}_x}\right)\right]\times U^{-1(a)}(\vec{k},z)\,U^{(b)}(\vec{k},z), \qquad (3.7)$$

where $\{U_{op}^{-1}U_{op}\}$ indicates that the product is not to be interpreted as exact product of an operator and its inverse.

We now prove a theorem useful for making U_{op} a similarity transformation up to an arbitrary order in the magnetic field strength without affecting the zero-order term $\tilde{H}^0(\vec{k},z)_\lambda\delta_{\lambda\lambda'}$ on the right-hand side of Eq. (3.3). The theorem states that $\{U_{op}^{-1}U_{op}\}$ can be made equal to unity up to an arbitrary order in the magnetic field strength B by means of successive multiplication by exponential operators on the left- and right-hand sides. We have

$$^{(n)}U_{op}^{-1}\;{}^{(n)}U_{op}=\prod_{i=n}^{1}e^{g_{op}^{(i)}}\{U_{op}^{-1}U_{op}\}\prod_{i=1}^{n}e^{g_{op}^{(i)}}=1+O(B^n), \qquad (3.8)$$

where each successive $g_{op}^{(i)}$ is so chosen so as to make the product unity up to order i in the magnetic field strength. To prove the theorem we need the expression for the lattice Weyl transform of an arbitrary operator A_{op} raised to any power n. This is given in Ref. 6, which can be rewritten, for problems involving uniform magnetic field and possessing translational symmetry, analogous to Eq. (3.3) as

$$A_{\rm op}^n \rightleftharpoons \cos\left[\frac{e\hbar B}{2c}\sum_{\substack{j,\bar{k}=1\\ j<\bar{k}}}^{n}\left(\frac{\partial^{(j)}}{\partial \bar{k}_x}\frac{\partial^{(k)}}{\partial \bar{k}_y}-\frac{\partial^{(j)}}{\partial \bar{k}_y}\frac{\partial^{(k)}}{\partial \bar{k}_x}\right)\right]$$

$$\times\frac{1}{2}\left(\prod_{l=1}^{n}A^{(l)}(\bar{k};B)+\prod_{l=n}^{1}A^{(l)}(\bar{k};B)\right). \quad (3.9)$$

The lattice Weyl transform of an exponential operator $e^{g_{\rm op}^{(i)}}$ can therefore be expressed as[6]

$$\exp(g_{\rm op}^{(i)}) \rightleftharpoons e^{g^{(i)}(\bar{k};B)}+R$$
$$=1+g^{(i)}(\bar{k},B)+\cdots+R, \quad (3.10)$$

where R represents the remaining terms and $g_{\rm op}^{(i)} \rightleftharpoons g^{(i)}(\bar{k},B)$. A complete iteration procedure for obtaining $S_{\rm op}^0$ in Eq. (3.4), up to an arbitrary order in B can now be defined. Let us write Eq. (3.7) as

$$\{U_{\rm op}^{-1}U_{\rm op}\} \rightleftharpoons 1+BS^{(1)}(\bar{k},z)+B^2S^{(2)}(\bar{k},z)+\cdots, \quad (3.11)$$

where the explicit dependence of B comes from the exponential "Poisson-bracket operator." We choose $g_{\rm op}^{(1)} \rightleftharpoons -\frac{1}{2}BS^{(1)}(\bar{k},z)$, obtaining

$$e^{g_{\rm op}^{(1)}}\{U_{\rm op}^{-1}U_{\rm op}\}e^{g_{\rm op}^{(1)}} \rightleftharpoons 1+B^2\,{}^{(1)}S^{(2)}(\bar{k},z)+{}^{(1)}\Delta_R. \quad (3.12)$$

We next choose $g_{\rm op}^{(2)} \rightleftharpoons -\frac{1}{2}B^2\,{}^{(1)}S^{(2)}(\bar{k};z)$ resulting in

$$e^{g_{\rm op}^{(2)}}e^{g_{\rm op}^{(1)}}\{U_{\rm op}^{-1}U_{\rm op}\}e^{g_{\rm op}^{(1)}}e^{g_{\rm op}^{(2)}} \rightleftharpoons 1+B^3\,{}^{(2)}S^{(3)}(\bar{k},z)+{}^{(2)}\Delta_R. \quad (3.13)$$

In general order n, we have

$${}^{(n)}U_{\rm op}^{-1}\,{}^{(n)}U_{\rm op} \rightleftharpoons 1+B^{n+1}\,{}^{(n)}S^{(n+1)}(\bar{k},z)+{}^{(n)}\Delta_R, \quad (3.14)$$

and $g_{\rm op}^{(n+1)}$ can be chosen such that $g_{\rm op}^{(n+1)} \rightleftharpoons -\frac{1}{2}B^{n+1}\,{}^{(n)}S^{(n+1)}(\bar{k},z)$. This completes the proof of the theorem. A trivial example is the following. Let $\{U_{\rm op}^{-1}U_{\rm op}\}=e^{BO_{\rm op}}e^{BO_{\rm op}}=1+2BO(\bar{k})+\Delta_R$, where $O_{\rm op} \rightleftharpoons O(\bar{k})$. Choosing $g_{\rm op}^{(1)} \rightleftharpoons -BO(\bar{k})$ we immediately obtain $e^{-BO_{\rm op}}e^{BO_{\rm op}}e^{BO_{\rm op}}e^{-BO_{\rm op}}=1$ to all orders in B and the similarity transformation $S_{\rm op}^0=1$.

We now proceed to the diagonalization of $\mathcal{H}_{\rm eff}$, Eq. (3.1). We assume that, by the method discussed above, we have obtained a similarity transformation which make the zero-order term in Eq. (3.3) free of interband terms. We denote this similarity transformation as $S_{\rm op}^0$, Eq. (3.4), and let us write

$$(S_{\rm op}^0)^{-1}\mathcal{H}_{\rm eff}S_{\rm op}^0 \rightleftharpoons \tilde{H}_\lambda^0(\bar{k},z)\delta_{\lambda\lambda'}+B(H^{(1)}(\bar{k},z)_{\lambda\lambda'})+\Delta_R. \quad (3.15)$$

Our task now is to diagonalize $\mathcal{H}_{\rm eff}$ by method of successive similarity transformation starting with $S_{\rm op}^0$, Eq. (3.4). For convenience in what follows, let us define "odd" and "even" operators and matrices. An even matrix is a diagonal matrix and the corresponding operator is called an even operator. An odd matrix and its corresponding operator is one where all diagonal (intraband) elements are zeros. Even operators and matrices commute, products of even matrices are even, whereas products of even and odd are odd. The zero-order term on the right-hand side of Eq. (3.15) is even, the remaining terms may be written as a sum of even and odd matrices. The rest of this section describes an iterative procedure for removing odd terms on the right-hand side of Eq. (3.15) up to arbitrary orders in the magnetic field strength. Odd terms in Eq. (3.15) correspond to the presence of interband terms in the effective Hamiltonian and its Weyl transform. To obtain the transformation represented by Eq. (3.1) up to any order in B, first we choose $G_{\rm op}^{(1)} \rightleftharpoons G^{(1)}(\bar{k},B,z)$ such that $[G^{(1)}(\bar{k};B,z),\tilde{H}^0(\bar{k};z)]=BH_{\rm odd}^{(1)}(\bar{k},z)$, where $H_{\rm odd}^{(1)}(\bar{k},z)$ is the odd part of $H^{(1)}(\bar{k},z)$ in Eq. (3.15), then it is easy to see that

$$e^{-G_{\rm op}^{(1)}}(S_{\rm op}^0)^{-1}\mathcal{H}_{\rm eff}S_{\rm op}^0e^{G_{\rm op}^{(1)}} \rightleftharpoons \tilde{H}_\lambda^0(\bar{k},z)\delta_{\lambda\lambda'}+BH_{\rm even}^{(1)}+B^2({}^{(1)}H_{\rm odd}^{(2)}+{}^{(1)}H_{\rm even}^{(2)})+{}^{(1)}\Delta_R, \quad (3.16)$$

showing that the right-hand side of Eq. (3.16) is even up to order B. Since $\tilde{H}^0(\bar{k},z)$ is even, $G^{(1)}(\bar{k},B,z)$ can be chosen odd. Its matrix elements is related to that of $H_{\rm odd}^{(1)}(\bar{k},z)$ and $\tilde{H}^0(\bar{k},z)$ by the relation

$$G_{ij}^{(1)}(\bar{k},B,z)=\begin{cases}B[H_{\rm odd}^{(1)}(\bar{k},z)]_{ij}\times[\tilde{H}_j^0(\bar{k},z)-\tilde{H}_i^0(\bar{k},z)]^{-1}, & i\neq j \quad (3.17)\\ 0, & i=j. \quad (3.18)\end{cases}$$

The procedure can now be reiterated, choosing $G_{\rm op}^{(2)} \rightleftharpoons G^{(2)}(\bar{k};B,z)$ such that $[G^{(2)}(\bar{k},B,z),\tilde{H}^0(\bar{k},z)]=B^2\,{}^{(1)}H_{\rm odd}^{(2)}(\bar{k},z)$ resulting in

$$e^{-G_{\rm op}^{(2)}}e^{-G_{\rm op}^{(1)}}S_{\rm op}^{0-1}\mathcal{H}_{\rm eff}S_{\rm op}^0e^{G_{\rm op}^{(1)}}e^{G_{\rm op}^{(2)}} \rightleftharpoons \tilde{H}^0(\bar{k},z)+BH_{\rm even}^{(1)}+B^2\,{}^{(1)}H_{\rm even}^{(2)}+B^3({}^{(2)}H_{\rm even}^{(3)}+{}^{(2)}H_{\rm odd}^{(3)})+{}^{(2)}\Delta_R, \quad (3.19)$$

with $G^{(2)}(\bar{k},B,z)$ given by

$$G_{ij}^{(2)}(\vec{k},B,z)=\begin{cases}B^2[{}^{(1)}H_{\text{odd}}^{(2)}(\vec{k},z)]_{ij}[\tilde{H}_j^0(\vec{k},z)-\tilde{H}_i^0(\vec{k},z)]^{-1}, & i\neq j, \quad (3.20)\\ 0, & i=j. \quad (3.21)\end{cases}$$

In general order n, we can choose $G_{\text{op}}^{(n+1)} \rightleftharpoons G^{(n+1)}(\vec{k},B,z)$ such that if

$$\prod_{i=n}^{1} e^{-G_{\text{op}}^{(n)}} S_{\text{op}}^{0-1}\mathcal{H}_{\text{eff}} S_{\text{op}}^0 \prod_{i=1}^{n} e^{G_{\text{op}}^{(n)}} \rightleftharpoons \tilde{H}^0(\vec{k},z)+\cdots+B^{n(n-1)}H_{\text{even}}^{(n)}(\vec{k},z)+B^{n+1}[{}^{(n)}H_{\text{odd}}^{(n+1)}(\vec{k},z)+{}^{(n)}H_{\text{even}}^{(n+1)}(\vec{k},z)]+{}^{(n)}\Delta_R, \quad (3.22)$$

then we have

$$G_{ij}^{(n+1)}(\vec{k},B,z)=\begin{cases}\dfrac{B^{n+1}[{}^{(n)}H_{\text{odd}}^{(n+1)}(\vec{k},z)]_{ij}}{\tilde{H}_j^0(\vec{k},z)-\tilde{H}_i^0(\vec{k},z)}, & i\neq j, \quad (3.23)\\ 0, & i=j. \quad (3.24)\end{cases}$$

We now have a complete iterative procedure for removing the interband terms in the lattice Weyl transform of $\mathcal{H}$ and, through Eq. (3.2), the resulting effective Hamiltonian becomes free of interband terms, yielding an effective Schrödinger equation for each band index λ. The procedure can, of course, only be guaranteed to converge for very small fields; for calculating the low-field susceptibility the removal of the interband terms up to second order in B is all that is required since higher-order terms do not contribute.

The removal of the interband terms in the lattice Weyl transform of $\mathcal{H}$, described above, suggests a second alternative but equivalent route for obtaining the lattice Weyl transform and effective Hamiltonian free of interband terms. This alternate route is believed to be straightforward for general Bloch bands although the first method may prove to be quite neat and elegant when there are very few bands involved, especially in cases where a small region in the Brillouin zone is all that is important.

First of all, we note that a lattice Weyl transform of $\mathcal{H}$ which is free of interband terms suggests the existence of magnetic Wannier function and magnetic Bloch function of interacting Bloch electrons. One can then proceed in a manner analogous to that used by Wannier and Upadhyaya,[12] which is a straightforward perturbative calculation employed for noninteracting Bloch electrons in a magnetic field, for obtaining the lattice Weyl transform and effective Hamiltonian, free of interband terms. As in the first method discussed above, we make the assumption that a well-defined Wannier function and Bloch function (in the absence of a magnetic field), which are in general energy dependent and biorthogonal, exist. This corresponds to having obtained the matrix $U(\vec{k},z)$ in Eq. (3.6).

The starting point in obtaining the lattice Weyl transform of $\mathcal{H}$, which is free of interband terms, is the equation defining the magnetic Wannier function on the corresponding equation defining the magnetic Bloch function. In the magnetic Wannier function representation we have

$$\mathcal{H}=\sum_{\lambda,\vec{q}',\vec{q}}\langle\lambda,\vec{q}',z,B|\mathcal{H}_0+\Sigma(z)|\lambda,\vec{q},z,B\rangle \times|\lambda,\vec{q}',z,B\rangle\langle\lambda,\vec{q},z,B|, \quad (3.25)$$

where the matrix elements of $\mathcal{H}_0+\Sigma(z)$ in general have dual magnetic Wannier functions on the left- and right-hand sides instead of the same wave function. The equation defining $|\lambda,\vec{q},z,B\rangle$ becomes

$$\mathcal{H}|\lambda,\vec{q},z,B\rangle=\sum_{\vec{q}'}\langle\lambda,\vec{q}',z,B|\mathcal{H}_0+\Sigma(z)|\lambda,\vec{q},z,B\rangle \times|\lambda,\vec{q}',z,B\rangle, \quad (3.26)$$

and that for $\langle\lambda,\vec{q},z,B|$ is

$$\langle\lambda,\vec{q}',z,B|\mathcal{H}=\sum_{\vec{q}'}\langle\lambda,\vec{q}',z,B|\mathcal{H}_0+\Sigma(z)|\lambda,\vec{q},z,B\rangle \times\langle\lambda,\vec{q},z,B|. \quad (3.27)$$

The form of $\langle\lambda,\vec{q}',z,B|\mathcal{H}_0+\Sigma(z)|\lambda,\vec{q},z,B\rangle$ is given in Appendix B which may be written

$$\langle\lambda,\vec{q}',z,B|\mathcal{H}_0+\Sigma(z)|\lambda,\vec{q},z,B\rangle =\exp[(ie/\hbar c)\vec{A}(\vec{q})\cdot\vec{q}']H_\lambda(\vec{q}-\vec{q}',B,z)\delta_{\lambda\lambda'}, \quad (3.28)$$

$$|\lambda,\vec{q},z,B\rangle = T(-\vec{q})|\lambda,0,z,B\rangle = \exp[(-ie/\hbar c)\vec{A}(\vec{r})\cdot\vec{q}]\,w_\lambda(\vec{r}-\vec{q},z,B), \quad (3.29)$$

where $T(-\vec{q})$ is the magnetic translation operator defined in Appendix B and $w_\lambda(\vec{r}-\vec{q},B,z)$ is the modified Wannier function centered at the lattice point $\vec{q}$. The equation satisfied by $|\lambda,0,z,B\rangle$ can explicitly be written

$$\mathcal{H}_0 w_\lambda(\vec{r},z,B) + \int d^3r'\,\Sigma(\vec{r},\vec{r}',z,B)\,w_\lambda(\vec{r}',z,B) = \sum_{\vec{q}'} H_\lambda(-\vec{q}',z,B)|\lambda,\vec{q}',z,B\rangle. \quad (3.30)$$

It is then easy to show that

$$\mathcal{H}|\lambda,\vec{q},z,B\rangle = T(-\vec{q})\mathcal{H}|\lambda,0,z,B\rangle, \quad (3.31)$$

which can be written explicitly as

$$\exp\left(-\frac{ie}{\hbar c}\vec{A}(\vec{r})\cdot\vec{q}\right)\mathcal{H}_0(\vec{r}-\vec{q})\,w_\lambda(\vec{r}-\vec{q},z,B) + \exp\left(\frac{-ie}{\hbar c}\vec{A}(\vec{r})\cdot\vec{q}\right)\int d^3r'\,\Sigma(\vec{r}-\vec{q},\vec{r}',z,B)\,w_\lambda(\vec{r}'-0,z,B)$$
$$= \sum_{\vec{q}'} \exp\left(\frac{ie}{\hbar c}\vec{A}(\vec{q})\cdot\vec{q}'\right) H_\lambda(\vec{q}-\vec{q}',z,B)\exp\left(\frac{-ie}{\hbar c}\vec{A}(\vec{r})\cdot\vec{q}'\right) w_\lambda(\vec{r}-\vec{q}',z,B). \quad (3.32)$$

Changing the variable of integration $\vec{r}'$ to $\vec{r}'-\vec{q}$, noting that by symmetry[3]

$$\Sigma(\vec{r},\vec{r}',z,B) = \exp[(-ie/\hbar c)\vec{A}(\vec{r})\cdot\vec{r}']\,\tilde{\Sigma}(\vec{r},\vec{r}',z,B), \quad (3.33)$$

where $\tilde{\Sigma}(\vec{r}-\vec{q},\vec{r}'-\vec{q},zB) = \tilde{\Sigma}(\vec{r},\vec{r}'z,B)$, dividing both sides of the equation by $\exp[(-ie/\hbar c)\vec{A}(\vec{r})\cdot\vec{q}]$ and taking the lattice Fourier transform [i.e., multiply both sides by $(1/N\hbar^3)^{1/2}\sum_{\vec{q}} e^{(i/\hbar)\vec{p}\cdot\vec{q}}$] we obtain

$$\mathcal{H}_0(\vec{p}-(e/c)\vec{A}(\vec{r}+i\nabla_{\vec{k}}),\vec{r})\,b_\lambda(\vec{r},\vec{k},B,z) + \int d^3r'\,e^{-(ie/\hbar c)\vec{A}(\vec{r})\cdot\vec{r}'}\tilde{\Sigma}(\vec{r},\vec{r}',z,B)\,b_\lambda\left(\vec{r}',\vec{k}+\frac{e}{\hbar c}\vec{A}(\vec{r}-\vec{r}');B,z\right)$$
$$= \sum_{\vec{q}} e^{i\vec{k}\cdot\vec{q}} H_\lambda(\vec{q},z,B)\,e^{(ie/\hbar c)\vec{A}(\vec{r})\cdot\vec{q}}\,b_\lambda\left(\vec{r},\vec{k}+\frac{e}{\hbar c}\vec{A}(\vec{q});B,z\right), \quad (3.34)$$

where the modified Bloch function $b_\lambda(\vec{r},\vec{k},B,z)$ is defined by

$$b_\lambda(\vec{r},\vec{k},B,z) = (N\hbar^3)^{-1/2}\sum_{\vec{q}} e^{i\vec{k}\cdot\vec{q}}\,w_\lambda(\vec{r}-\vec{q},z,B) \equiv e^{i\vec{k}\cdot\vec{r}}u_\lambda(\vec{r},\vec{k},z,B). \quad (3.35)$$

The equation satisfied by $u_\lambda(\vec{k},\vec{r},z,B)$ is

$$\mathcal{H}_0\left(\vec{p}+\hbar\vec{k}-\frac{e}{c}\vec{A}(i\nabla_{\vec{k}});\vec{r}\right)u_\lambda(\vec{r},\vec{k},z,B) + \int d^3r'\,e^{i\vec{k}\cdot(\vec{r}'-\vec{r})}\tilde{\Sigma}(\vec{r},\vec{r}',z,B)\,u_\lambda\left(\vec{r},\vec{k}+\frac{e}{\hbar c}\vec{A}(\vec{r}-\vec{r}'),z,B\right)$$
$$= \sum_{\vec{q}} e^{i\vec{k}\cdot\vec{q}} H_\lambda(\vec{q},z,B)\,u_\lambda\left(\vec{r},\vec{k}+\frac{e}{\hbar c}\vec{A}(\vec{q}),z,B\right). \quad (3.36)$$

Thereafter, a straightforward perturbative solution can be carried out by expanding all quantities in powers of B with zero-order terms given by the field-free quantities. To calculate the low-field χ we only need to expand all quantities to second order in B. The procedure is similar to that used by Wannier and Upadhyaya for noninteracting Bloch electrons except for the fact that here matrix elements are taken with dual wave functions, owing to the non-Hermitian nature of the self-energy. Let us write

$$\mathcal{H}_0 = \mathcal{H}_0^0 + B\mathcal{H}_0^{(1)} + B^2\mathcal{H}_0^{(2)}, \quad (3.37)$$

$$u_\lambda(\vec{r},\vec{k},z,B) = u_\lambda^0(\vec{r},\vec{k},z) + Bu_\lambda^{(1)}(\vec{r},\vec{k},z) + B^2u_\lambda^{(2)}(\vec{r},\vec{k},z) + \cdots, \quad (3.38)$$

$$\tilde{\Sigma}(\vec{r},\vec{r}',z,B) = \tilde{\Sigma}^0(\vec{r},\vec{r}',z) + B\tilde{\Sigma}^{(1)}(\vec{r},\vec{r}',z) + B^2\tilde{\Sigma}^{(2)}(\vec{r},\vec{r}',z) + \cdots, \quad (3.39)$$

$$u_\lambda[\vec{r},\vec{k}+(e/\hbar c)\vec{A}(\alpha),z,B] = e^{(e/\hbar c)\vec{A}(\alpha)\cdot\nabla_{\vec{k}}}\,u_\lambda(\vec{r},\vec{k},z,B). \quad (3.40)$$

We expand both sides of Eq. (3.36) up to second order in B and equate the coefficients on both sides. Multiplying both sides of the resulting equations by the dual set of wave functions $\langle u_\delta(\vec{r},\vec{k},z)|$, determined by Eq. (2.18) biorthogonal to $|u_\delta(\vec{r},\vec{k},z)\rangle\rangle$, and integrating, we obtain for $\delta=\lambda$ the expression for $H_\lambda^{(1)}(\vec{k},z)$ and $H_\lambda^{(2)}(\vec{k},z)$, where

$$H_\lambda^{(i)}(\vec{k},z)=\sum_{\vec{q}} e^{i\vec{k}\cdot\vec{q}}H_\lambda^{(i)}(\vec{q},z). \tag{3.41}$$

We have the following:

$$\begin{aligned}H_\lambda^{(1)}(\vec{k},z)=&\left\langle u_\lambda^0\middle|\mathcal{H}_0^{(1)}+\frac{e}{B\hbar c}[\vec{A}(\nabla_{\vec{k}})\tilde{H}_\lambda^0(\vec{k},z)]\cdot\nabla_{\vec{k}}\middle|u_\lambda^0\right\rangle\\&+\left\langle u_\lambda^0(\vec{r},\vec{k},z)\middle|\int d^3r'\,e^{i\vec{k}\cdot(\vec{r}\,'-\vec{r})}\tilde{\Sigma}^0(\vec{r},\vec{r}\,',z)\frac{e}{B\hbar c}\vec{A}(\vec{r}-\vec{r}\,')\cdot\nabla_{\vec{k}}u_\lambda^0(\vec{r}\,',\vec{k},z)\right\rangle\\&+\left\langle u_\lambda^0(\vec{r},\vec{k},z)\middle|\int d^3r'\,e^{i\vec{k}\cdot(\vec{r}\,'-\vec{r})}\tilde{\Sigma}^{(1)}(\vec{r},\vec{r}\,',z)u_\lambda^0(\vec{r}\,',\vec{k},z)\right\rangle,\end{aligned}\tag{3.42}$$

$$\begin{aligned}H_\lambda^{(2)}(\vec{k},z)=&\langle u_\lambda^0|\mathcal{H}_0^{(2)}|u_\lambda^0\rangle+\langle u_\lambda^0|\mathcal{H}_0^{(1)}|u_\lambda^{(1)}\rangle-\left\langle u_\lambda^0\middle|\sum_{\vec{q}}e^{i\vec{k}\cdot\vec{q}}\tilde{H}_\lambda^0(\vec{q},z)\frac{1}{2!}\left(\frac{e}{B\hbar c}\vec{A}(\vec{q})\cdot\nabla_{\vec{k}}\right)^2u_\lambda^0\right\rangle\\&+\left\langle u_\lambda^0\middle|\frac{e}{B\hbar c}[\vec{A}(\nabla_{\vec{k}})\tilde{H}_\lambda^0(\vec{k},z)]\cdot i\nabla_{\vec{k}}u_\lambda^{(1)}\right\rangle+\left\langle u_\lambda^0\middle|\frac{e}{B\hbar c}[\vec{A}(\nabla_{\vec{k}})H_\lambda^{(1)}(\vec{k},z)]\cdot i\nabla_{\vec{k}}u_\lambda^0\right\rangle-H_\lambda^{(1)}(\vec{k},z)\langle u_\lambda^0|u_\lambda^{(1)}\rangle\\&+\left\langle u_\lambda^0(\vec{r},\vec{k},z)\middle|\int d^3r'\,e^{i\vec{k}\cdot(\vec{r}\,'-\vec{r})}\tilde{\Sigma}^0(\vec{r},\vec{r}\,',z)\frac{1}{2!}\left(\frac{e}{B\hbar c}\vec{A}(\vec{r}-\vec{r}\,')\cdot\nabla_{\vec{k}}\right)^2u_\lambda^0(\vec{r}\,',\vec{k},z)\right\rangle\\&+\left\langle u_\lambda^0(\vec{r},\vec{k},z)\middle|\int d^3r'\,e^{i\vec{k}\cdot(\vec{r}\,'-\vec{r})}\tilde{\Sigma}^0(\vec{r},\vec{r}\,',z)\frac{e}{B\hbar c}\vec{A}(\vec{r}-\vec{r}\,')\cdot\nabla_{\vec{k}}u_\lambda^{(1)}(\vec{r}\,',\vec{k},z)\right\rangle\\&+\left\langle u_\lambda^0(\vec{r},\vec{k},z)\middle|\int d^3r'\,e^{i\vec{k}\cdot(\vec{r}\,'-\vec{r})}\tilde{\Sigma}^{(1)}(\vec{r},\vec{r}\,',z)\frac{e}{B\hbar c}\vec{A}(\vec{r}-\vec{r}\,')\cdot\nabla_{\vec{k}}u_\lambda^0(\vec{r}\,',\vec{k},z)\right\rangle\\&+\left\langle u_\lambda^0(\vec{r},\vec{k},z)\middle|\int d^3r'\,e^{i\vec{k}\cdot(\vec{r}\,'-\vec{r})}\tilde{\Sigma}^{(1)}(\vec{r},\vec{r}\,',z)u_\lambda^{(1)}(\vec{r}\,',\vec{k},z)\right\rangle\\&+\left\langle u_\lambda^0(\vec{r},\vec{k},z)\middle|\int d^3r'\,e^{i\vec{k}\cdot(\vec{r}\,'-\vec{r})}\tilde{\Sigma}^{(2)}(\vec{r},\vec{r}\,',z)\,u_\lambda^0(\vec{r}\,',\vec{k},z)\right\rangle.\end{aligned}\tag{3.43}$$

To obtain $H_\lambda^{(2)}(\vec{k},z)$ we need $u_\lambda^{(1)}(\vec{r},\vec{k},z)$, which can be written

$$|u_\lambda^{(1)}(\vec{r},\vec{k},z)\rangle\rangle=\sum_\delta\beta_{\lambda\delta}|u_\delta^0(\vec{r},\vec{k},z)\rangle\rangle, \tag{3.44}$$

and for $\lambda\neq\delta$, $\beta_{\lambda\delta}$ can de determined from the same set of equations λ which determined $H_\lambda^{(i)}(\vec{k},z)$. It is given by ($\beta_{\lambda\delta}=\langle u_\delta^0|u_\lambda^{(1)}\rangle$)

$$\langle u_\delta^0|u_\lambda^{(1)}\rangle=-[\tilde{H}_\delta^0(\vec{k},z)-\tilde{H}_\lambda^0(\vec{k},z)]^{-1}\langle u_\delta^0|H_\lambda^{(1)\text{op}}|u_\lambda^0\rangle, \tag{3.45}$$

where $\langle u_\delta^0|H_\lambda^{(1)\text{op}}|u_\lambda^0\rangle$ is given by Eq. (3.42) with the band index λ replaced by δ on the left-hand wave function. It is easy to see that had we started with Eq. (3.27) we arrive at

$$\langle u_\lambda^{(1)}(\vec{r},\vec{k},z)|=\sum_\delta\beta_{\delta\lambda}\langle u_\delta^0(\vec{r},\vec{k},z)|, \tag{3.46}$$

where for $\delta\neq\lambda$

$$\beta_{\delta\lambda}=-[\tilde{H}_\delta^0(\vec{k},z)-\tilde{H}_\lambda^0(\vec{k},z)]^{-1}\langle u_\lambda^0|H_\lambda^{(1)\text{op}}|u_\delta^0\rangle, \tag{3.47}$$

which is nothing but the complex conjugate of $\beta_{\lambda\delta}$ if $H_\lambda^{(1)\text{op}}$ is a Hermitian operator and $\tilde{H}_\alpha^0(\vec{k},z)$ are real quantities. Thus our results here serve to generalize the result of Wannier and Upadhyaya obtained for the cases where $\mathcal{H}$ is a completely Hermitian operator and its Weyl transform (and hence its eigenvalues) is real. For $\delta=\lambda$, $\beta_{\lambda\lambda}$ can be obtained from the requirement that the magnetic Wannier functions are biorthogonal.[9,12] This is expressed by the equation

$$\int d^3r\exp\left(\frac{1}{2}\frac{ie}{\hbar c}(\vec{B}\times\vec{r})\cdot(\vec{q}\,'-\vec{q})\right)\Omega_\lambda^*(\vec{r}-\vec{q}\,',z,B)\times w_\lambda(\vec{r}-\vec{q},z,B)=\delta_{\vec{q}\vec{q}\,'}, \tag{3.48}$$

where we have written

$$\langle\lambda,\vec{q}\,',z,B|=\exp\left(\frac{1}{2}\frac{ie}{\hbar c}(\vec{B}\times\vec{r})\cdot\vec{q}\,'\right)\Omega_\lambda^*(\vec{r}-\vec{q}\,',z,B). \tag{3.49}$$

Expanding the left-hand side of Eq. (3.48) in powers of B we obtain the following relations:

$$\langle\lambda',\vec{q}',z|\lambda,\vec{q},z\rangle=\delta_{qq'},\tag{3.50}$$

$$\langle\lambda,\vec{q}',z|w_\lambda^{(1)}(\vec{r}-\vec{q}',z)\rangle\!\rangle+\langle\!\langle\Omega_\lambda^{(1)*}(\vec{r}-\vec{q}',z)|\lambda,\vec{q},z\rangle$$
$$+\tfrac{1}{2}(ie/\hbar c)\langle\!\langle(\hat{z}\times\vec{r})\cdot(\vec{q}'-\vec{q})\Omega_\lambda^{0*}(\vec{r}-\vec{q}',z)$$
$$\times w_\lambda^0(\vec{r}-\vec{q},z)\rangle\!\rangle=0\ ,\tag{3.51}$$

where $\Omega_\lambda^{0*}(\vec{r}-\vec{q}',z)\equiv\langle\lambda,\vec{q}',z|$ and $w_\lambda^0(\vec{r}-\vec{q},z)\equiv|\lambda,\vec{q},z\rangle$. By virtue of the identity

$$(\hat{z}\times\vec{r})\cdot(\vec{q}'-\vec{q})=\hat{z}\cdot[(\vec{r}-\vec{q}')\times(\vec{r}-\vec{q})-(\vec{q}'\times\vec{q})]$$

and of Eq. (3.50) we obtain from Eq. (3.51), after lattice Fourier transformation,

$$\langle u_\lambda^0|u_\lambda^{(1)}\rangle+\langle u_\lambda^{(1)}|u_\lambda^0\rangle=\frac{1}{2}\frac{e}{\hbar c}\left(\frac{\partial}{\partial\vec{k}_y}X_\lambda-\frac{\partial}{\partial\vec{k}_x}Y_\lambda\right),\tag{3.52}$$

where

$$X_\lambda=\left\langle u_\lambda^0\left|i\frac{\partial}{\partial\vec{k}_x}u_\lambda^0\right.\right\rangle,\tag{3.53}$$

$$Y_\lambda=\left\langle u_\lambda^0\left|i\frac{\partial}{\partial\vec{k}_y}u_\lambda^0\right.\right\rangle.\tag{3.54}$$

Equation (3.52) yields the expression for $\beta_{\lambda\lambda}$,

$$\beta_{\lambda\lambda}=\frac{1}{4}\frac{e}{\hbar c}\left(\frac{\partial}{\partial\vec{k}_y}X_\lambda-\frac{\partial}{\partial\vec{k}_x}Y_\lambda\right).\tag{3.55}$$

The last result completely determines $H_\lambda^{(1)}(\vec{k},z)$ and $H_\lambda^{(2)}(\vec{k},z)$ in the expansion of $\tilde{H}_\lambda(\vec{k},z)$ in powers of B. The lattice Weyl transform, which is free of interband terms, is obtained by replacement of $\hbar\vec{k}$ by $[\hbar\vec{k}-(e/c)\vec{A}(\vec{q})]$ in $\tilde{H}_\lambda(\vec{k},z)$ (see Appendix B). Thus the right-hand side of Eq. (3.1) written up to second order in its explicit dependence in B, beyond the vector potential, is given by

$$\tilde{H}_\lambda[\vec{p}-(e/c)\vec{A}(\vec{q}),B,z]$$
$$=\tilde{H}_\lambda^0[\vec{p}-(e/c)\vec{A}(\vec{q}),z]+BH_\lambda^{(1)}[\vec{p}-(e/c)\vec{A}(\vec{q}),z]$$
$$+B^2H_\lambda^{(2)}[\vec{p}-(e/c)\vec{A}(\vec{q}),z]+\cdots.\tag{3.56}$$

IV. DERIVATION OF GENERAL FORMULA FOR χ

In this section we will derive the most general expression for χ using the temperature Green's-function formalism of Luttinger and Ward.[13] The magnetic susceptibility for a system of volume V is given by

$$\chi=\frac{1}{V}\lim_{B\to0}\frac{\partial^2}{\partial B^2}\left(\frac{1}{\beta}\ln Z\right),\tag{4.1}$$

where Z is the grand partition function. At zero-temperature limit, we may write[14]

$$\chi=\frac{1}{V}\lim_{\substack{B\to0\\ \beta\to\infty}}\frac{\partial^2}{\partial B^2}\left(\frac{\partial}{\partial\beta}\ln Z\right).\tag{4.2}$$

The expression for $\ln Z$ as a functional of the temperature Green's function $\mathcal{G}_{\zeta_l}$ is given by Luttinger and Ward,[13,14]

$$-\ln Z=\Phi(\mathcal{G}_{\zeta_l})-\mathrm{Tr}\,\Sigma(\mathcal{G}_{\zeta_l})\mathcal{G}_{\zeta_l}+\mathrm{Tr}\ln(-\mathcal{G}_{\zeta_l}),\tag{4.3}$$

where the temperature Green's-function operator $\mathcal{G}_{\zeta_l}$ is defined formally by

$$\mathcal{G}_{\zeta_l}^{-1}=\zeta_l-\mathcal{H}_0-\Sigma_{\zeta_l},\tag{4.4}$$

$$\zeta_l=(2l+1)\pi i/\beta+\mu.\tag{4.5}$$

Tr is defined as $\sum_l\tilde{\mathrm{T}}\mathrm{r}$, where $\tilde{\mathrm{T}}\mathrm{r}$ refers to taking the trace in any convenient representation. The functional $\Phi(\mathcal{G}_{\zeta_l})$ is defined[13-16] as

$$\Phi(\mathcal{G}_{\zeta_l})=\lim_{\lambda\to1}\mathrm{Tr}\sum_n\frac{\lambda^n}{2n}\Sigma^{(n)}(\mathcal{G}_{\zeta_l})\mathcal{G}_{\zeta_l}.\tag{4.6}$$

$\Sigma^{(n)}(\mathcal{G}_{\zeta_l})$ is the nth-order self-energy part where only the interaction parameter λ occurring explicitly in (4.6) is used to determine the order. Indeed, $\Phi(\mathcal{G}_{\zeta_l})$ is defined through the decomposition of $\Sigma^{(n)}(\mathcal{G}_{\zeta_l})$ into skeleton diagrams. There are $2n$ $\mathcal{G}_{\zeta_l}$ lines for the nth-order diagram in $\Phi(\mathcal{G}_{\zeta_l})$. Differentiation of $\Phi(\mathcal{G}_{\zeta_l})$ with respect to $\mathcal{G}_{\zeta_l}$ has the effect of "opening" any of the $2n$ lines of an nth-order diagram and each will give the same contribution when $\tilde{\mathrm{T}}\mathrm{r}$ is taken.[13] The reader is referred to Ref. 13 and to the work of Baym,[14] Bloch,[15] and the book of Nozières[16] for more discussion of the functional $\Phi(\mathcal{G}_{\zeta_l})$.

It is convenient to work in the coordinate representation as a first step to simplify the right-hand side of Eq. (4.1). The total Hamiltonian in this representation takes the form

$$\mathcal{H}=\int d^3r\,\psi_\alpha^\dagger(\vec{r})\mathcal{H}_0\psi_\alpha(\vec{r})$$
$$+\tfrac{1}{2}\int d^3r\,d^3r'\;\psi_\alpha^\dagger(\vec{r})\,\psi_\beta^\dagger(\vec{r}')v_{\alpha\beta\gamma s}(\vec{r},\vec{r}')\,\psi_\gamma(\vec{r}')\,\psi_\delta(\vec{r}),\tag{4.7}$$

where repeated spin indices are summed over, and for simplicity, we may take Eq. (2.2) for $\mathcal{H}_0$. $v_{\alpha\beta\gamma s}(\vec{r},\vec{r}')$ is the interaction between a pair of particles assumed to be velocity independent; this immediately implies that in coordinate representation the field dependence of $\ln Z$ in (4.3) occurs only through the field dependence of $\mathcal{G}_{\zeta_l}(\vec{r},\vec{r}')$. To take spin into account explicitly, both $\mathcal{G}_{\zeta_l}$ and Σ_{ζ_l} must be considered as 2×2 matrices in spin indices. The form of $\mathcal{G}_{\zeta_l}(\vec{r},\vec{r}')$ and $\Sigma_{\zeta_l}(\vec{r},\vec{r}')$ is given by Eq. (3.33) by gauge invariance. It is convenient for our purpose to expand $\Sigma_{\zeta_l}(\vec{r},\vec{r}')$ in powers of its explicit dependence on the magnetic field (beyond the Peierls phase factor) and write

$$\Sigma_{\zeta_l}(\vec{r},\vec{r}')=\Sigma^0_{\zeta_l}(\vec{r},\vec{r}')+B\Sigma^{(1)}_{\zeta_l}(\vec{r},\vec{r}')+B^2\Sigma^{(2)}_{\zeta_l}(\vec{r},\vec{r}')+\cdots, \tag{4.8}$$

where the remaining field dependence of $\Sigma^0_{\zeta_l}(\vec{r},\vec{r}')$, $\Sigma^{(1)}_{\zeta_l}(\vec{r},\vec{r}')$, and $\Sigma^{(2)}_{\zeta_l}(\vec{r},\vec{r}')$ occurs only through the Peierls phase factor. We now wish to evaluate $\partial^2 \ln Z/\partial B^2$ using Eq. (4.3). We have, using the definition of $\Phi(\mathcal{G}_{\zeta_l})$, the following relations:

$$\frac{\partial^2\Phi(\mathcal{G}_{\zeta_l})}{\partial B^2}\bigg|_{B\to 0}=\sum_l\int d^3r\,d^3r'\left(\tilde{\Sigma}^{(1)}_{\zeta_l}(\vec{r},\vec{r}')\frac{\partial\tilde{\mathcal{G}}_{\zeta_l}}{\partial B}(\vec{r},\vec{r}',B)\bigg|_{B\to 0}+\tilde{\Sigma}^0_{\zeta_l}(\vec{r},\vec{r}')\frac{\partial^2}{\partial B^2}\mathcal{G}_{\zeta_l}(\vec{r},\vec{r}',B)\bigg|_{B\to 0}\right), \tag{4.9}$$

$$\frac{-\partial^2}{\partial B^2}\mathrm{Tr}\Sigma_{\zeta_l}\mathcal{G}_{\zeta_l}\bigg|_{B\to 0}=-\sum_l\int d^3r\,d^3r'\left(2\tilde{\Sigma}^{(2)}_{\zeta_l}(\vec{r},\vec{r}')\tilde{\mathcal{G}}_{\zeta_l}(\vec{r},\vec{r}',B)\bigg|_{B\to 0}+2\tilde{\Sigma}^{(1)}_{\zeta_l}(\vec{r},\vec{r}')\frac{\partial}{\partial B}\tilde{\mathcal{G}}_{\zeta_l}(\vec{r},\vec{r}',B)\bigg|_{B\to 0}+\tilde{\Sigma}^0_{\zeta_l}(\vec{r},\vec{r}')\frac{\partial^2}{\partial B^2}\tilde{\mathcal{G}}_{\zeta_l}(\vec{r},\vec{r}',B)\bigg|_{B\to 0}\right). \tag{4.10}$$

The above relations lead to a more convenient expression for χ,

$$\chi=-\frac{1}{V}\left(\frac{\partial^2}{\partial B^2}\frac{1}{\beta}\mathrm{Tr}\ln(-\mathcal{G}_{\zeta_l})\right)_{B\to 0}+\frac{1}{V}\left(\frac{1}{\beta}\mathrm{Tr}2\tilde{\Sigma}^{(2)}_{\zeta_l}\tilde{\mathcal{G}}_{\zeta_l}+\frac{1}{\beta}\mathrm{Tr}\tilde{\Sigma}^{(1)}_{\zeta_l}\frac{\partial}{\partial B}\tilde{\mathcal{G}}_{\zeta_l}\right)_{B\to 0}, \tag{4.11}$$

where $\tilde{\Sigma}^{(i)}_{\zeta_l}$ are field-independent quantities. The advantage of this expression, aside from calculational convenience in what follows, is that it already displays some familiar features. The first term in Eq. (4.11) has exactly the same form[13] as that of the noninteracting Fermi systems, except for the replacement of the "noninteracting $\mathcal{G}_{\zeta_l}$" by the exact $\mathcal{G}_{\zeta_l}$ for the interacting, free, or Bloch, electrons. The second term can be immediately recognized as correction to the "crystalline induced diamagnetism" calculated from the first term. The last term turns out to contain corrections to both the "crystalline paramagnetism" and "crystalline induced diamagnetism" as calculated from the first term in Eq. (4.11).

We now take advantage of the fact that, for systems possessing translational symmetry, the trace over wave vector $\vec{k}$ and band index λ can, conveniently, be carried out in terms of a Weyl transform, discussed at length in Sec. III. We are, in the present case, of course, interested in the effective one-particle Schrödinger Hamiltonian[17]

$$\mathcal{H}_{\zeta_l}=\mathcal{H}_0+\Sigma_{\zeta_l}, \tag{4.12}$$

which is formally the same as that of Eq. (2.1), with the replacement $z\to\zeta_l$ (we have chosen to indicate the discrete frequency dependence of operators by a subscript). Therefore, all the results of Sec. III can be formally carried over to apply to the effective Hamiltonian given above. The beauty and power in the use of the Weyl transform is that the Weyl transform of an operator is a physically meaningful quantity and faithfully corresponds to the original quantum-mechanical operator. Moreover, it provides a natural way of calculating the trace of any function of $\mathcal{H}_{\zeta_l}$ as a power-series expansion in $\hbar$, Planck's constant, which is equivalent to an expansion in the magnetic field strength for Fermi systems possessing translational symmetry. We have, for an arbitrary function $F(\mathcal{H}_{\zeta_l})$, the following expression[6,7]:

$$\tilde{\mathrm{T}}\mathrm{r}F(\mathcal{H}_{\zeta_l})=\left(\frac{1}{2\pi}\right)^3\sum_\lambda\int d^3k\,d^3q\left\{F(\tilde{H}_\lambda(\vec{k},B,\zeta_l))-\frac{1}{24}\left(\frac{eB}{\hbar c}\right)^2F''(\tilde{H}^0_\lambda(\vec{k},\zeta_l))\left[\frac{\partial^2\tilde{H}^0_\lambda}{\partial\vec{k}_x^2}\frac{\partial\tilde{H}^0_\lambda}{\partial\vec{k}_y^2}-\left(\frac{\partial^2\tilde{H}^0_\lambda}{\partial\vec{k}_x\,\partial\vec{k}_y}\right)^2\right]\right\}+O(B^4), \tag{4.13}$$

where, $\vec{p}-(e/c)\vec{A}(\vec{q})$ in (3.56) is replaced by $\hbar\vec{k}$ in Eq. (4.13). In the above expression, it is assumed that $\tilde{H}^0_\lambda(\vec{k},\zeta_l)$ is diagonal in spin indices; this is generally true for nonferromagnetic systems.[7] The first term in Eq. (4.13) can then be expanded up to second order in B using the expansion given in Eq. (3.56). Applying this result to the first term of Eq. (4.11), we obtain

$$-\frac{1}{V}\left[\frac{\partial^2}{\partial B^2}\left(\frac{1}{\beta}\mathrm{Tr}\ln(-\mathcal{G}_{\zeta_l})\right)\right]_{B\to 0}=\chi_{\mathrm{LP}}+\chi_{\mathrm{CP}}+\chi_{\mathrm{ID}}, \tag{4.14}$$

where

$$\chi_{\text{LP}} = \frac{1}{12}\left(\frac{e}{\hbar c}\right)^2 \sum_\lambda \left(\frac{1}{2\pi}\right)^3 \int d^3k\, k_B T \times \sum_l \left[\frac{\partial^2 \tilde{H}^0_\lambda}{\partial \vec{k}_x^2}\frac{\partial^2 \tilde{H}^0_\lambda}{\partial \vec{k}_y^2} - \left(\frac{\partial^2 \tilde{H}^0_\lambda}{\partial \vec{k}_x \partial \vec{k}_y}\right)^2\right] \times \mathcal{G}^2_\lambda(\vec{k},\zeta_l), \tag{4.15}$$

$$\chi_{\text{CP}} = -\sum_\lambda \left(\frac{1}{2\pi}\right)^3 \int d^3k\, k_B T \times \sum_l \left[\tilde{H}^{(1)}_\lambda(\vec{k},\zeta_l)\right]^2 \mathcal{G}^2_\lambda(\vec{k},\zeta_l), \tag{4.16}$$

$$\chi_{\text{ID}} = -\sum_\lambda \left(\frac{1}{2\pi}\right)^3 \int d^3k\, k_B T \sum_l 2\tilde{H}^{(2)}_\lambda(\vec{k},\zeta_l)\mathcal{G}_\lambda(\vec{k},\zeta_l), \tag{4.17}$$

$$\mathcal{G}_\lambda(\vec{k},\zeta_l) = [\zeta_l - \tilde{H}^0_\lambda(\vec{k},\zeta_l)]^{-1}. \tag{4.18}$$

In Eqs. (4.15), (4.16), and (4.17), taking the trace over spin indices is implied. χ_{LP} is a generalized Landau-Peierls formula for the orbital diamagnetism of free and Bloch electrons. It is for the case of an interacting free-electron gas that this term was derived by Fukuyama and McClure.[4] In the limit of vanishing self-energy parts, Eq. (4.14) exactly reproduces the expression for χ of Bloch electrons, both with or without spin-orbit coupling, as given by Roth, and by Wannier and Upadhyaya,[12] respectively. Moreover, when the self-energy part is assumed to be independent of ζ_l, which holds true in Hartree-Fock approximation, the form of Eq. (4.14), after summation over ζ_l, is exactly the same as that of the noninteracting case. χ_{CP}, which includes the effect of free-electron spin, will be referred to as the crystalline paramagnetism, and χ_{ID}, the induced diamagnetism, although its sign cannot be determined *a priori* even in the Hartree-Fock approximation and in the noninteracting case.[12]

We consider the correction terms represented by the last two terms of Eq. (4.11). As we have mentioned earlier, these corrections only modify χ_{CP} and χ_{ID}, but do not affect χ_{LP}. Let us recast the last two terms of Eq. (4.11), which we now denote by χ_{corr}, and write them as follows:

$$\chi_{\text{corr}} = \frac{1}{V}\lim_{B\to 0}\frac{\partial}{\partial B}\text{Tr}\,\frac{1}{\beta}(\Sigma^{(1)}_{\zeta_l} + 2B\Sigma^{(2)}_{\zeta_l})\mathcal{G}_{\zeta_l}. \tag{4.19}$$

Recall that in the coordinate representation, the Peierls phase factors occurring in $\Sigma^{(i)}_{\zeta_l}$ and $\mathcal{G}_{\zeta_l}$ cancel. However, it is convenient to retain these phase factors in Eq. (4.19) as the trace will now be taken using the biorthogonal magnetic function representation discussed in Sec. III. The trace would then be expressed in terms of the Weyl transform, where indeed the Weyl transform of $\mathcal{G}_{\zeta_l}$ is diagonal in band indices, resulting in much simplification. We have[6]

$$\chi_{\text{corr}} = \lim_{B\to 0}\frac{\partial}{\partial B}\sum_\lambda\left(\frac{1}{2\pi}\right)^3\int d^3k\, k_B T \times \sum_l[\Sigma^{(1)}_{\lambda\lambda}(\vec{k},B,\zeta_l) + 2B\Sigma^{(2)}_{\lambda\lambda}(\vec{k},B,\zeta_l)] \times \mathcal{G}_\lambda(\vec{k},B,\zeta_l), \tag{4.20}$$

where in the last equation a familiar change of variable has been made, $\vec{p} - (e/c)\vec{A}(\vec{q}) \to \hbar\vec{k}$, and from Eq. (3.9) we have

$$\mathcal{G}_\lambda(\vec{k},B,\zeta_l) = [\zeta_l - \tilde{H}_\lambda(\vec{k},B,\zeta_l)]^{-1} + O(B^2). \tag{4.21}$$

$\tilde{H}_\lambda(\vec{k},B,\zeta_l)$ is of the form given by Eq. (3.56) with the replacement $z\to\zeta_l$. Since we need $\Sigma^{(2)}_{\lambda\lambda}(\vec{k},B,\zeta_l)$ only to zero order in the field, the calculation of the second term in Eq. (4.20) is trivial. Denoting this contribution as $\chi^{(2)}_{\text{corr}}$, we have

$$\chi^{(2)}_{\text{corr}} = \sum_\lambda\left(\frac{1}{2\pi}\right)^3\int d^3k\, k_B T\sum_l 2\left\langle u^0_\lambda(\vec{r},\vec{k},\zeta_l)\left|\int d^3r'\, e^{i\vec{k}\cdot(\vec{r}'-\vec{r})}\Sigma^{(2)}_{\zeta_l}(\vec{r},\vec{r}')u^0_\lambda(\vec{r}',\vec{k},\zeta_l)\right.\right\rangle \mathcal{G}_\lambda(\vec{k},\zeta_l). \tag{4.22}$$

$\chi^{(2)}_{\text{corr}}$ is indeed a correction to χ_{ID} as can be seen from Eqs. (4.17) and (3.43). Further clarification of the above result can be obtained from the calculation $\Sigma^{(1)}(\vec{k},B,\zeta_l)$. To find $\Sigma^{(1)}(\vec{k},B,\zeta_l)$, we utilize the results of Appendix B [in particular (B14)] and write down the effect of operating $\Sigma^{(1)}_{\zeta_l}$ on the magnetic Bloch function (same relation holds for $\Sigma^{(2)}_{\zeta_l}$)

$$\Sigma^{(1)}_{\zeta_l}|\vec{p},\lambda,\zeta_l,B\rangle = \sum_{\vec{q},\lambda'} e^{i\vec{p}\cdot\vec{q}/\hbar}[\Sigma^{(1)}_{\zeta_l}(\vec{q},B)]_{\lambda\lambda'} \times|\vec{p}+(e/c)\vec{A}(\vec{q}),\lambda',\zeta_l,B\rangle. \tag{4.23}$$

The Weyl transform of $\Sigma^{(1)}_{\zeta_l}$, as defined by (A4), is

$$\Sigma^{(1)}_{\lambda\lambda'}(\vec{p},\vec{q},\zeta_l,B) = \sum_{\vec{u}} e^{(2i/\hbar)\vec{q}\cdot\vec{u}}\langle\vec{p}+\vec{u},\lambda,\zeta_l,B|\Sigma^{(1)}_{\zeta_l}|\vec{p}-\vec{u},\lambda',\zeta_l,B\rangle, \tag{4.24}$$

and by virtue of Eq. (4.23) we obtain

$$\Sigma^{(1)}_{\lambda\lambda'}(\vec{p},\vec{q},\zeta_l,B) = \sum_{\vec{u}} e^{(2i/\hbar)\vec{q}\cdot\vec{u}} \sum_{\vec{v}} \delta_{u,(e/c)\vec{A}(\vec{v})/2}\, e^{(i/\hbar)\vec{p}\cdot\vec{v}} [\Sigma^{(1)}_{\zeta_l}(\vec{v},B)]_{\lambda\lambda'} = \sum_{\vec{v}} \exp\left[\frac{1}{\hbar}\left(\vec{p}-\frac{e}{c}\vec{A}(\vec{q})\right)\cdot\vec{v}\right][\Sigma^{(1)}_{\zeta_l}(\vec{v},B)]_{\lambda\lambda'}, \tag{4.25}$$

which in turn yields

$$\Sigma^{(1)}_{\lambda\lambda'}(\vec{p},\vec{q},\zeta_l,B)\big|_{\vec{p}-(e/c)\vec{A}(\vec{q})-\hbar\vec{k}} = \sum_{\vec{v}} e^{i\vec{k}\cdot\vec{v}}[\Sigma^{(1)}_{\zeta_l}(\vec{v},B)]_{\lambda\lambda'}. \tag{4.26}$$

We are therefore interested in the right-hand side of Eq. (4.26), to obtain this we may proceed in a manner quite similar to that used in Sec. III, i.e., Eqs. (3.30)–(3.43). However, at this stage, Eq. (4.23) provides a very good starting point. The relation between $|\vec{p},\lambda,\zeta_l,B\rangle$ and the modified Bloch function $b_\lambda(\vec{r},\vec{k},B,\zeta_l)$, used in the perturbation theory of Sec. III, can be easily deduced from Eqs. (3.29) and (3.35)

$$|\vec{p},\lambda,\zeta_l,B\rangle = b_\lambda[\vec{r},\vec{k}-(e/\hbar c)\vec{A}(\vec{r}),B,\zeta_l]. \tag{4.27}$$

Let us make the substitution $\vec{p}\to\vec{p}'+(e/c)\vec{A}(\vec{r})$ in Eq. (4.23) and obtain the relation

$$\int e^{-(ie/\hbar c)\vec{A}(\vec{r})\cdot\vec{r}'}\tilde{\Sigma}^{(1)}_{\zeta_l}(\vec{r},\vec{r}')b_\lambda\left(\vec{r}',\vec{p}'+\frac{e}{c}\vec{A}(\vec{r}-\vec{r}'),B,\zeta_l\right)d^3r' = \sum_{\vec{q},\lambda'}\exp\left[\frac{i}{\hbar}\left(\vec{p}'+\frac{e}{c}\vec{A}(\vec{r})\right)\cdot\vec{q}\right][\Sigma^{(1)}_{\zeta_l}(\vec{q},B)]_{\lambda\lambda'}b_{\lambda'}\left(\vec{r},\vec{p}'+\frac{e}{c}\vec{A}(\vec{q}),B,\zeta_l\right). \tag{4.28}$$

The equation in terms of the modified periodic function $u_\lambda(\vec{r},\vec{k},\zeta_l,B)$ is therefore given by

$$\int e^{i\vec{k}\cdot(\vec{r}'-\vec{r})}\tilde{\Sigma}^{(1)}_{\zeta_l}(\vec{r},\vec{r}')u_\lambda\left(\vec{r}',\vec{k}+\frac{e}{\hbar c}\vec{A}(\vec{r}-\vec{r}'),\zeta_l,B\right)d^3r' = \sum_{\vec{q},\lambda'}e^{i\vec{k}\cdot\vec{q}}[\Sigma^{(1)}_{\zeta_l}(\vec{q},B)]_{\lambda\lambda'}u_{\lambda'}\left(\vec{r},\vec{k}+\frac{e}{\hbar c}\vec{A}(\vec{q}),\zeta_l,B\right). \tag{4.29}$$

Equation (4.29) corresponds to Eq. (3.36) of Sec. III. Perturbative treatment can then be carried out, using Eqs. (3.38) and (3.39), and solution is obtained up to first order in B for $\Sigma^{(1)}_{\lambda\lambda}(\vec{k},B,\zeta_l)$. Writing

$$\Sigma^{(1)}_{\lambda\lambda}(\vec{k},B,\zeta_l) = \Sigma^{(1)0}_{\lambda\lambda}(\vec{k},\zeta_l) + B\Sigma^{(1)(1)}_{\lambda\lambda}(\vec{k},\zeta_l)+\cdots, \tag{4.30}$$

we get, by equating the zero- and first-order coefficients of B, the following relations:

$$\int e^{i\vec{k}\cdot(\vec{r}'-\vec{r})}\tilde{\Sigma}^{(1)}_{\zeta_l}(\vec{r},\vec{r}')u^0_\lambda(\vec{r}',\vec{k},\zeta_l)\,d^3r' = \sum_{\vec{q},\lambda'}e^{i\vec{k}\cdot\vec{q}}[\Sigma^{(1)0}_{\zeta_l}(\vec{q})]_{\lambda\lambda'}u^0_{\lambda'}(\vec{r},\vec{k},\zeta_l), \tag{4.31}$$

$$\int e^{i\vec{k}\cdot(\vec{r}'-\vec{r})}\tilde{\Sigma}^{(1)}_{\zeta_l}(\vec{r},\vec{r}')u^{(1)}_\lambda(\vec{r}',\vec{k},\zeta_l)\,d^3r' + \int e^{i\vec{k}\cdot(\vec{r}'-\vec{r})}\tilde{\Sigma}^{(1)}_{\zeta_l}(\vec{r},\vec{r}')\frac{e}{B\hbar c}\vec{A}(\vec{r}-\vec{r}')\cdot\nabla_{\vec{k}}u^0_\lambda(\vec{r}',\vec{k},\zeta_l)\,d^3r$$
$$= \sum_{\vec{q},\lambda'}e^{i\vec{k}\cdot\vec{q}}\left([\Sigma^{(1)0}_{\zeta_l}(\vec{q})]_{\lambda\lambda'}\frac{e}{B\hbar c}\vec{A}(\vec{q})\cdot\nabla_{\vec{k}}u^0_{\lambda'}(\vec{r},\vec{k},\zeta_l) + [\Sigma^{(1)0}_{\zeta_l}(\vec{q})]_{\lambda\lambda'}u^{(1)}_{\lambda'}(\vec{r},\vec{k},\zeta_l) + [\Sigma^{(1)(1)}_{\zeta_l}(\vec{q})]_{\lambda\lambda'}u^0_{\lambda'}(\vec{r},\vec{k},\zeta_l)\right). \tag{4.32}$$

These relations yield for $\Sigma^{(1)0}_{\zeta_l}(\vec{k},\zeta_l)$ and $\Sigma^{(1)(1)}_{\lambda\lambda}(\vec{k},\zeta_l)$ the following expressions:

$$\Sigma^{(1)0}_{\lambda\lambda}(\vec{k},\zeta_l) = \left\langle u^0_\lambda(\vec{r},\vec{k},\zeta_l)\right|\left.\int d^3r'\,e^{i\vec{k}\cdot(\vec{r}'-\vec{r})}\tilde{\Sigma}^{(1)}_{\zeta_l}(\vec{r},\vec{r}')u^0_\lambda(\vec{r}',\vec{k},\zeta_l)\right\rangle, \tag{4.33}$$

$$\begin{aligned}\Sigma^{(1)(1)}_{\lambda\lambda}(\vec{k},\zeta_l) &= \left\langle u^0_\lambda(\vec{r},\vec{k},\zeta_l)\right|\left.\int d^3r'\,e^{i\vec{k}\cdot(\vec{r}'-\vec{r})}\tilde{\Sigma}^{(1)}_{\zeta_l}(\vec{r},\vec{r}')u^{(1)}_\lambda(\vec{r}',\vec{k},\zeta_l)\right\rangle \\ &+ \left\langle u^0_\lambda(\vec{r},\vec{k},\zeta_l)\right|\left.\int d^3r'\,e^{i\vec{k}\cdot(\vec{r}'-\vec{r})}\tilde{\Sigma}^{(1)}_{\zeta_l}(\vec{r},\vec{r}')\frac{e}{B\hbar c}\vec{A}(\vec{r}-\vec{r}')\cdot\nabla_{\vec{k}}u^0_\lambda(\vec{r}',\vec{k},\zeta_l)\right\rangle \\ &+ \left\langle u^0_\lambda(\vec{r},\vec{k},\zeta_l)\right|\sum_{\lambda'}\left(\frac{e}{B\hbar c}\vec{A}(\nabla_{\vec{k}})\sum_{\vec{q}}e^{i\vec{k}\cdot\vec{q}}[\tilde{\Sigma}^{(1)0}_{\zeta_l}(\vec{q})]_{\lambda\lambda'}\right)\cdot i\nabla_{\vec{k}}u^0_{\lambda'}(\vec{r},\vec{k},\zeta_l)\Big\rangle \\ &- \sum_{\lambda'}\Sigma^{(1)0}_{\lambda\lambda'}(\vec{k},\zeta_l)\langle u^0_\lambda(\vec{r},\vec{k},\zeta_l)|u^{(1)}_{\lambda'}(\vec{r},\vec{k},\zeta_l)\rangle.\end{aligned} \tag{4.34}$$

The first and last terms of Eq. (4.34) can be combined through the use of Eqs. (3.44), (3.45), and (4.31) to yield

$$\left\langle u_\lambda^0(\vec{r},\vec{k},\zeta_l)\right| \int d^3r'\, e^{i\vec{k}\cdot(\vec{r}'-\vec{r})}\tilde{\Sigma}_{\zeta_l}^{(1)}(\vec{r},\vec{r}')u_\lambda^{(1)}(\vec{r}',\vec{k},\zeta_l)\Big\rangle - \sum_{\lambda'}\Sigma_{\lambda\lambda'}^{(1)0}(\vec{k},\zeta_l)\langle u_\lambda^0(\vec{r},\vec{k},\zeta_l)|u_{\lambda'}^{(1)}(\vec{r},\vec{k},\zeta_l)\rangle$$
$$= -\sum_{\lambda'\neq\lambda} 2(\tilde{H}_{\lambda'}^0-\tilde{H}_\lambda^0)^{-1}\langle u_\lambda^0|\mathcal{H}_\delta^{(1)}u_{\lambda'}^0\rangle\langle u_{\lambda'}^0|\mathcal{H}_\delta^{(1)}u_\lambda^0\rangle$$
$$-\sum_{\lambda'\neq\lambda}(\tilde{H}_{\lambda'}^0-\tilde{H}_\lambda^0)^{-1}(\langle u_{\lambda'}^0|\mathcal{H}_\Delta^{(1)}u_\lambda^0\rangle\langle u_\lambda^0|\mathcal{H}_\delta^{(1)}u_{\lambda'}^0\rangle + \langle u_\lambda^0|\mathcal{H}_\Delta^{(1)}u_{\lambda'}^0\rangle\langle u_{\lambda'}^0|\mathcal{H}_\delta^{(1)}u_\lambda^0\rangle), \tag{4.35}$$

where the operators $\mathcal{H}_\Delta^{(1)}$ and $\mathcal{H}_\delta^{(1)}$ are defined such that $\langle u_\lambda^0|\mathcal{H}_\Delta^{(1)}u_\lambda^0\rangle$ is given by the first two terms, and $\langle u_\lambda^0|\mathcal{H}_\delta^{(1)}u_\lambda^0\rangle$ by the last term, of Eq. (3.42) ($z\to\zeta_l$ and ζ_l occur as subscripts in $\Sigma^{(1)}$). With the aid of Eq. (4.31) and noting that the vector potential function used is in symmetric gauge, the second term of Eq. (4.34) can be shown to be equal to the third term. Putting all these results together, Eqs. (4.22), (4.30), and (4.33)–(4.35) in Eq. (4.20), we obtain the total susceptibility correction $\chi_{\rm corr}$ as

$$\chi_{\rm corr} = \sum_\lambda\left(\frac{1}{2\pi}\right)^3\int d^3k\, k_BT\sum_l 2\left\langle u_\lambda^0(\vec{r}',\vec{k},\zeta_l)\right|\int d^3r'\, e^{i\vec{k}\cdot(\vec{r}'-\vec{r})}\tilde{\Sigma}_{\zeta_l}^{(2)}(\vec{r},\vec{r}')u_\lambda^0(\vec{r}',\vec{k},\zeta_l)\Big\rangle\, \mathcal{G}_\lambda(\vec{k},\zeta_l)$$
$$+\sum_\lambda\left(\frac{1}{2\pi}\right)^3\int d^3k\, k_BT\sum_l\langle u_\lambda^0|\mathcal{H}_\delta^{(1)}u_\lambda^0\rangle\tilde{H}_\lambda^{(1)}(\vec{k},\zeta_l)\mathcal{G}_\lambda^2(\vec{k},\zeta_l)$$
$$+\sum_\lambda\left(\frac{1}{2\pi}\right)^3\int d^3k\, k_BT\sum_l 2\left\langle u_\lambda^0(\vec{r},\vec{k},\zeta_l)\right|\int d^3r'\, e^{i\vec{k}\cdot(\vec{r}'-\vec{r})}\tilde{\Sigma}_{\zeta_l}^{(1)}(\vec{r},\vec{r}')\frac{e}{B\hbar c}\vec{A}(\vec{r}-\vec{r}')\cdot\nabla_{\vec{k}}u_\lambda^0(\vec{r}',\vec{k},\zeta_l)\Big\rangle\,\mathcal{G}_\lambda(\vec{k},\zeta_l)$$
$$-\sum_\lambda\left(\frac{1}{2\pi}\right)^3\int d^3k\, k_BT\sum_l 2\sum_{\lambda'\neq\lambda}(\tilde{H}_{\lambda'}^0-\tilde{H}_\lambda^0)^{-1}\langle u_{\lambda'}^0|\mathcal{H}_\delta^{(1)}u_\lambda^0\rangle\langle u_\lambda^0|\mathcal{H}_\delta^{(1)}u_{\lambda'}^0\rangle\mathcal{G}_\lambda(\vec{k},\zeta_l)$$
$$-\sum_\lambda\left(\frac{1}{2\pi}\right)^3\int d^3k\, k_BT\sum_l\sum_{\lambda'\neq\lambda}(\tilde{H}_{\lambda'}^0-\tilde{H}_\lambda^0)^{-1}(\langle u_{\lambda'}^0|\mathcal{H}_\Delta^{(1)}u_\lambda^0\rangle\langle u_\lambda^0|\mathcal{H}_\delta^{(1)}u_{\lambda'}^0\rangle$$
$$+\langle u_\lambda^0|\mathcal{H}_\Delta^{(1)}u_{\lambda'}^0\rangle\langle u_{\lambda'}^0|\mathcal{H}_\delta^{(1)}u_\lambda^0\rangle)\,\mathcal{G}_\lambda(\vec{k},\zeta_l). \tag{4.36}$$

The second term gives a correction to $\chi_{\rm CP}$ and the rest are corrections to $\chi_{\rm ID}$. We shall see that these corrections to $\chi_{\rm CP}$ and $\chi_{\rm ID}$ lead, among other things, to the cancellation of the appearance of quadratic terms in $\Sigma_{\zeta_l}^{(1)}$ as well as the total cancellation of the appearance of $\Sigma_{\zeta_l}^{(2)}$. This important cancellation is expected and is in agreement with the work of Philippas and McClure.[3] Using Eqs. (3.42) and (3.43) to write down $\chi_{\rm CP}$ and $\chi_{\rm ID}$ explicitly and denoting the corrected $\chi_{\rm CP}$ and $\chi_{\rm ID}$ by $\chi_{\rm CP}^\Sigma$ and $\chi_{\rm ID}^\Sigma$, respectively, we may write the total magnetic susceptibility of interacting free and Bloch electrons as

$$\chi = \chi_{\rm LP} + \chi_{\rm CP}^\Sigma + \chi_{\rm ID}^\Sigma. \tag{4.37}$$

$\chi_{\rm LP}$ is given by Eq. (4.15), $\chi_{\rm CP}^\Sigma$ and $\chi_{\rm ID}^\Sigma$ are given by the following relations:

$$\chi_{\rm CP}^\Sigma = -\sum_\lambda\left(\frac{1}{2\pi}\right)^3\int d^3k\, k_BT\sum_l\{[\tilde{H}_\lambda^{(1)}(\vec{k},\zeta_l)_\Delta]^2 + H_\lambda^{(1)}(\vec{k},\zeta_l)_\Delta\tilde{H}_\lambda^{(1)}(\vec{k},\zeta_l)_\delta\}\,\mathcal{G}_\lambda^2(\vec{k},\zeta_l), \tag{4.38}$$

$$\chi_{\rm ID}^\Sigma = -\sum_\lambda\left(\frac{1}{2\pi}\right)^3\int d^3k\, k_BT\sum_l 2W_\lambda^{(2)}(\vec{k},\zeta_l)\mathcal{G}_\lambda(\vec{k},\zeta_l), \tag{4.39}$$

where

$$\tilde{H}_\lambda^{(1)}(\vec{k},\zeta_l)_\Delta = \langle u_\lambda^0|\mathcal{H}_0^{(1)} + (e/B\hbar c)[\vec{A}(\nabla_{\vec{k}})\tilde{H}_\lambda^0(\vec{k},\zeta_l)]\cdot\nabla_{\vec{k}}u_\lambda^0\rangle$$
$$+\left\langle u_\lambda^0(\vec{r},\vec{k},\zeta_l)\right|\int d^3r'\, e^{i\vec{k}\cdot(\vec{r}'-\vec{r})}\tilde{\Sigma}_{\zeta_l}^0(\vec{r},\vec{r}')\frac{e}{B\hbar c}\vec{A}(\vec{r}-\vec{r}')\cdot\nabla_{\vec{k}}u_\lambda^0(\vec{r}',\vec{k},\zeta_l)\Big\rangle, \tag{4.40}$$

$$\tilde{H}_\lambda^{(1)}(\vec{k},\zeta_l)_\delta = \left\langle u_\lambda^0(\vec{r},\vec{k},\zeta_l)\right|\int d^3r'\, e^{i\vec{k}\cdot(\vec{r}'-\vec{r})}\tilde{\Sigma}_{\zeta_l}^{(1)}(\vec{r},\vec{r}')u_\lambda^0(\vec{r}',\vec{k},\zeta_l)\Big\rangle = \Sigma_{\lambda\lambda}^{(1)0}(\vec{k},\zeta_l), \tag{4.41}$$

$$W_\lambda^{(2)}(\vec{k},\zeta_l)=\langle u_\lambda^0|\mathcal{H}_0^{(2)}|u_\lambda^0\rangle+\langle u_\lambda^0|\mathcal{H}_0^{(1)}|u_\lambda^{(1)}\rangle-\left\langle u_\lambda^0\right|\sum_{\vec{q}}e^{i\vec{k}\cdot\vec{q}}\tilde{H}_\lambda^0(\vec{q},\zeta_l)\frac{1}{2!}\left(\frac{e}{B\hbar c}\vec{A}(\vec{q})\cdot\nabla_{\vec{k}}\right)^2u_\lambda^0\Big\rangle$$
$$+\left\langle u_\lambda^0\right|\frac{e}{B\hbar c}[\vec{A}(\nabla_{\vec{k}})\tilde{H}_\lambda^0(\vec{k},\zeta_l)]\cdot i\nabla_{\vec{k}}u_\lambda^{(1)}\Big\rangle$$
$$+\left\langle u_\lambda^0\right|\frac{e}{B\hbar c}[\vec{A}(\nabla_{\vec{k}})\tilde{H}_\lambda^{(1)}(\vec{k},\zeta_l)]\cdot i\nabla_{\vec{k}}u_\lambda^0\Big\rangle-\tilde{H}_\lambda^{(1)}(\vec{k},\zeta_l)_\Delta\frac{1}{4}\frac{e}{\hbar c}\left(\frac{\partial}{\partial\vec{k}_y}\left\langle u_\lambda^0\right|i\frac{\partial}{\partial\vec{k}_x}u_\lambda^0\Big\rangle-\frac{\partial}{\partial\vec{k}_x}\left\langle u_\lambda^0\right|i\frac{\partial}{\partial\vec{k}_y}u_\lambda^0\Big\rangle\right)$$
$$+\left\langle u_\lambda^0(\vec{r},\vec{k},\zeta_l)\right|\int d^3r'\,e^{i\vec{k}\cdot(\vec{r}'-\vec{r})}\tilde{\Sigma}_{\zeta_l}^0(\vec{r},\vec{r}')\frac{1}{2!}\left(\frac{e}{B\hbar c}\vec{A}(\vec{r}-\vec{r}')\cdot\nabla_{\vec{k}}\right)^2u_\lambda^0(\vec{r}',\vec{k},\zeta_l)\Big\rangle$$
$$+\left\langle u_\lambda^0(\vec{r},\vec{k},\zeta_l)\right|\int d^3r'\,e^{i\vec{k}\cdot(\vec{r}'-\vec{r})}\tilde{\Sigma}_{\zeta_l}^0(\vec{r},\vec{r}')\frac{e}{B\hbar c}\vec{A}(\vec{r}-\vec{r}')\cdot\nabla_{\vec{k}}u_\lambda^{(1)}(\vec{r}',\vec{k},\zeta_l)\Big\rangle$$
$$-\tfrac{1}{2}\sum_{\lambda'\neq\lambda}(\tilde{H}_{\lambda'}^0-\tilde{H}_\lambda^0)^{-1}(\langle u_{\lambda'}^0|\mathcal{H}_\Delta^{(1)}u_\lambda^0\rangle\langle u_\lambda^0|\mathcal{H}_\delta^{(1)}u_{\lambda'}^0\rangle-\langle u_\lambda^0|\mathcal{H}_\Delta^{(1)}u_{\lambda'}^0\rangle\langle u_{\lambda'}^0|\mathcal{H}_\delta^{(1)}u_\lambda^0\rangle).\tag{4.42}$$

Indeed, χ is a linear function of the operator $\Sigma_{\zeta_l}^{(1)}$ and is independent of $\Sigma_{\zeta_l}^{(2)}$.[3] For reasons which maybe clarified in some well-known cases, we will refer to the $\Sigma_{\zeta_l}^{(1)}$ term in χ_{CP}^Σ as the "enhancement term." Consequently, we will also refer to the $\Sigma_{\zeta_l}^{(1)}$ terms in χ_{ID}^Σ as the "second-order effect of the enhancement."

V. APPLICATION OF GENERAL FORMULA TO SOME KNOWN CASES

It would be enlightening to apply the general expression, Eq. (4.37), for χ to some very well-known cases. We will continue in this section by applying the general formula to (a) a Fermi liquid and to (b) a system of strongly correlated electrons in a narrow band represented by the Hubbard model. We will treat this last case only in Hartree-Fock approximation for simplicity. In what follows, electric charge $e\to-e$.

A. Fermi liquid

Since the periodic wave function $u_\lambda^0(\vec{r},\vec{k},\zeta_l)$ occurring in Eqs. (4.40) and (4.42) is a constant quantity for Fermi liquids,[9] we can immediately write down the magnetic susceptibility of the quasiparticles as

$$\chi=\chi_{LP}+\chi_{CP}^\Sigma.\tag{5.1}$$

We obtain using Eqs. (4.62), (4.67), and (4.69) of Ref. 18, the total quasiparticle energy [more appropriately the Weyl transform with $\vec{p}+(e/c)\vec{A}(\vec{q})\to\hbar\vec{k}$] in a magnetic field as

$$\tilde{H}_\lambda(\vec{k},B,\zeta_l)=e^0(\vec{k})\begin{pmatrix}1&0\\0&1\end{pmatrix}+B\mu_B\begin{pmatrix}1&0\\0&-1\end{pmatrix}+\frac{B\chi_{CP}^\Sigma}{\mu_B}\frac{\vec{\pi}^2\hbar^2}{m^*k_F}B_0\begin{pmatrix}-1&0\\0&1\end{pmatrix},\tag{5.2}$$

where $m^*=(1+\frac{1}{3}A_1)m$; A_1 and B_0 are well-known Fermi-liquid parameters. We immediately identify, upon examination of Eqs. (3.56), (4.40), and (4.41), the following relations:

$$\tilde{H}_\lambda^0(\vec{k},\zeta_l)=e^0(\vec{k})\begin{pmatrix}1&0\\0&1\end{pmatrix},\tag{5.3}$$

$$\tilde{H}_\lambda^{(1)}(\vec{k},\zeta_l)_\Delta=\mu_B\begin{pmatrix}1&0\\0&-1\end{pmatrix},\tag{5.4}$$

$$\tilde{H}_\lambda^{(1)}(\vec{k},\zeta_l)_\delta=\frac{\chi_{CP}^\Sigma}{\mu_B}\frac{\vec{\pi}^2\hbar^2}{m^*k_F}B_0\begin{pmatrix}-1&0\\0&1\end{pmatrix}.\tag{5.5}$$

Substituting these quantities in χ_{CP}^Σ, Eq. (4.38), we get

$$\chi_{CP}^\Sigma=[(1+\tfrac{1}{3}A_1)/(1+B_0)]\chi_P^0,\tag{5.6}$$

where χ_P^0 is the Pauli spin susceptibility for a noninteracting electron gas. The calculation of χ_{LP} is very elementary and the total χ is thus given by

$$\chi=(1+\tfrac{1}{3}A_1)^{-1}\chi_{LP}^0+[(1+\tfrac{1}{3}A_1)/(1+B_0)]\chi_P^0.\tag{5.7}$$

This is a very well-known result for the orbital and spin susceptibility of Fermi liquids. Note that a small effective mass enhances χ_{LP}^0.

B. Hubbard model in Hartree-Fock approximation

The model under consideration assumes that there is only one band of interest energetically far removed from the other bands. For a very narrow band we may write

$$\chi\simeq\chi_{CP}^\Sigma+\chi_{ID}^\Sigma.\tag{5.8}$$

Upon transforming Eqs. (4.75) and (4.76) of Ref. 18 to k space, we have for the expression of the total Hubbard Hamiltonian in a magnetic field in the Hartree-Fock approximation as[19]

$$H = \sum_{\vec{k},\sigma} e(\vec{k})n(\vec{k},\sigma) + \sum_{\vec{k},\sigma} I\langle n(\vec{k},\sigma)\rangle n(\vec{k},-\sigma) + \tfrac{1}{2} g\ \mu_B B \sum_{\vec{k}} [n(\vec{k},\uparrow) - n(\vec{k},\downarrow)]. \quad (5.9)$$

Therefore, $\tilde{H}_\lambda(\vec{k}, B, \zeta_l)$ is given by

$$\tilde{H}_\lambda(\vec{k}, B, \zeta_l) = e(\vec{k})\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} + I\begin{pmatrix}\langle n(\vec{k},\downarrow)\rangle & 0\\ 0 & \langle n(\vec{k},\uparrow)\rangle\end{pmatrix} + \tfrac{1}{2} g\mu_B B\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \quad (5.10)$$

In view of the fact that $\langle n(\vec{k},\downarrow)\rangle$ is greater than $\langle n(\vec{k},\uparrow)\rangle$, we may write

$$\langle n(\vec{k},\downarrow)\rangle = n + \delta n, \quad (5.11)$$

$$\langle n(\vec{k},\uparrow)\rangle = n - \delta n, \quad (5.12)$$

$$(2N\delta n/V)\tfrac{1}{2} g\mu_B = \chi^{\Sigma}_{\mathrm{CP}}\ B, \quad (5.13)$$

and readily obtain

$$\tilde{H}^0_\lambda(\vec{k}, \zeta_l) = [e(\vec{k}) + In]\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \quad (5.14)$$

$$\tilde{H}^{(1)}_\lambda(\vec{k}, \zeta_l)_\Delta = \tfrac{1}{2} g\mu_B\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \quad (5.15)$$

$$\tilde{H}^{(1)}_\lambda(\vec{k}, \zeta_l)_\delta = \frac{I(V/N)\chi^{\Sigma}_{\mathrm{CP}}}{g\mu_B}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \quad (5.16)$$

Upon substitution of these quantities in Eq. (4.38), we obtain

$$\chi^{\Sigma}_{\mathrm{CP}} = \chi_0\left(1 - \frac{2I(V/N)\chi_0}{(g\mu_B)^2}\right)^{-1}, \quad (5.17)$$

leading to the Stoner criterion for the appearance of ferromagnetism.[18] To obtain $\chi^{\Sigma}_{\mathrm{ID}}$, we note that

$$W^{(2)}_\lambda(\vec{k}, \zeta_l) \simeq \langle u^0_\lambda(\vec{r},\vec{k})|\mathcal{H}^{(2)}_0|u^0_\lambda(\vec{r},\vec{k})\rangle, \quad (5.18)$$

the second term, representing a Van Vleck paramagnetism, and last term of Eq. (4.42) are neglected since the band of interest is energetically far removed from other bands. The third up to sixth term, inclusive, are neglected by the assumption of a very narrow band and the rest of Eq. (4.42) is neglected due to the δ-function locality[19] of $\Sigma^0_{\zeta_l}(\vec{r},\vec{r}')$. Expressing $e^{i\vec{k}\cdot\vec{r}}u_\lambda(\vec{r},\vec{k},\zeta_l)$ as a linear combination of atomic orbitals we obtain, upon substitution in Eq. (4.39), a familiar "atomic diamagnetism" multiplied by the total number of electrons N in the band

$$\chi^{\Sigma}_{\mathrm{ID}} = -(Ne^2/4mc^2)\langle\phi_\lambda(\vec{r})|\ x^2 + y^2|\ \phi_\lambda(\vec{r})\rangle, \quad (5.19)$$

where $\phi_\lambda(\vec{r})$ is the atomic orbital of the band. For most purposes $\chi^{\Sigma}_{\mathrm{ID}}$ is neglected and $\chi \simeq \chi^{\Sigma}_{\mathrm{CP}}$.

VI. DISCUSSION

The results presented in this paper provide a powerful and rounded theory of the dynamics of a Fermi system possessing translational symmetry. Moreover, the derivation of χ sheds more light and understanding on the role of symmetry arguments in unifying the calculation of χ for Fermi systems, interacting or noninteracting, possessing translational symmetry in a uniform magnetic field. We have obtained a most general expression for χ which includes both the spin and orbital susceptibility and have at the same time given a more general proof of the validity of the Sampson-Seitz prescription,[1] applied to χ_{LP}, for cases where the self-energy part is independent of frequency.

To avoid confusion, the discussions of Secs. I–V did not explicitly take into account the presence of spin indices; this has been only briefly alluded to in Ref. 7. As mentioned in that reference, the method discussed in this paper requires that in the absence of the magnetic field the eigenvalues of $W_{\lambda\lambda'}(\vec{\pi}, B, \zeta_l)$ [Eqs. (2.8)–(2.10)] [$W_{\lambda\lambda'}(\vec{\pi}, B, \zeta_l) = H^0_{\lambda\lambda'}(\vec{p}, \zeta_l)$ in the absence of B] are nondegenerate and for each band index λ these eigenvalues which we represent by $\tilde{H}^0_\lambda$, Eq. (2.16), are proportional to $\delta_{\alpha\beta}$ in spin indices, thus commuting with other 2×2 matrices. This appropriately limits our discussion to nonferromagnetic substances. In the presence of a magnetic field the self-energy operator in Eq. (2.1) becomes spin dependent,[20] therefore, $H^{(1)}_\lambda(\vec{p} - (e/c)\vec{A}(\vec{q}), \zeta_l)$ and $H^{(2)}_\lambda(\vec{p} - (e/c)\vec{A}(\vec{q}), \zeta_l)$ obtained from Eqs. (3.42) and (3.43), respectively, are 2×2 matrices. In other words, each band index λ is a two-dimensional space. Intraband as well as interband matrix elements, in the perturbation theory of Sec. III, are to be understood as 2×2 matrices, and hence, taking the trace over spin indices is implicit in all expressions for $\tilde{\mathrm{T}}\mathrm{r}$.

We now wish to make some general comments regarding spin indices. Spin degeneracy occurs, both for noninteracting or interacting Fermi systems, with or without spin-orbit coupling, in nonferromagnetic crystals with inversion symmetry in the absence of the magnetic field. When spin-orbit coupling is taken into account in the Hamiltonian of Eq. (2.1), we add to $\mathcal{H}_0$ of Eq. (2.2) a term

$$\frac{\hbar}{4m^2c^2}\nabla_{\vec{r}}V(\vec{r})\times\left(\frac{\hbar}{i}\nabla_{\vec{r}} - \frac{e}{c}\vec{A}(\vec{r})\right)\cdot\vec{\sigma}$$

and Σ_{ζ_l} describes, as before, the residual electron-electron interactions.[21] Usual space and time-reversal symmetry arguments[22] then lead to spin degeneracy both for noninteracting and interacting Fermi systems in nonferromagnetic crystals with inversion symmetry in the absence of B. The general treatment regarding spin goes as follows. Each band index λ is treated as consisting of two degenerate states[23] (with spin-orbit coupling these states cannot be pure spin states) and in the $(\vec{p}-\vec{q})$ dynamical representation, $f_\lambda(\vec{p})$ and $f_\lambda(\vec{q})$ in Eqs. (2.8) and (2.9) will be two-component functions for each band index λ and each element $W_{\lambda\lambda'}(\vec{\pi}, B, \zeta_l)$ will be a 2×2 matrix. In the absence of magnetic field the eigenvectors of $H^0_{\lambda\lambda'}(\vec{p}, \zeta_l)$ determine the transformation from the $\Sigma_{\zeta_l}=0$ degenerate states to the $\Sigma_{\zeta_l}\neq 0$ degenerate states, labeled by a band index λ. $H^{(1)}_\lambda(\vec{p}-(e/c)\vec{A}(\vec{q}), \zeta_l)$ and $H^{(2)}_\lambda(\vec{p}-(e/c)\vec{A}(\vec{q}), \zeta_l)$ as well as matrix elements in the perturbation theory are, themselves, 2×2 matrices. In this way discussion of problems with or without spin-orbit coupling are formally identical.

ACKNOWLEDGMENTS

The author is grateful to Dr. D. L. Hunter for his hospitality at the Department of Physics, St. Francis Xavier University and wishes to thank Dr. T. McMullen and Dr. J. P. Carbotte for some informative discussions.

APPENDIX A: DERIVATION OF THE EFFECTIVE HAMILTONIAN

The transformation of the one-particle effective Hamiltonian expressed in "bare" dynamical variables into an effective Hamiltonian in terms of crystal-momentum and lattice-position operators[5] can be carried out in rigorous fashion using the Weyl-Wigner formalism[6,7] of the quantum theory of solids. Let $w_\lambda(\vec{r}, \vec{q})$ be any complete set of localized states labeled by a band index λ and a lattice point $\vec{q}$ and let $b_\lambda(\vec{r}, \vec{p})$ be its lattice Fourier transform. We use ket and bra notations.[6] The following identity holds for an arbitrary operator A_{op}:

$$A_{\mathrm{op}} = (N\hbar^3)^{-1} \sum_{\vec{p}\vec{q}\lambda\lambda'} A_{\lambda\lambda'}(\vec{p}, \vec{q})\Delta_{\lambda\lambda'}(\vec{p}, \vec{q}), \tag{A1}$$

where $A_{\lambda\lambda'}(\vec{p}, \vec{q})$ and $\Delta_{\lambda\lambda'}(\vec{p}, \vec{q})$ are given by ($\vec{q}$ and $\vec{v}$ are restricted to lattice vectors)

$$\Delta_{\lambda\lambda'}(\vec{p}, \vec{q}) = \sum_{\vec{v}} e^{(2i/\hbar)\vec{p}\cdot\vec{v}} \langle \vec{q}-\vec{v}, \lambda | A_{\mathrm{op}} | \vec{q}+\vec{v}, \lambda'\rangle, \tag{A2}$$

$$\Delta_{\lambda\lambda'}(\vec{p}, \vec{q}) = \sum_{\vec{u}} e^{(2i/\hbar)\vec{q}\cdot\vec{u}} | \vec{p}-\vec{u}, \lambda\rangle\langle \vec{p}+\vec{u}, \lambda' |, \tag{A3}$$

or by the equivalent expressions

$$A_{\lambda\lambda'}(\vec{p}, \vec{q}) = \sum_{\vec{u}} e^{(2i/\hbar)\vec{q}\cdot\vec{u}} \langle \vec{p}+\vec{u}, \lambda | A_{\mathrm{op}} | \vec{p}-\vec{u}, \lambda'\rangle, \tag{A4}$$

$$\Delta_{\lambda\lambda'}(\vec{p}, \vec{q}) = \sum_{\vec{v}} e^{(2i/\hbar)\vec{p}\cdot\vec{v}} | \vec{q}+\vec{v}, \lambda\rangle\langle \vec{q}-\vec{v}, \lambda' |. \tag{A5}$$

We now introduce a lattice-position operator $\vec{Q}$ and a crystal-momentum operator $\vec{P}$, defined with the aid of $w_\lambda(\vec{r}, \vec{q})$ and $b_\lambda(\vec{r}, \vec{p})$, as

$$\vec{P}|\vec{p}, \lambda\rangle = \vec{p}|\vec{p}, \lambda\rangle, \tag{A6}$$

$$\vec{Q}|\vec{q}, \lambda\rangle = \vec{q}|\vec{q}, \lambda\rangle. \tag{A7}$$

The significance of $\vec{P}$ and $\vec{Q}$ can be appreciated by showing that they provide the appropriate canonically conjugate dynamical variables very useful in discussing band dynamics.[5] The Weyl transform of the commutator of $\vec{P}$ and $\vec{Q}$ is[6]

$$[\vec{P}_l, \vec{Q}_j]_{\lambda\lambda'}(\vec{p}, \vec{q}) = (\hbar/i)\delta_{jl}\delta_{\lambda\lambda'}, \tag{A8}$$

and hence $[\vec{P}_l, \vec{Q}_j] = (\hbar/i)\delta_{jl}$. Moreover, using Eqs. (5) and (6) of Ref. 6, we can write

$$\vec{Q}|\vec{p}, \lambda\rangle = (\hbar/i)\nabla_{\vec{p}}|\vec{p}, \lambda\rangle, \tag{A9}$$

$$\vec{P}|\vec{q}, \lambda\rangle = -(\hbar/i)\nabla_{\vec{q}}|\vec{q}, \lambda\rangle, \tag{A10}$$

and for any function $\psi(\vec{r})$, expanded in terms of the complete set $|\vec{q}, \lambda\rangle$ or $|\vec{p}, \lambda\rangle$, we have

$$\vec{P}\psi(\vec{r}) = \sum_{\vec{p},\lambda} [\vec{p} f_\lambda(\vec{p})]|\vec{p}, \lambda\rangle, \tag{A11}$$

$$\vec{P}\psi(\vec{r}) = \sum_{\vec{q},\lambda} \left(\frac{\hbar}{i}\nabla_{\vec{q}} f_\lambda(\vec{q})\right)|\vec{q}, \lambda\rangle, \tag{A12}$$

$$\vec{Q}\psi(\vec{r}) = \sum_{\vec{q},\lambda} [\vec{q} f_\lambda(\vec{q})]|\vec{q}, \lambda\rangle, \tag{A13}$$

$$\vec{Q}\psi(\vec{r}) = \sum_{\vec{p},\lambda} \left(-\frac{\hbar}{i}\nabla_{\vec{p}} f_\lambda(\vec{p})\right)|\vec{p}, \lambda\rangle. \tag{A14}$$

These results enable us to express the quantum dynamics of band electrons entirely in $\vec{p}$-$\vec{q}$ space. The above results depend, of course, on the existence of continuous functions of $\vec{q}$, having infinite radius of convergence, which give the right values at the lattice points.[6,10]

The following identities can easily be verified:

$$|\vec{q}+\vec{v}, \lambda\rangle = \exp[-(2i/\hbar)\vec{P}\cdot\vec{v}]|\vec{q}-\vec{v}, \lambda\rangle, \tag{A15}$$

$$|\vec{q}-\vec{v}, \lambda\rangle\langle\vec{q}-\vec{v}, \lambda'| = (N\hbar^3)^{-1}\sum_{\vec{u}} \exp\left(\frac{2i}{\hbar}(\vec{q}-\vec{v}-\vec{Q})\cdot\vec{u}\right)\Omega_{\lambda\lambda'}, \tag{A16}$$

where

$$\Omega_{\lambda\lambda'} = \sum_{\vec{q}} |\vec{q}, \lambda\rangle\langle\vec{q}, \lambda'|, \tag{A17}$$

$$\Omega_{\lambda\lambda'} = \sum_{\vec{p}} |\vec{p}, \lambda\rangle\langle\vec{p}, \lambda'|, \tag{A18}$$

and by virtue of the above identities we may therefore write

$$\Delta_{\lambda\lambda'}(\vec{p},\vec{q}) = (N\hbar^3)^{-1}\sum_{\vec{v},\vec{u}} \exp\left(\frac{2i}{\hbar}(\vec{p}-\vec{P})\cdot\vec{v}\right) \times \exp\left(\frac{2i}{\hbar}(\vec{q}-\vec{v}-\vec{Q})\cdot\vec{u}\right)\Omega_{\lambda\lambda'}, \tag{A19}$$

and find

$$A_{op}\psi(\vec{r}) = (N\hbar^3)^{-2}\sum_{\substack{\vec{p},\vec{q},\lambda\lambda'\\ \vec{v},\vec{u},\vec{q}'}} A_{\lambda\lambda'}(\vec{p},\vec{q})\exp\left[\frac{2i}{\hbar}\left(\vec{p}-\frac{\hbar}{i}\nabla_{\vec{q}'}\right)\cdot\vec{v}\right] \times \exp\left(\frac{2i}{\hbar}(\vec{q}-\vec{v}-\vec{q}')\cdot\vec{u}\right) \times f_{\lambda'}(\vec{q}')\,|\vec{q}',\lambda\rangle. \tag{A20}$$

Equating the right-hand side of Eq. (A36) to $E\psi(\vec{r})$ to obtain an eigenvalue equation, we have in $\vec{p}$-$\vec{q}$ space,

$$(N\hbar^3)^{-2}\sum_{\substack{\vec{p},\vec{q},\lambda'\\ \vec{v},\vec{u}}} A_{\lambda\lambda'}(\vec{p},\vec{q})\exp\left[\frac{2i}{\hbar}\left(\vec{p}-\frac{\hbar}{i}\nabla_{\vec{q}'}\right)\cdot\vec{v}\right] \times \exp\left(\frac{2i}{\hbar}(\vec{q}-\vec{v}-\vec{q}')\cdot\vec{u}\right)f_{\lambda'}(\vec{q}') = Ef_{\lambda}(\vec{q}'). \tag{A21}$$

Now let us take the operator A_{op} to be the effective one-particle Hamiltonian $\mathcal{H}$ defined in Eq. (2.1). It is shown in Appendix B that the lattice Weyl transform $\mathcal{H}$ is of the form where $\vec{p}$ and $\vec{q}$ occur only in the combination $\vec{p}-(e/c)\vec{A}(\vec{q})$. Using this result in (A21) we have

$$(N\hbar^3)^{-2}\sum_{\substack{\vec{p}',\vec{q},\lambda'\\ \vec{u},\vec{v}}} H_{\lambda\lambda'}(\vec{p}';B,z) \times \exp\left[\frac{2i}{\hbar}\left(\vec{p}'+\frac{e}{c}\vec{A}(\vec{q})-\frac{\hbar}{i}\nabla_{\vec{q}'}\right)\cdot\vec{v}\right] \times \exp\left(\frac{2i}{\hbar}(\vec{q}-\vec{v}-\vec{q}')\cdot\vec{u}\right)f_{\lambda'}(\vec{q}') = Ef_{\lambda}(\vec{q}'). \tag{A22}$$

Performing a summation over $\vec{q}$ and $\vec{u}$, we obtain, after some simplification the following

$$(N\hbar^3)^{-1}\sum_{\vec{p}',\lambda',\vec{v}} H_{\lambda\lambda'}(\vec{p}';B,z)e^{(2i/\hbar)(\vec{p}'-\vec{\pi})\cdot\vec{v}}f_{\lambda'}(\vec{q}) = Ef_{\lambda}(\vec{q}), \tag{A23}$$

where $\vec{\pi} = (\hbar/i)\nabla_{\vec{q}} - (e/c)\vec{A}(\vec{q})$. Because of the noncommutivity of the components of $\vec{\pi}$, the summation of $\vec{p}'$ and $\vec{v}$ does not simply result in the replacement of $\vec{p}'$ by $\vec{\pi}$ in $H_{\lambda\lambda'}(\vec{p}';B,z)$.[7] The replacement rule is only valid if $H_{\lambda\lambda'}(\vec{p}',B,z)$ is a polynomial of order 2 in $\vec{p}'$. Thus in general we must write the effective Hamiltonian in $\vec{q}$ space as, Eqs. (2.8),

$$\sum_{\lambda'} W_{\lambda\lambda'}(\vec{\pi};B,z)f_{\lambda'}(\vec{q}) = Ef_{\lambda}(\vec{q}). \tag{A24}$$

The corresponding equation in $\vec{p}$ space can easily be deduced from Eqs. (A11)–Eq. (A14). This is given by Eqs. (2.9) and (2.12). Indeed in the absence of the magnetic field and for $\Sigma(z)=0$ in Eq. (2.1), we have $W_{\lambda\lambda'}(p)=E_{\lambda}(p)\delta_{\lambda\lambda'}$, where $E_{\lambda}(p)$ is the energy-band function, with trivial solutions

$$f(\vec{p}) = \text{const} \quad\text{and}\quad f(\vec{q}) = (N\hbar^3)^{-1/2}e^{(i/\hbar)\vec{p}\cdot\vec{q}}.$$

Because of the complicated many-body character of $\Sigma(z)$ due to its dependence in the energy variable, the effective Hamiltonian in Eq. (A24) is in general non-Hermitian; the eigenfunctions, though complete,[9] are not orthogonal. Thus one needs to solve the adjoint problem and this has been discussed in Sec. II. Except for the extra dependence on the energy variable z, magnetic field, etc., relations (5)–(15) of Ref. 6 hold for the biorthogonal Wannier functions and biorthogonal Bloch functions and using these as basis states the effective Hamiltonian assumes a "diagonal" form. Thus in the absence of the field we have

$$\tilde{\mathcal{H}}^0_{\text{eff}} = (N\hbar^3)^{-2}\sum_{\substack{\vec{p},\vec{q},\lambda\\ \vec{u},\vec{v}}} \tilde{H}^0_{\lambda}(\vec{p},z)\exp\left(\frac{2i}{\hbar}(\vec{p}-\vec{P})\cdot\vec{v}\right) \times \exp\left(\frac{2i}{\hbar}(\vec{q}-\vec{v}-\vec{Q})\cdot\vec{u}\right)\Omega_{\lambda\lambda}, \tag{A25}$$

where

$$\Omega_{\lambda\lambda} = \sum_{\vec{p}} |\vec{p},\lambda,z\rangle\langle\vec{p},\lambda,z|, \tag{A26}$$

$$\Omega_{\lambda\lambda} = \sum_{\vec{q}} |\vec{q},\lambda,z\rangle\langle\vec{q},\lambda,z|. \tag{A27}$$

$\tilde{H}^0_{\lambda}(\vec{p},z)$ is given by Eq. (2.21) or (2.22) and $|\vec{p},\lambda,z\rangle$, $\langle\vec{p},\lambda,z|$, $|\vec{q},\lambda,z\rangle$, and $\langle\vec{q},\lambda,z|$ are defined by Eqs. (2.17)–(2.20). In the presence of the magnetic field, we have shown in the first part of Sec. III that the lattice Weyl transform of $\mathcal{H}_0+\Sigma(z)$ and the effective Hamiltonian in $\vec{p}$-$\vec{q}$ space can be reduced to an even (diagonal) form. This important result suggests the existence of biorthogonal magnetic Wannier functions and biorthogonal magnetic Bloch functions satisfying the relations (5)–(15) of Ref. 6 and this idea leads to another method, discussed in the second part of Sec. III, for obtaining the lattice Weyl transform, free of interband terms.

APPENDIX B: LATTICE WEYL TRANSFORM OF ONE-PARTICLE EFFECTIVE HAMILTONIAN

The lattice Weyl transform of the one-particle effectic-Hamiltonian operator is defined by (A2) or (A4) with the arbitrary operator A_{op} replaced by $\mathcal{H}_0 + \Sigma(z)$, Eq. (2.1). It is convenient to introduce the magnetic translation operator[5,24] defined by

$$T(\vec{q}) = \exp\left[\frac{i}{\hbar}\left(\frac{\hbar}{i}\nabla_{\vec{r}} + \frac{e}{c}\vec{A}(\vec{r})\right)\cdot\vec{q}\right] , \quad \text{(B1)}$$

where $\vec{A}(\vec{r})$ is the vector potential, $\vec{A}(\vec{r}) = \frac{1}{2}\vec{B}\times\vec{r}$, and $\vec{q}$ is the crystal lattice vector. In terms of this operator the following relation holds for the magnetic Wannier functions:

$$|\vec{q},\lambda\rangle = T(\vec{q})\,|0,\lambda\rangle . \quad \text{(B2)}$$

In other words, $T(\vec{q})$ generates all the magnetic Wannier functions belonging to a band index λ from a given magnetic Wannier function centered at at the origin. Using notation in Appendix A we have

$$w_\lambda(\vec{r}, -\vec{q}) = T(-\vec{q})\,w_\lambda(\vec{r},0) = \exp\left(-\frac{i}{\hbar}\frac{e}{c}\vec{A}(\vec{r})\cdot\vec{q}\right)w_\lambda(\vec{r}-\vec{q}) . \quad \text{(B3)}$$

$T(\vec{q})$ commutes with $\mathcal{H}_0$ and moreover

$$T(\vec{q})T(\vec{p}) = \exp\left(\frac{ie}{\hbar c}\vec{A}(\vec{q})\cdot\vec{p}\right)T(\vec{q}+\vec{p}) . \quad \text{(B4)}$$

By virtue of the last equation we can write the matrix element of $\mathcal{H}_0 + \Sigma(z)$ between two magnetic Wannier functions as

$$\langle\vec{q}+\vec{p},\lambda|\mathcal{H}_0+\Sigma(z)|\vec{q}+\vec{p}\,',\lambda'\rangle = e^{(ie/\hbar c)\vec{A}(\vec{q})\cdot(\vec{p}-\vec{p}\,')}\{\langle\vec{p},\lambda|\mathcal{H}_0|\vec{p}\,',\lambda'\rangle + \langle\vec{p},\lambda|T^\dagger(\vec{q})\Sigma(z)T(\vec{q})|\vec{p}\,',\lambda'\rangle\} . \quad \text{(B5)}$$

The second term within the curly brackets can be written

$$\langle\vec{p},\lambda|T^\dagger(\vec{q})\Sigma(z)T(\vec{q})|\vec{p}\,',\lambda'\rangle = \int d^3r\,d^3r'\,e^{-(ie/\hbar c)\vec{A}(\vec{r})\cdot\vec{p}}w_\lambda^*(\vec{r}+\vec{p})e^{-(ie/\hbar c)\vec{A}(\vec{r})\cdot\vec{q}}\Sigma(\vec{r}-\vec{q},\vec{r}\,',z)$$
$$\times e^{(ie/\hbar c)\vec{A}(\vec{r}\,')\cdot\vec{q}}e^{(ie/\hbar c)\vec{A}(\vec{r}\,'+\vec{q})\cdot\vec{p}\,'}w_{\lambda'}(\vec{r}\,'+\vec{q}+\vec{p}\,') . \quad \text{(B6)}$$

Changing the variable of integration $\vec{r}\,'\to\vec{r}\,'-\vec{q}$, with Jacobian unity, we obtain

$$\langle\vec{p},\lambda|T^\dagger(\vec{q})\Sigma(z)T(\vec{q})|\vec{p}\,',\lambda'\rangle = \int d^3r\,d^3r'e^{-(ie/\hbar c)\vec{A}(\vec{r})\cdot\vec{p}}\,w_\lambda^*(\vec{r}+\vec{p})\,e^{-(ie/\hbar c)\vec{A}(\vec{r})\cdot\vec{q}}\Sigma(\vec{r}-\vec{q},\vec{r}\,'-\vec{q},z)e^{(ie/\hbar c)\vec{A}(\vec{r}\,')\cdot\vec{q}}$$
$$\times e^{(ie/\hbar c)\vec{A}(\vec{r}\,')\cdot\vec{p}\,'}w_{\lambda'}(\vec{r}\,'+\vec{p}\,') . \quad \text{(B7)}$$

We now make use of the form[3] of $\Sigma(r,r',z)$ given by Eq. (3.33). Substituting in (B7), we obtain the result

$$\langle\vec{p},\lambda|T^\dagger(\vec{q})\Sigma(z)T(\vec{q})|\vec{p}\,',\lambda'\rangle = \langle\vec{p},\lambda|\Sigma(z)|\vec{p}\,',\lambda'\rangle , \quad \text{(B8)}$$

and thus we can write (B5) as

$$\langle\vec{q}+\vec{p},\lambda|\mathcal{H}_0+\Sigma(z)|\vec{q}+\vec{p}\,',\lambda'\rangle = e^{(ie/\hbar c)\vec{A}(\vec{q})\cdot(\vec{p}-\vec{p}\,')}\langle\vec{p},\lambda|\mathcal{H}_0+\Sigma(z)|\vec{p}\,',\lambda'\rangle . \quad \text{(B9)}$$

The last equation implies

$$\langle\vec{p},\lambda|\mathcal{H}_0+\Sigma(z)|\vec{p}\,',\lambda'\rangle = e^{(ie/\hbar c)\vec{A}(\vec{p}\,')\cdot\vec{p}}F_{\lambda\lambda'}(\vec{p}\,'-\vec{p}) , \quad \text{(B10)}$$

where $F_{\lambda\lambda'}(\vec{p}\,'-\vec{p})$ is a function which depends on $\vec{p}\,'-\vec{p}$,

$$F_{\lambda\lambda'}(\vec{p}\,'-\vec{p}) = \langle\vec{p}-\vec{p}\,',\lambda|\mathcal{H}_0+\Sigma(z)|0,\lambda'\rangle , \quad \text{(B11)}$$

$$F_{\lambda\lambda'}(\vec{p}\,'-\vec{p}) = \langle 0,\lambda|\mathcal{H}_0+\Sigma(z)|\vec{p}\,'-\vec{p},\lambda'\rangle . \quad \text{(B12)}$$

The Hamiltonian $\mathcal{H}_0+\Sigma(z)$ operating on magnetic Wannier function is therefore given by

$$\mathcal{H}|\vec{q},\lambda\rangle = \sum_{\vec{q}\,',\lambda'} e^{(ie/\hbar c)\vec{A}(\vec{q})\cdot\vec{q}\,'}F_{\lambda'\lambda}(\vec{q}-\vec{q}\,')|\vec{q}\,',\lambda'\rangle . \quad \text{(B13)}$$

Taking the lattice Fourier transform of (B13), we obtain the effect of operating $\mathcal{H}_0+\Sigma(z)$ on the magnetic Bloch function

$$\mathcal{H}|\vec{p}\rangle = \sum_{\vec{q},\lambda'} e^{(i/\hbar)\vec{p}\cdot\vec{q}}F_{\lambda'\lambda}(\vec{q})\,|\vec{p}+(e/c)\vec{A}(\vec{q}),\lambda'\rangle . \quad \text{(B14)}$$

It is now a trivial task to take the lattice Weyl transform of $\mathcal{H}_0+\Sigma(z)$, defined by (A2) and (A4). Using (B13) and the identity $(\vec{q}+\vec{v})\times(\vec{q}-\vec{v}) = -2\vec{q}\times\vec{v}$, we obtain

$$H_{\lambda\lambda'}(\vec{p},\vec{q}) = \sum_{\vec{v}}\exp\left[\frac{i}{\hbar}\left(\vec{p}-\frac{e}{c}\vec{A}(\vec{q})\right)\cdot 2\vec{v}\right]F_{\lambda\lambda'}(2\vec{v}) . \quad \text{(B15)}$$

Writing

$$F_{\lambda\lambda'}(2\vec{v}) = (N\hbar^3)^{-1} \sum_{\vec{p}'} H_{\lambda\lambda'}(\vec{p}')e^{-(i/\hbar)\vec{p}'\cdot 2\vec{v}}, \quad \text{(B16)}$$

we end up with

$$H_{\lambda\lambda'}(\vec{p},\vec{q}) = H_{\lambda\lambda'}(\vec{p} - (e/c)\vec{A}(\vec{q}); B, z). \quad \text{(B17)}$$

Equation (B17) will of course be diagonal in band index if biorthogonal magnetic Wannier functions or biorthogonal magnetic Bloch functions, discussed in Sec. III, are used. This will result in an effective Schrödinger equation in $\vec{p}-\vec{q}$ space for each band index λ, following Eq. (A23). A WKB solution of this equation has indeed been recently employed by the author[25] in discussing the influence of scattering or magnetic breakdown in zinc alloys, assuming for simplicity that the imaginary part of $W_\lambda(\vec{\pi})\delta_{\lambda\lambda'}$ is a constant.

---

*Work supported in part by the National Research Council of Canada and partly by the University Council for Research.

[1]J. B. Sampson and F. Seitz, Phys. Rev. 58, 633 (1940); H. Kanasawa and N. Matsudaira, Prog. Theor. Phys. 23, 433 (1960); E. Fujita and T. Usui, *ibid.* 23, 799 (1960); M. J. Stephen, Proc. R. Soc. A 267, 215 (1962); R. M. Rockmore, Phys. Rev. 129, 926 (1963); J. T. Tsai, M. Wadati, and A. Isihara, Phys. Rev. A 4, 1219 (1971); A. K. Rajagopal and K. P. Jain, *ibid.* 5, 1475 (1972).

[2]H. Fukuyama, Prog. Theor. Phys. 45, 704 (1971).

[3]M. A. Philippas and J. W. McClure, Phys. Rev. B 6, 2051 (1972).

[4]H. Fukuyama and J. W. McClure, Phys. Rev. B 9, 975 (1974).

[5]G. H. Wannier, Rev. Mod. Phys. 34, 645 (1962).

[6]F. A. Buot, Phys. Rev. B 10, 3700 (1974). Formalism discussed in this paper has been useful in many-body problems in several instances; see, for example, N. R. Werthamer, Phys. Rev. 132, 663 (1963); G. A. Baraff and S. Borowitz, *ibid.* 121, 1704 (1961); G. A. Baraff, *ibid.* 123, 2087 (1961); D. F. Dubois and M. G. Kivelson, *ibid.* 127, 1182 (1962).

[7]F. A. Buot, Phys. Rev. A 8, 1570 (1973); 9, 2811 (1974). In the presence of the magnetic field each matrix element $W_{\lambda\lambda'}(\vec{\pi}, B, z)$ must itself be considered as a 2×2 matrix to take into account spin explicitly and hence each vector component $f_\lambda(\vec{p}, z)$ a two-component column vector just as in the Pauli representation of positive energy electrons. The only requirement for the results of the paper to be valid is that $\tilde{H}^0_\lambda$ of Eq. (2.16), for each band index λ, is proportional to $\delta_{\alpha\beta}$ in spin indices. This is generally true for nonferromagnetic systems in the absence of external magnetic field; see, for example, A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinki, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Englewood Cliffs, N. J., 1963), pp. 19–21 and 52. Extension of this consideration to problems with spin-orbit coupling is given in Sec. VI.

[8]R. A. Craig, Ann. Phys. (N.Y.) 64, 149 (1971).

[9]A. J. Layzer, Phys. Rev. 129, 897 (1963); for a definition of biorthogonal functions, see P. M. Morse and H. Feshback, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), p. 884 ff.

[10]E. I. Blount, Phys. Rev. 128, 2454 (1962); see also E. I. Blount, in *Solid State Physics*, edited by F. Seitz and D. Turnball (Academic, New York, 1961), Vol. 13, p. 305.

[11]L. G. Suttorp and S. R. de Groot, Nuovo Cimento A 65, 245 (1970).

[12]L. M. Roth, J. Phys. Chem. Solids 23, 433 (1962); G. H. Wannier and U. N. Upadhyaya, Phys. Rev. 136, A803 (1964). Although the derivation given by Roth and by Wannier and Upadhyaya basically accomplishes the same thing, the use of magnetic Wannier functions as basis states greatly simplifies the work of Wannier and Upadhyaya.

[13]J. M. Luttinger and J. C. Ward, Phys. Rev. 118, 1417 (1960).

[14]G. Baym, Phys. Rev. 127, 1391 (1962).

[15]C. Bloch, in *Studies in Statistical Mechanics* (North-Holland, Amsterdam, 1965), Vol. 3.

[16]P. Nozières, *Theory of Interacting Fermi Systems* (Benjamin, New York, 1964), p. 221 ff.; see also Russian authors of Ref. 7; L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, New York, 1962). See also, A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (Gordon and Breach, New York, 1969).

[17]J. M. Luttinger, Phys. Rev. 119, 1153 (1960); 121, 1251 (1961).

[18]R. M. White, *Quantum Theory of Magnetism* (McGraw-Hill, New York, 1970), p. 106 ff.

[19]S. Lundqvist, in *Electrons in Crystalline Solids* (IAEA, Vienna, 1973), p. 281.

[20]L. Hedin and S. Lundqvist, in *Solid State Physics*, edited by F. Seitz, D. Turnball, and H. Ehrenreich (Academic, New York, 1969), p. 1.

[21]W. M. Lomer, in *Theory of Magnetism in Transition Metals*, edited by W. Marshall (Academic, New York, 1967), p. 12.

[22]E. P. Wigner, *Group Theory* (Academic, New York, 1959), p. 325 ff.; J. W. McClure (private communication).

[23]Y. Yafet, in *Solid State Physics*, edited by F. Seitz and D. Turnball (Academic, New York, 1963), Vol. 14, p. 11 ff.

[24]E. Brown, Phys. Rev. 133, A1038 (1964). See also, for example, W. G. Chambers, *ibid.* 149, 493 (1966).

[25]F. A. Buot, P. L. Li, and J. O. Strom-Olsen, J. Low Temp. Phys. 22, 535 (1976).