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Theory of a Possible Ordered Diamagnetic State*

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Because of the nature of the one-electron states in a metal in a magnetic field, the possibility exists that the charge density of the ground state does not have the periodicity of the lattice. We present an elementary theory which suggests the possibility of a laminar arrangement of electron density with planes parallel to the magnetic field. We show that such a state is consistent with group theory. If observable at all, this state should experimentally be seen only at extremely low temperatures and strong magnetic fields.

I. INTRODUCTION

The interaction between electrons in a solid is too strong and of too long a range to be neglected, or to be treated by means of perturbation theory. Nevertheless the independent-particle model seems to yield a good picture for describing low-lying excitations of a solid. Much of our understanding of the effect of electron correlation is based on the treatment of an electron gas by Pines and others.[1] This treatment has led to a description of the gas in terms of weakly interacting quasiparticles. It is generally assumed that the same results hold true in the presence of a periodic lattice. Since the charge density associated with the one-particle Bloch states has the periodicity of the lattice, such a description is self-consistent. This periodicity is destroyed by the presence of a magnetic field. It is known[2] that the states are localizable in at least one direction normal to the field. Therefore, it may be expected that it is not sufficient to treat the behavior of electrons in crystals under an applied magnetic field merely by modifying the one-electron Hamiltonian to incorporate the magnetic field. The lattice potential itself must be altered to some extent in order to incorporate the effects associated with the modified electron distribution in solids. The purpose of this investigation is to examine the question of the modified electronic charge distribution in a strong magnetic field in order to see whether any observable phenomena may be associated with it. Instead of attempting a complete theory of the problem, including correlation, we will approach the problem in the spirit of the independent-particle model, making those modifications which seem reasonable from our current understanding of many-body theory.

The nature of the eigenstates of a charged particle in a periodic lattice in a uniform magnetic field is by now fairly well understood.[3] The first treatment of this problem is due to Landau,[2] who treated the lattice potential as constant. Subsequent work by Peierls and others[4–12] has shed much light on the effect of the lattice. Recently much work on the degenerate electron gas in a strong magnetic field has been done by Quinn, Lee, Greene, Rodriguez, and others.[13] They solved simultaneously the equations of motion for the electrons in a self-consistent electromagnetic field and the Maxwell equations. One of their important results is the possibility for the existence of thermodynamic equilibrium states with a broken symmetry of interacting electrons in a strong magnetic field. Such a system can spontaneously adopt a state that is spatially nonuniform in the plane perpendicular to the applied uniform magnetic field. We are considering the possibility of a somewhat different structure here. A group-theoretical approach, which is applicable to this problem, has been developed by one of us.[14] This provides a convenient formulation on which much of our analysis is based. In Sec. II, we discuss the irreducible representations of the many-electron magnetic translation group. These representations are then obtained in Sec. III in terms of the product representations. It is shown there, for self-consistency, that the lattice potential must be modified to incorporate the two-dimensional probability density of electrons. The discrepancy between the modified potential and the periodic potential is treated as a perturbation in Sec. IV. In Sec. V, the perturbation calculation is carried out in the free-electron limit.

II. GENERALIZED MAGNETIC TRANSLATION OPERATORS

We state briefly the group-theoretical results.[3,14] Assume a magnetic field $\vec{B}$ along the $\vec{\tau}_3$ direction. The magnetic flux through a two-dimensional unit cell (τ_1, τ_2) is assumed to be a rational number l/N. Our unit is the quantum of flux hc/e. For convenience, the crystal dimensions are chosen as $N_1N\tau_1$, $N_1N\tau_2$, $N_3\tau_3$, and periodic boundary conditions are assumed. The magnetic translation group (a ray group) G consists of the operators defined as

$$T(\vec{\tau}) = \exp[i/\hbar)\vec{\tau}\cdot(\vec{\pi} - \hbar\vec{r}\times\vec{\beta})], \tag{1}$$

where

$$\vec{\beta} = e\vec{\beta}/\hbar c = (2\pi/\Omega)(l/N)\vec{\tau}_3,$$

$$\Omega = (\vec{\tau}_1 \times \vec{\tau}_2)\cdot\vec{\tau}_3, \quad \vec{\pi} = \vec{p} + e\vec{A}/c,$$

$\vec{A}$ is the vector potential, $-e$ is the electronic charge, and $\vec{\tau}$ is an arbitrary lattice vector. The operators do not affect the spin states, but commute with the single-electron Hamiltonian $H = \pi^2/2m + V(\vec{r})$. From the gauge invariant relation

$$T(\vec{\tau}_n)T(\vec{\tau}_m) = \exp[i(\vec{\tau}_n \times \vec{\tau}_m)\cdot\vec{\beta}]\; T(\vec{\tau}_m)T(\vec{\tau}_n), \quad (2)$$

there follows the useful special cases

$$T(\vec{\tau}_1)T(\vec{\tau}_2) = \exp(i2\pi l/N)\; T(\vec{\tau}_2)T(\vec{\tau}_1), \quad (3)$$

$$[T(\vec{\tau}_3),\; T(\vec{\tau})] = [T(N\vec{\tau}_1),\; T(\vec{\tau})] = [T(N\vec{\tau}_2),\; T(\vec{\tau})] = 0. \quad (4)$$

Consequently, $N\vec{\tau}_1$, $N\vec{\tau}_2$, and $\vec{\tau}_3$ serve as basis vectors for a magnetic superlattice. The imaginary crystal generated by the magnetic unit cell of volume $(N\vec{\tau}_1 \times N\vec{\tau}_2)\cdot\vec{\tau}_3 = N^2\Omega$ has the symmetry of the conventional translation group. Consequently the irreducible representations (IR) are characterized by wave vectors $\vec{q}$ in the magnetic zone of domain $(K_1/N, K_2/N, K_3)$. The representation matrices are N by N, given as

$$D^{\vec{q}}_{m,n}(\vec{\tau}_1) = \delta_{m,n}\exp[i\vec{q}\cdot\vec{\tau}_1 + im(2\pi l/N)], \quad (5a)$$

$$D^{\vec{q}}_{m,n}(\vec{\tau}_2) = \delta_{m,n+1}\exp[i\vec{q}\cdot\vec{\tau}_2] \quad (\mathrm{Mod}\,N). \quad (5b)$$

The translation through $\vec{\tau}_3$, i.e., in the direction of $\vec{B}$, is not interesting and will not be considered here. The N-fold degenerate wave functions are no longer of the Bloch type. However, the partner function for a given $\vec{q}$th IR, $B(\vec{q} + n_2 l\vec{K}_1/N;\, r)$, where $n_2 = 0, 1, 2, \cdots, N-1$, satisfy the equations

$$T(\vec{\tau}_1)B(\vec{q} + n_2 l\vec{K}_1/N;\, \vec{r}) = \exp[i\vec{q}\cdot\vec{\tau}_1 + in_2(2\pi l/N)]B(\vec{q} + n_2 l\vec{K}_1/N;\, \vec{r}), \quad (6a)$$

$$T(\vec{\tau}_2)B(\vec{q} + n_2 l\vec{K}_1/N;\, \vec{r}) = \exp[i\vec{q}\cdot\vec{\tau}_2]B(\vec{q} + (n_2+1)l\vec{K}_1/N;\, \vec{r}). \quad (6b)$$

The states of a single energy band can be viewed as decomposing into N magnetic sub-bands, clustered in sets of l. As is shown in Appendix A, for any magnetic field now available, it is a sufficient approximation to consider only the case $l = 1$.

The Hamiltonian of $\mathfrak{N}$ interacting electrons in the presence of a periodic lattice potential V_L and a magnetic field $\vec{B} = \vec{\nabla}\times\vec{A}$ is given by

$$\mathcal{H} = \sum_{i=1}^{\mathfrak{N}}\left[\frac{1}{2m}\left(\vec{p}_i + \frac{e\vec{A}(\vec{r}_i)}{c}\right)^2 + V_L(\vec{r}_i)\right] + \sum_{i,j=1}^{\mathfrak{N}}\frac{1}{2}\frac{e^2}{r_{ij}}. \quad (7)$$

Clearly $[\mathcal{H}, T_i(\vec{\tau})] \neq 0$, where $T_i(\vec{\tau})$ operates only on the ith electron. However, $\mathcal{H}$ is invariant under a magnetic translation $\mathcal{T}(\vec{\tau})$, operating on all the electrons simultaneously, viz., $[\mathcal{H}, \mathcal{T}(\vec{\tau})] = 0$, provided that periodic boundary conditions are imposed.[15] The operator $\mathcal{T}(\vec{\tau})$ is defined as

$$\mathcal{T}(\vec{\tau}) = \prod_{i=1}^{\mathfrak{N}} T_i(\vec{\tau}). \quad (8)$$

The set of such operators also forms a ray group $\mathcal{G}$ because of the relations

$$\mathcal{T}(\vec{\tau}_n)\mathcal{T}(\vec{\tau}_m) = \exp[i\mathfrak{N}(\vec{\tau}_n \times \vec{\tau}_m)\cdot\vec{\beta}]\; \mathcal{T}(\vec{\tau}_n), \quad (9a)$$

$$\mathcal{T}(\vec{\tau}_1)\mathcal{T}(\vec{\tau}_2) = \exp[i2\pi\mathfrak{N}/N]\; \mathcal{T}(\vec{\tau}_2)\mathcal{T}(\vec{\tau}_1), \quad (9b)$$

$$[\mathcal{T}(\vec{\tau}_3), \mathcal{T}(\vec{\tau}_1)] = [\mathcal{T}(\vec{\tau}_3), \mathcal{T}(\vec{\tau}_2)] = 0. \quad (9c)$$

If $\mathfrak{N}$ and N have any factor in common, it will henceforth be assumed that $\mathfrak{N}/N$ has been brought to lowest terms (i.e., $\mathfrak{N}$ no longer need refer to the number of particles in the system, and a corresponding change is possible in the definition of N).[16] Equation (9a) differs from Eq. (2) because of the factor $\mathfrak{N}$ which appears in the phase. Thus the results obtained for G also apply to $\mathcal{G}$, with substitution of $\mathfrak{N}/N$ for l/N. Each IR is characterized by a vector $\vec{Q}$ in a newly defined magnetic zone as

$$\mathfrak{D}^{\vec{Q}}_{m,n}(\vec{\tau}_1) = \delta_{m,n}\exp[i\vec{Q}\cdot\vec{\tau}_1 + im(2\pi\mathfrak{N}/N)], \quad (10a)$$

$$\mathfrak{D}^{\vec{Q}}_{m,n}(\vec{\tau}_2) = \delta_{m,n+1}\exp(i\vec{Q}\cdot\vec{\tau}_2) \quad (\mathrm{Mod}_2 N). \quad (10b)$$

The periodicity of the wave functions and the degeneracy are also changed accordingly.

The degeneracy N of the many-body state is sensitive to the number of electrons in the system. Correspondingly, so are the translational properties of the many-body wave functions. For example, if the number of electrons is the same as the originally defined value of N, $(N = N_0)$, the phase factor of Eq. (9a) disappears and the many-particle state has the same translational behavior as a Bloch function. Conversely, if the number is not a multiple of N_0, the many-particle state does not have Bloch character with respect to the originally defined lattice, so that the charge density associated with such a state need not have the periodicity of the crystal. Thus, it is not rigorous to assume, in the presence of a magnetic field, that the self-consistent potential has the original periodicity of the lattice. Although such deviations from periodicity can be assumed small on experimental as well as theoretical grounds, it is our purpose to see whether any experimentally observable effects may be associated with such changes.

III. IRREDUCIBLE REPRESENTATIONS AND BASIS FUNCTIONS

Basis functions for an IR of the group $\mathcal{G}$ can be obtained as linear combinations of products of one-electron basis functions of the group G. Define the product functions as

$$B^{\mu_i,\vec{q}_i}(\vec{r}_i)=\prod_{i=1}^{\mathfrak{N}} B(\vec{q}_i+\mu_i\vec{K}_1/N;\vec{r}_i), \tag{11}$$

where $\mu_i=0,1,2,\cdots,N-1$. Note that the notation $B^{\mu_i,\vec{q}_i}(\vec{r}_i)$ indicates a $\mathfrak{N}$-electron wave function, where the ith electron occupies a one-electron state specified by μ_i and $\vec{q}_i$. The functions $B^{\mu_i,\vec{q}_i}(\vec{r}_i)$ are Bloch type along the x and z axes, but are not necessarily Bloch-like in the y direction. Let $\nu_j=\mu_j-\mu_1$ where $j=1,2,\cdots,\mathfrak{N}$. For a fixed choice of ν_i and $\vec{q}_i$, consider the set of N product functions

$$B_\alpha^{\nu_i,\vec{q}_i}(\vec{r}_i)=\prod_{i=1}^{\mathfrak{N}} B(\vec{q}_i+[(\alpha-1)+\nu_i]\vec{K}_1/N;\vec{r}_i), \tag{12}$$

where $\alpha=1,2,\ldots,N$, and $\alpha+\nu_i$ has modulus N. It can be shown by using Eqs. (6a), (6b), (8), and (11) that

$$\mathcal{T}(\vec{\tau}_1)B_\alpha^{\nu_i,\vec{q}_i}(\vec{r}_i)=\exp\left(i\sum_{j=1}^{\mathfrak{N}}[\vec{q}_j\cdot\vec{\tau}_1+(\alpha+\nu_j-1)2\pi/N]\right)\times B_\alpha^{\nu_i,\vec{q}_i}(\vec{r}_i), \tag{13a}$$

$$\mathcal{T}(\vec{\tau}_2)B_\alpha^{\nu_i,\vec{q}_i}(\vec{r}_i)=\exp\left(i\sum_{j=1}^{\mathfrak{N}}\vec{q}_j\cdot\vec{\tau}_2\right)\times B_\alpha^{\nu_i,\vec{q}_i}(\vec{r}_i)\quad(\mathrm{Mod}\,N). \tag{13b}$$

The functions defined by Eq. (12) serve as a basis for a reducible representation of $\mathcal{G}$. The matrices of this representation, denoted by $(\nu_i,\vec{q}_i)$ for the elements $\vec{\tau}_1$ and $\vec{\tau}_2$, are given by

$$D_{m,n}^{(\nu_i,\vec{q}_i)}(\vec{\tau}_1)=\exp\left(i\sum_{j=1}^{\mathfrak{N}}[\vec{q}_j\cdot\vec{\tau}_1+(\alpha+\nu_j-1)2\pi/N]\right)\delta_{m,n}, \tag{14}$$

$$D_{m,n}^{(\nu_i,\vec{q}_i)}(\vec{\tau}_2)=\exp\left(i\sum_{j=1}^{\mathfrak{N}}\vec{q}_j\cdot\vec{\tau}_2\right)\delta_{m,n+1}\quad(\mathrm{Mod}\,N). \tag{15}$$

The remaining matrices are easily obtained from these.

If M is the largest common factor of $\mathfrak{N}$ and N, and if $N=MN'$, the normalized basis functions which we seek turn out to be

$$B_\alpha^{\nu_i,\vec{q}_i,\gamma}(\vec{r}_i)=M^{-1/2}\sum_{j=0}^{m-1}\exp[-2\gamma\pi(\alpha+jN')/N]\times B_{\alpha+jN'}^{\nu_i,\vec{q}_i}(\vec{r}_i), \tag{16}$$

where $\alpha=1,2,\ldots,N'$; $\gamma=1,2,\ldots,M$. The representation label $\vec{Q}$ is obtained from ν_i, $\vec{q}_i$, and γ by the relation

$$\vec{Q}=\sum_{j=1}^{\mathfrak{N}}[\vec{q}_j+(\nu_j-1)\vec{K}_1/N+\gamma\vec{K}_2/\mathfrak{N}N]. \tag{17}$$

Let us examine the behavior of the functions $B_\alpha^{\nu_i,\vec{q}_i,\gamma}(\vec{r}_i)$ as a function of y. We consider for illustrative purpose the case for $N=6$, $\mathfrak{N}=2$. Figure 1 shows the magnetic zone corresponding to this case. The vectors $\vec{q}_1$, $\vec{q}_2$ label the representations of the one-electron states which are used in the product wave function. The product function $B_\alpha^{\nu_i,\vec{q}_i}(\vec{r}_i)$ illustrated in Fig. 2 corresponds to $\mu_1=\mu_2=0$. This is one of six partner functions of the reducible representation ($\nu_1=\nu_2=0$, $\vec{q}_1$, $\vec{q}_2$). The remaining partners come from the other products for which $\mu_1=\mu_2$. These six functions are schematically shown in Fig. 2, column III. From these six functions we can form three which transform according to a representation labeled by $\vec{Q}_1$ (see Fig. 1), and another three which transform according to $\vec{Q}_2$. One of these linear combinations is indicated in column IV of Fig. 2.

We now consider what happens in terms of the independent-electron picture. If, in such a picture, one has a state of completely filled Landau levels, the many-particle state is consistent with a periodic lattice potential. This is similar to the closed-shell configuration which leads to a spherical potential in the atomic analog. As in the atomic case, all one needs to consider are those electrons outside of closed shell (i.e., filled Landau levels). The potential which results from these electrons will be referred to as the residual potential.

The rational field was introduced for convenience only. Any physical property which depends on the precise value of $\mathfrak{N}/N$ is not likely to be observable. This point was discussed by one of us in connection with the independent-particle model, where l/N is the important parameter.[3]

IV. RESIDUAL POTENTIAL

We assume as our unperturbed Hamiltonian H_0 the usual independent particle one, which is characterized by the self-consistent potential $V(\vec{r})$. We thus assume

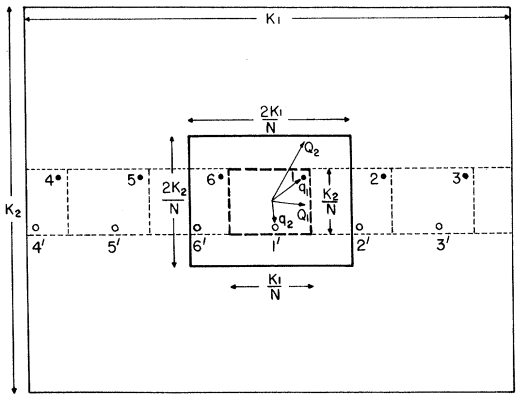

FIG. 1. Two-dimensional reciprocal spaces for $\vec{k}$ (the first Broullin zone) for $\vec{q}$ (the magnetic zone indicated by the dashed line) and for $\vec{Q}$ (the heavy-lined region). The magnetic field corresponds to $N=6'$, the number of electrons, $\mathfrak{N}=2$.

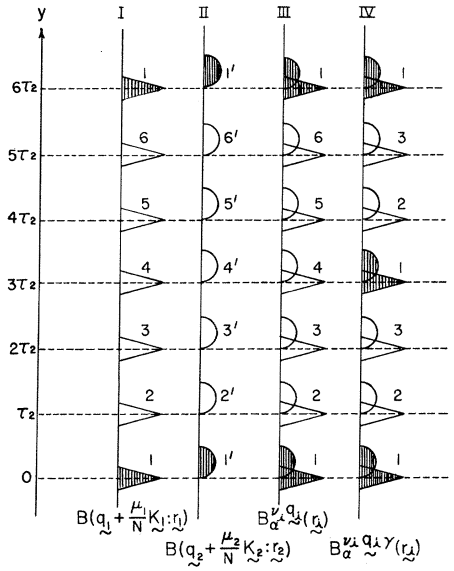

FIG. 2. Symbolic profile of the laminar states (for $N=6$ and $N=2$) along the y axis. The shadow states are under consideration. They correspond to $\mu_1=\mu_2=\nu_1=\nu_2=0$.

$$H_0=\sum_{i=1}^{\mathfrak{N}}[(1/2m)(\vec{p}_i+e\vec{A}(\vec{r}_i)/c)^2+V(\vec{r}_i)]. \tag{18}$$

We further assume we can solve for the associated one-electron states by first solving the band problem corresponding to $\vec{A}=0$. Secondly, we use the effective Hamiltonian method to incorporate the effect of the magnetic field. This procedure has been discussed in a number of places.[17-23]

We can determine, in principle, the one-electron states associated with the last unfilled Landau level. We now consider the complete Hamiltonian of the system. If we now let $\mathfrak{N}$ denote the number of electrons in this level, we can use as a perturbing term the expression

$$H_1=\sum_{i,j=1}^{\mathfrak{N}}{}'\frac{e^2}{2r_{ij}}-\sum_{i=1}^{\mathfrak{N}}ev(\vec{r}_i), \tag{19}$$

where $v(\vec{r}_i)$ is the periodic part of the potential contributed by these electrons. The antisymmetrized wave functions belonging to the $(\nu_i, \vec{q}_i, \gamma)$th IR are

$$\Psi_\alpha^{(\nu_i,\vec{q}_i\gamma)}(\vec{r}_i;\, s_i)=(\mathfrak{N}!)^{-1/2}\sum(-1)^{\mathcal{P}}\mathcal{P}B_\alpha^{(\nu_i,\vec{q}_i,\gamma)}(\vec{r}_i;\, s_i), \tag{20}$$

where $\mathcal{P}$ is the conventional notation for a permutation operator and s_i denotes the spin coordinate. Since H_1 commutes with $\mathcal{G}$, it is generally known from group theory that

$$(\Psi_\alpha^{\vec{Q}}|H_1|\Psi_\beta^{\vec{P}})=\frac{1}{N'}\cdot\sum_{m=1}^{N'}(\Psi_m^{\vec{Q}}|H_1|\Psi_m^{\vec{Q}})\,\delta_{\vec{Q},\vec{P}}\,\delta_{\alpha\beta}. \tag{21}$$

There are many sets of $(\nu_i, \vec{q}_i, \gamma)$ corresponding to the same vector $\vec{Q}$. Let these sets be labeled as ζ_n, $n=1, 2, \ldots, t$. We then have to diagonalize a t by t matrix, the eigenfunctions for which are of the form

$$\sum_{i=1}^{t}C_{\zeta_i}\Psi_\alpha^{\zeta_i}.$$

For a particular choice of $(\nu_i, \vec{q}_i, \gamma)$, we only need to calculate the matrix element $(H_1)_{1,1}$. From Appendix A, we have

$$\begin{aligned}
&[\Psi_1^{(\nu_i,\vec{q}_i,\gamma)}(\vec{r}_i;\, s_i)|H_1|\Psi_1^{(\nu_i,\vec{q}_i,\gamma)}(\vec{r}_i;\, s_i)]\\
&=\sum_{i=1}^{\mathfrak{N}}(-e)\left[B\left(\vec{q}_i+\frac{\nu_i\vec{K}_1}{N};\vec{r},\, s_i\right)\middle|v(\vec{r})\middle|B\left(\vec{q}_i+\frac{\nu_i\vec{K}_1}{N};\vec{r},\, s_i\right)\right]\\
&+\frac{1}{2}\sum_{i,j=1}^{\mathfrak{N}}\left[B\left(\vec{q}_i+\frac{\nu_i\vec{K}_1}{N};\vec{r}_1,\, s_i\right)B\left(\vec{q}_j+\frac{\nu_j\vec{K}_1}{N};\vec{r}_2;\, s_j\right)\middle|\frac{e^2}{r_{12}}\middle|\right.\\
&\left.\times B\left(\vec{q}_i+\frac{\nu_i\vec{K}_1}{N};\vec{r}_1,\, s_i\right)B\left(\vec{q}_j+\frac{\nu_j\vec{K}_1}{N};\vec{r}_2,\, s_j\right)\right]\\
&-\frac{1}{2}\sum_{i,j=1}^{\mathfrak{N}}\left[B\left(\vec{q}_i+\frac{\nu_i\vec{K}_1}{N};\vec{r}_1,\, s_i\right)B\left(\vec{q}_j+\frac{\nu_j\vec{K}_1}{N};\vec{r}_2,\, s_j\right)\middle|\frac{e^2}{r_{12}}\middle|\right.\\
&\left.\times B\left(\vec{q}_i+\frac{\nu_i\vec{K}_1}{N};\vec{r}_2,\, s_i\right)B\left(\vec{q}_j+\frac{\nu_j\vec{K}_1}{N};\vec{r}_1,\, s_j\right)\right]\delta_{s_i,s_j}\,.
\end{aligned} \tag{22}$$

The two-body terms come from the Coulomb and exchange interactions between two sets of planar states. The one-body potential term can be viewed as resulting from a positive background with lattice

periodicity. Note that Eq. (22) is γ independent. This is because γ was introduced as a phase factor to distinguish the planar states which have similar density probability.

We could equally well have chosen $\mathfrak{D}(\vec{\tau}_2)$ to be diagonal, instead of $\mathfrak{D}(\vec{\tau}_1)$, in which case the laminar orbitals would be localized along the x axis. This result yields an equivalent picture of the electron system as far as group theory is concerned. There could however be a directional effect in the plane normal to the magnetic field even though the original Hamiltonian has no preferred orientation. (This is analogous to the alignment of spins in a ferromagnetic domain in a cubic crystal.) The electron-electron interaction can thus be regarded as a symmetry-breaking term, which could yield a laminar structure in the electron density. This structure would yield a self-consistent potential with the periodicity of the planes. Such a structure is consistent with group theory and could possibly occur at low temperatures. We will try to obtain an estimate of the "binding energy" of such a state in Sec. V.

V. EMPTY-LATTICE CALCULATION

We first estimate the residual Coulomb energy for the empty-lattice model. The unperturbed Hamiltonian is

$$H_0=\sum_{i=1}^{\mathfrak{N}}(1/2m)(\vec{\mathfrak{p}}_i+e\vec{A}(\vec{r}_i)/c)^2. \tag{23}$$

In the Landau gauge, $\vec{A}=B(-y,0,0)'$, the solutions are

$$\psi^n_{k_x,k_z}(\vec{r})=(L_xL_z)^{-1/2}\exp[i(k_xx+k_zz)-\tfrac{1}{2}\beta(y-y_0)^2]\times H_n[\beta^{1/2}(y-y_0)], \tag{24}$$

$$E_{n,k_z}=(n+\tfrac{1}{2})\hbar\omega_c+\hbar^2k_z^2/2m, \tag{25}$$

where $H_n[\beta^{1/2}(y-y_0)]$ is a normalized Hermite function centered at $y_0=-k_x/\beta$. The basis function for the $\vec{q}$th IR of group G are generated by using projection operators:

$$B^n(\vec{q}+\mu\vec{K}_1/N;\vec{r})=(N_2)^{-1/2}\sum_{t=0}^{N_2-1}\exp[-i(tN+\mu)\vec{q}\cdot\vec{\tau}_2]\times T[(tN+\mu)\vec{\tau}_2]\psi^n_{k_xk_z}(\vec{r}), \tag{26}$$

where $\vec{q}$ is restricted to a magnetic zone and $q_x=k_x$; $q_z=k_z$. Those Hermite functions centered outside the crystal are chopped off. Note that τ_1, τ_2, τ_3 and therefore N are not uniquely defined. We assume a set of lattice vectors and treat them as adjustable parameters. For a ground state consisting of $\mathfrak{N}$ electrons in a partially filled shell, the product functions are

$$B_\alpha^{(n_i,\nu_i,\vec{q}_i)}(\vec{r}_i)=(N_2)^{-1/2}\prod_{i=1}^{\mathfrak{N}}\sum_{t=1}^{N_2}\exp[-i(tN+\alpha+\nu_i-1)\vec{q}_i\cdot\vec{\tau}_2]\times T[(tN+\alpha+\nu_i-1)\vec{\tau}_2]\psi^{n_i}_{q_xq_z}(\vec{r}_i), \tag{27}$$

$$B_\alpha^{(n_i,\nu_i,\vec{q}_i,\gamma)}(\vec{r}_i)=\sum_{j=0}^{M-1}(M)^{-1/2}\exp[i2\pi\gamma(\alpha+jN')/N]B^{(n_i,\nu_i,\vec{q}_i)}_{\alpha+jN'}(\vec{r}_i), \tag{28}$$

where $\alpha=1,2,\ldots,N'$ and $\gamma=1,2,\ldots,M$. Geometrically the single-particle states $B^n(\vec{q}+\mu\vec{K}_1/N;\vec{r})$ consist of N_2 planar functions $\psi^n_{q_xq_z}(\vec{r})$ centered along the y axis. Their equilibrium points are equally spaced at $y_0=(-q_x/\beta+\mu\tau_2)+tN\tau_2$, where $t=1,2,\ldots,N_2$. The width of each plane is

$$2q_0=2[(2n+1)/\beta]^{1/2}=2[(n+1/2)N\tau_1\tau_2/\pi]^{1/2}. \tag{29}$$

We are interested in the case of negligible intraband tunneling; i.e., we assume $2q_0<N\tau_2$.

The $\mathfrak{N}$-electron wave function is simply $\mathfrak{N}$ mutually penetrating sets of parallel laminar orbitals. In a region $\Delta y=N\tau_2$ on the y axis, there are $\mathfrak{N}$ such planes. Each one belongs to a different electron. The analytic form of the perturbation energy is derived in Appendix B. In principle, the ground state is determined by minimizing the energy treating n_i, $\vec{q}_i$, and ν_i as parameters. However, it is difficult to get an accurate estimate of the energy from the analytic solution. We will therefore estimate the order of magnitude by a semiclassical approach.

The residual Coulomb energy of $\mathfrak{N}$ electrons in states belonging to the same n and k_z will be first estimated. This is the electrostatic energy of $\mathfrak{N}$ electrons immersed in a uniform positive-charged background of charge density $\mathfrak{N}e/V$. The Coulomb energy of these $\mathfrak{N}$ sets of penetrating laminar states will be a minimum if all the planar orbitals are equally separated by $\Delta=N\tau_2/\mathfrak{N}$. Also, it is less for smaller $N\tau_2$. However, we have $N\tau_2\geq 2q_0$; hence, we approximate the ground state by setting $N\tau_2=2q_0$ and then determine $\tau_1=2\pi/N\tau_2\beta=\pi/q_0\beta$. In the semiclassical approach we assume, for the electronic density probability of the planar orbitals, the classical value $P(y)=(1/\pi)[q_0^2-(y-y_0)^2]^{-1/2}$. Then the electrostatic energy density $\frac{1}{2}E^2$ is obtained by solving $\vec{\nabla}\cdot\vec{E}=4\pi\rho(y)$, where $\rho(y)$ is the resultant charge density.

The density distribution, along the y axis, of $\mathfrak{N}$ electrons in the ground state is found by first periodically extending $P(y)=(1/\pi)[q_0^2-(y-y_0)^2]^{-1/2}$ along the y axis with period $2q_0$. Call the new function $S(y-y_0)$. Then $\mathfrak{N}$ such functions $S(y-m\Delta)$, where $m=1,2,\ldots,\mathfrak{N}$, are superimposed. Including

the contribution of the positive-charged background, it is easy to find the electrostatic energy per electron of the system as

$$\epsilon = (e^2 q_0^2/8\pi^2 V)(1 - 2/3\mathfrak{N}). \tag{30}$$

Since $\mathfrak{N}$ is large, the residual Coulomb energy per electron for a given n and k_z can be rewritten as

$$\epsilon = (e^2 q_0^2/8\pi^2 V) = (e^2/8\pi^2 V)[(2n+1)/\beta], \tag{31}$$

where V is the volume of the crystal.

In real system, all the Landau levels on the Fermi surface with different n and k_z are partially filled. The residual Coulomb energy can be estimated by the same process. Its upper limit can be easily obtained by setting $q_0 = Q_0$ in Eq. (31), where Q_0 is the maximum spread of the Landau levels involved. Then we have

$$\epsilon\,|_{\max} = (e^2 Q_0^2/8\pi^2 V) = (e^2/8\pi^2 V)[(2N_0+1)/\beta], \tag{32}$$

where N_0 specifies the Laudau level for Q_0.

The volume V can not be arbitrarily small due to the restriction of periodic boundary conditions. For a thin film of thickness 500 Å, the area of the film should be at least $10^4 Q_0^2$. Putting these values into Eq. (32), we obtain

$$\epsilon\,|_{\max} \simeq 3\times 10^{-8}\ \text{Ry}.$$

For metal with conduction electrons approximated by free electrons, we have to take into account the lattice constants. The result is

$$\epsilon\,|_{\max} = (e^2 N\tau_2 Q_0)/16\pi^2 V. \tag{33}$$

For a thin film of volume $V = (500\tau_3)(100N\tau_1) \times (100N\tau_2)$ and a strong magnetic field $B \simeq 10^6$ G, for which $N \simeq 10^4$, the residual Coulomb energy per electron is about 10^{-8} Ry.

We can not find a semiclassical approximation for the residual exchange energy, but it is presumed to be of the same order of magnitude as the Coulomb energy. Consequently, the correction energy is negligibly small. Thus we would estimate that no alignment into a laminar structure could be observed in a free-electron metal at a temperature above $\simeq 0.001$ °K. Even at such a temperature we are not in position to predict from this elementary approach how such a state would manifest itself. We have not investigated the possibility of the electrons arranging themselves into domains with different orientations of the planes for example. It is possible that if such a state did exist and extended to the surface of the metal, there might be diffraction effects associated with the periodic surface density, as in a reflection grating. Since ϵ involves only the partially filled Landau levels at the Fermi surface, the de Haas–van Alphen–type oscillation of ϵ versus $1/B$ may also exist.

VI. CONCLUSION

The analytic expression for the residual interaction energy is too complicated to be evaluated numerically. Although the semiclassical calculation is much less exact, its accuracy is sufficient to give an estimate of the residual interaction for a reasonable density of electrons. In the empty-lattice model it was found that the interaction is very small. Such a calculation may be expected to yield an order-of-magnitude estimate for most metals, at least those described by a nearly free-electron picture at the Fermi surface.

According to Eq. (32) it appears that the residual interaction energy is inversely proportional to $B^{3/2}$. It should be pointed out that this seemingly nonphysical result is not to be taken literally. Equation (32) is derived using the nonphysical assumption of periodic boundary conditions. These can be invoked only if B exceeds some value (of the order of 10^3 G for a solid of dimension about 1 cm). Since we make use of rational fields throughout, the theory pertains only to values of B substantially larger than this. The falling off with B is not expected to be valid for fields greater than 10^8–10^9 G in which case B changes the one-electron wave functions significantly over atomic dimensions.

The residual interaction seems to be several orders of magnitude too small to give rise to observable effects even at helium temperatures. These calculations thus support the usual view that the behavior of solids in applied magnetic fields can be understood in terms of the picture in which one merely replaces the momentum operator $\vec{p}$ in the Hamiltonian for the individual electron by the kinetic momentum $\vec{p} + e\vec{A}/c$. This assumption, which has been used extensively, is thus expected to yield quite reliable predictions.

It is to be noted that we have not carried out a fully rigorous treatment of the correlation problem. This problem is too difficult to be carried out in any detail. We have merely assumed that true correlation terms are not measurably altered by a magnetic field.

In summary, we say that a state of lowered energy can exist in a strong magnetic field at sufficiently low temperatures, which results in a superlattice structure with a periodic laminar structure. We have not considered in this elementary theory the residual interactions which are responsible for superconductivity. In the strong magnetic fields which we are considering we do not expect the kind of correlated behavior which are associated with superconductivity.

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APPENDIX A: APPROXIMATING RATIONAL FIELD $l=1$

For a crystal of dimensions $(NN_1\tau_1, NN_2\tau_2, N_3\tau_3)$ in a magnetic field $\beta \propto 1/N$, the symmetrized functions are

$$B^n(\vec{q}+\mu\vec{K}_1/N;\ \vec{r}) = (N_2)^{-1/2}\sum_{t=1}^{N_2}\exp[-i(tN+\mu)\vec{q}\cdot\vec{\tau}_2] \times T[(tN+\mu)\vec{\tau}_2]\psi^n_{\vec{q}}(\vec{r}), \tag{A1}$$

where $\psi^n_{\vec{q}}(\vec{r})$ are Landau functions with

$$\vec{q} = n_1\vec{k}_1/N_1N + n_2\vec{K}_2/N_2N + n_3\vec{K}_3/N_3\ , \tag{A2}$$

and $\mu = 1, 2, \ldots, N$; $n_i = 1, 2, \ldots, N_i$ with $i = 1, 2, 3$. With a slight change of magnetic field from $1/N$ to $l/N' = l/(lN+m)$, where $m \ll N$, the new symmetrized functions are

$$b^{n,\alpha}(\vec{s}+\delta l\vec{K}_1/N';\ \vec{r}) = (N_2')^{-1/2}\sum_{t=1}^{N_2'}\exp[-i(pN'+\delta)(\vec{s}+(\alpha-1)\vec{K}_1/N')\cdot\vec{\tau}_2] \times T[(pN'+\delta)\vec{\tau}_2]\psi^n_{\vec{s}+(\alpha-1)\vec{K}_1/N'}(\vec{r})\ , \tag{A1'}$$

where

$$\vec{s} = n_1'\vec{K}_1/N_1'N' + n_2'\vec{K}_2/N_2'N' + n_3\vec{K}_3/N_3\ , \tag{A2'}$$

and $\alpha = 1, 2, \ldots, l$; $n_i' = 1, 2, \ldots, N_i'$ with $i = 1, 2$; $\delta = 1, 2, \ldots, N'$; $N_1'N' = N_1N$, $N_2'N' = N_2N$. The index α describes explicitly which of the l clustered bands is referred. Note that the domain of $\vec{q}$ is not exactly l^2 times as large as the domain of $\vec{s}$. The discrepancy in each dimension is $mK_1/N(lN+m)$ [or $mK_2/N(lN+m)$]. This small difference does not affect many of the physical quantities which depend on the magnetic field. However, it does have significant importance to the IR's of the magnetic translation group in the sense of completeness of the basis functions. The inverse transform of Eq. (A1') gives

$$\psi^n_{\vec{s}+(\alpha-1)\vec{K}_1/N'}(\vec{r}) = (N_2')^{-1/2}\sum_{s_y}\exp[i(pN'+\delta)\vec{s}\cdot\vec{\tau}_2] \times T[-(pN'+\delta)\vec{\tau}_2]\, b^{n,\alpha}(\vec{s}+\delta l\vec{K}_1/N';\ \vec{r}) = (N_2')^{-1/2}\sum_{s_y} b^{n,\alpha}(\vec{s};\ \vec{r})\ . \tag{A3}$$

For $m \ll N$, we have the fairly good approximation $N' \simeq lN$, $N_1' \simeq N'/l$, $N_2' \simeq N_2/l$, and $s_x + (\alpha-1)K_1/N' = q_x$ for a proper choice of α. We change the notation by extending the domain of s_x l times larger; then we can omit the index α and set $s_x = q_x$. For a pair of $\psi^n_{\vec{q}}(\vec{r})$ and $\psi^n_{\vec{s}}(\vec{r})$ with $\vec{q} = \vec{s}$, the centers of the two Hermite functions are slightly shifted by

$$|y_0(\vec{q}) - y_0(\vec{s})| = \Omega q_x m/2\pi\tau_3 l\ .$$

It is negligibly small compared to the width of the planar functions. Hence we can approximate $\psi^n_{\vec{q}}(\vec{r})$ by $\psi^n_{\vec{s}}(\vec{r})$ for $\vec{q} = \vec{s}$. Substituting Eq. (A3) into Eq. (A1), using the new notation without the appearance of α, we have

$$B^n(\vec{q}+\mu\vec{K}_1/N;\ \vec{r}) = l^{-1/2}\, e^{-i2\pi\mu m/lN}\sum_{t=1}^{l} e^{-itN\vec{q}\cdot\vec{\tau}_2} \times T(tN\vec{\tau}_2)\, b^n(\vec{s}+\mu\vec{K}_1/N - \xi\vec{K}_2/lN;\ \vec{r})\ , \tag{A4}$$

where ξ is an integer such that $q_y - \xi K_2/lN$ falls in the range $\pm K_2/2_lN$.

The derivation of Eq. (A4) depends on the approximation $N' \simeq lN$. This is a very good approximation for the highest achievable field, or even higher. If the magnetic field is so strong that the approximation collapses, then both l and N are small. In this case, it is not necessary to use the approximating field $l = 1$. Equation (A4) indicates that the field $\beta \propto l/N'$ can be replaced by the field $\beta \propto 1/(N'/l) = 1/N$, with negligible effect on the physical quantities which depend on the strength of the magnetic field.

APPENDIX B: ANALYTICAL EXPRESSION FOR RESIDUAL INTERACTION ENERGY

The matrix of the residual interaction is the product of a constant and a unit matrix. Using Eq. (24) for $\alpha = 1$, we obtain

$$\Psi_1^{(n_i\nu_i\vec{q}_i\gamma)}(\vec{r}_i,\ s_i) = (\mathfrak{N}!)^{-1/2}\sum_{\mathcal{P}}(-1)^{\mathcal{P}}\,\mathcal{P}B_1^{(n_i\nu_i\vec{q}_i\gamma)}(\vec{r}_i,\ s_i)\ . \tag{B1}$$

The constant is given by

$$(\Psi_1^{(n_i\nu_i\vec{q}_i\gamma)}(\vec{r}_i,\ s_i)\,|\,H_1\,|\,\Psi_1^{(n_i\nu_i\vec{q}_i\gamma)}(\vec{r}_i,\ s_i)) = (MN!)^{-1}\sum_{u,\,s=0}^{M-1}\exp\left(-i2\gamma\pi\frac{u-s}{M}\right)\left[\sum_{\mathcal{P}}(-1)^{\mathcal{P}}\,\mathcal{P}\prod_{i=1}^{N}B^{n_i}\left(\vec{q}_i+(\nu_i+sN')\frac{\vec{K}_1}{N};\ \vec{r}_i,\ s_i\right)\right.$$

$$\times\left|\sum_{\xi,\eta}{}'\frac{e^2}{2r_{\xi\eta}}-\sum_{\xi=1}^{N}ev(\vec{r}_\xi)\left|\sum_{\mathcal{P}}(-1)^{\mathcal{P}}\mathcal{P}\prod_{i=1}^{N}B^{n_i}\left(\vec{q}_i+(\nu_i+uN')\frac{\vec{K}_1}{N};\vec{r}_i s_i\right)\right.\right]$$

$$=\sum_{\xi=1}^{\mathfrak{N}}(-e)\left(B\left(\vec{q}_\xi+\frac{\nu_\xi\vec{K}_1}{N};\vec{r},s_\xi\right)|v(\vec{r})|B\left(\vec{q}_\xi+\frac{\nu_\xi\vec{K}_1}{N};\vec{r},s_\xi\right)\right)$$

$$+(M)^{-1}\sum_{u=0}^{M-1}\left\{\sum_{\xi,\eta}{}'\left[B^{n_\xi}\left(\vec{q}_\xi+(\nu_\xi+uN')\frac{\vec{K}_1}{N};\vec{r}_1,s_\xi\right)B^{n_\eta}\left(\vec{q}_\eta+(\nu_\eta+uN')\frac{\vec{K}_1}{N};\vec{r}_2,s_\eta\right)\right.\right.$$

$$\times\left|\frac{e^2}{2r_{12}}\right|B^{n_\xi}\left(\vec{q}_\xi+(\nu_\xi+uN')\frac{\vec{K}_1}{N};\vec{r}_1,s_\xi\right)B^{n_\eta}\left(\vec{q}_\eta+(\nu_\eta+uN')\frac{\vec{K}_1}{N};\vec{r}_2,s_\eta\right)\Big]$$

$$-\sum_{\xi,\eta}{}'\left[B^{n_\xi}\left(\vec{q}_\xi+(\nu_\xi+uN')\frac{\vec{K}_1}{N};\vec{r}_1,s_\xi\right)B^{n_\eta}\left(\vec{q}_\eta+(\nu_\eta+uN')\frac{\vec{K}_1}{N};\vec{r}_2,s_\eta\right)\right.$$

$$\times\left|\frac{e^2}{2r_{12}}\right|B^{n_\xi}\left(\vec{q}_\xi+(\nu_\xi+uN')\frac{\vec{K}_1}{N};\vec{r}_2,s_\xi\right)B^{n_\eta}\left(\vec{q}_\eta+(\nu_\eta+uN')\frac{\vec{K}_1}{N};\vec{r}_1,s_\eta\right)\Big]\delta_{s_\xi,s_\eta}\Big\}. \tag{B2}$$

Since e^2/r_{12} commutes with the operator $T_1(-u\vec{\tau}_2)\,T_2(-u\vec{\tau}_2)$, the value of u has no effect on the matrix elements in Eq. (B2). Hence we set $u=0$ for all the matrix elements, and Eq. (B2) reduces to Eq. (22).

We will treat the residual Coulomb energy $(H_{12})_C$ and the residual exchange energy $(H_{12})_{ex}$ separately for the empty-lattice model. For Coulomb energy, we assume a single spin for simplicity. Using Eq. (26), we have

$$(H_{12})_c=(N_2)^{-2}\sum_{\xi,\eta}{}'\sum_{t_i=1}^{N_2}\exp\{-i[N(t_3-t_1)\vec{q}_\xi+N(t_4-t_2)\vec{q}_\eta]\cdot\vec{\tau}_2\}\,\{T_1[(t_1N+\nu_\xi)\vec{\tau}_2]\,\psi^{n_\xi}_{\vec{q}_\xi}(\vec{r}_1)\,T_2[(t_2N+\nu_\eta)\vec{\tau}_2]$$
$$\times\psi^{n_\eta}_{\vec{q}_\eta}(\vec{r}_2)|e^2/2r_{12}|\,T_1[(t_3N+\nu_\xi)\vec{\tau}_2]\,\psi^{n_\xi}_{\vec{q}_\xi}(\vec{r}_1)\,T_2[(t_4N+\nu_\eta)\vec{\tau}_2]\,\psi^{n_\eta}_{\vec{q}_\eta}(\vec{r}_2)\}\,.$$

Substituting in the Fourier transform of the two-body potential and integrating over x and z, we obtain

$$(H_{12})_c=(2N_2^2)^{-1}\sum_{\xi,\eta}{}'\sum_{t_i=1}^{N_2}(4e^2\pi/V)\delta_{(t_1-t_3),(t_4-t_2)}\exp\{-i[N(t_3-t_1)\vec{q}_\xi+N(t_4-t_2)\vec{q}_\eta]\cdot\vec{\tau}_2\}\sum_{\vec{q}}[\{1/[(t_1-t_3)^2K_1^2+q^2]\}$$
$$\times\exp(\{-[(t_3-t_1)K_1+iq]^2-2q^2+i2q\beta\tau_2[(t_2-t_1)N+(\nu_\eta-\nu_\xi)]-i2q(q_{\xi_x}-q_{\eta_x})\}/2\beta)$$
$$\times\int dy\,(\exp\{-[\beta y+(q_{\xi_x}-\tfrac{1}{2}iq)+(t_3-t_1)\tfrac{1}{2}K_1]^2/\beta\}\,H^*_{n_\xi}[\beta^{1/2}(y+\tfrac{1}{2}q_{\xi_x})]\,H_{n_\xi}\{\beta^{1/2}y+[q_{\xi_x}+(t_3-t_1)K_1]\beta^{-1/2}\})$$
$$\times\int dy\,(\exp\{-[\beta y+(q_{\eta_x}+\tfrac{1}{2}iq)-(t_3-t_1)\tfrac{1}{2}K_1]^2/\beta\}$$
$$\times H^*_{n_\eta}[\beta^{1/2}(y+\tfrac{1}{2}q_{\eta_x})]\,H_{n_\eta}\{\beta^{1/2}y+[q_{\eta_x}-(t_3-t_1)K_1]\beta^{-1/2}\})]\,.$$

The two integrals can be evaluated using generating function

$$S(\xi,t)=e^{-t^2+2t\xi}=\sum_{n=0}^{\infty}H_n(\xi)t^n(n!)^{-1}\,.$$

Omitting the detailed algebraic work, the final result becomes

$$(H_{12})_c=(2\pi e^2/N_2^2V)\sum_{\xi,\eta=1}^{N}\sum_{t_1t_2t_3=1}^{N_2}\sum_{q=-\infty}^{\infty}\exp\{-[(t_3-t_1)^2K_1^2+q^2]/2\beta\}$$
$$\times\exp\{-iN(t_3-t_1)(\vec{q}_\xi-\vec{q}_\eta)\cdot\vec{\tau}_2+iq\tau_2[(t_2-t_3)N+(\nu_\eta-\nu_\xi)]-iq(q_{\xi_x}-q_{\eta_x})/\beta\}$$
$$\times\sum_{m=0}^{n_\xi}\sum_{n=0}^{n_\eta}\frac{(-1)^{m+n}n_\xi!\,n_\eta!\,[(t_3-t_1)^2K_1^2+q^2]^{n_\xi+n_\eta-m-n-1}}{m!\,n!\,[(n_\xi-m)!]^2\,[(n_\eta-n)!]^2\,(2\beta)^{n_\xi+n_\eta-m-n-1}}\,. \tag{B3}$$

The exchange energy is obtained by the same procedure as

$$(H_{12})_{ex} = (-2\pi e^2/N_2^2 V) \sum_{\xi,\eta=1}^{\eta} \sum_{t_1 t_2 t_3=1}^{N_2} \sum_{q=-\infty}^{\infty} \exp\{-[(\rho - q_{\xi_x} + q_{\eta_x})^2 + q^2]/2\beta\} \exp\{-iN(t_3 - t_1)\,(\vec{q}_\xi - \vec{q}_\eta)\cdot\vec{\tau}_2\}$$

$$\times\{[(t_3 - t_1)K_1 + (\nu_\eta - \nu_\xi)K_1/N + (q_{\eta_x} - q_{\xi_x})]^2 + q^2\}^{-1}$$

$$\times \sum_{m,n=0}^{(n_\xi | n_\eta)} \frac{(-1)^{m+n} n_\xi!\, n_\eta!\, [(q_{\xi_x} - q_{\eta_x} - \rho)^2 + q^2]^{n_\eta - m} [(q_{\eta_x} - q_{\xi_x} - \rho)^2 + q^2]^{n_\xi - n}}{m!\, n!\, (n_\xi - m)!\, (n_\eta - n)!\, (n_\xi - n)!\, (n_\eta - m)!\, (2\beta)^{n_\xi + n_\eta - m - n}}, \tag{B4}$$

where

$$\rho = (t_3 - t_1)K_1 + (\nu_\eta - \nu_\xi)K_1/N$$

and $(n_\xi | n_\eta)$ is the smaller value of n_ξ and n_η.

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