Influence of Collisions on the Magnetic Susceptibility of an Electron Gas. I

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Using a simple model, a determination is made of the influence of collisions on the magnetic susceptibility of an electron gas without assuming the existence of a relaxation time. The model consists of noninteracting free electrons being elastically scattered by randomly distributed impurity centers in the presence of a strong uniform magnetic field. The free energy for this simple system is expanded in ascending powers of the strength of the scattering potential and is evaluated for impurities represented by a screened Coulomb potential. The result for the oscillatory part of the magnetic susceptibility is in agreement with that obtained by Dingle to the order considered and provides an explicit expression for the collision relaxation time and the corresponding Dingle temperature.

I. INTRODUCTION

THIS study is concerned with the problem of calculating on as rigorous a basis as possible the influence of collisions on the magnetic susceptibility of an electron gas. It is known that the discrete nature of the energy levels of an electron in a magnetic field, which gives rise to Landau diamagnetism,[1] is connected with the fact that the classical electron orbits are periodic.[2] If electrons are subject to collisions, corresponding corrections to the susceptibility might be expected when the mean time τ between collisions is comparable with the cyclotron resonance frequency $\omega_0=eB/mc$, where B is the magnetic field strength, or equivalently when $\hbar\omega_0\approx\hbar/\tau$ in terms of characteristic energies. However, Peierls,[3] who first considered the problem, showed that the constant part of the diamagnetic susceptibility at least is unaffected by collisions provided

$$KT\gg\hbar/\tau, \tag{1.1}$$

where K is Boltzmann's constant and T is the absolute temperature. He has since indicated[4] that this is probably not a necessary condition for the validity of the expression for the constant part of the susceptibility but that it is probably sufficient to have

$$\eta\gg\hbar/\tau, \tag{1.2}$$

where η is the Fermi energy.

More recently, Dingle[5] has given a more detailed treatment of the problem. He calculated the collision broadening of the energy levels semiclassically and obtained an expression for the magnetic susceptibility in terms of an average collision time which was introduced rather arbitrarily. His expression for the magnetic susceptibility shows that the periodic part (the de Haas–van Alphen effect) is important only when $\hbar\omega_0\gtrsim KT$, while the effect of collisions is negligible when

$$\hbar\omega_0\gg\hbar/\tau, \tag{1.3}$$

which is then equivalent to Peierl's inequality (1.1). The constant part of Dingle's expression for the susceptibility depends on τ only through even powers of the factor $\hbar/\eta\tau$, indicating that collisions do not affect it provided the inequality (1.2) is satisfied, just as Peierls has suggested.

It is generally assumed in discussions of phenomena taking place in a magnetic field that the interactions between electrons and phonons or between electrons and impurities are unaffected by the external magnetic field. Since the effects of strong magnetic fields are interesting and not too transparent, it is important to investigate just what effects the magnetic field might have on the scattering mechanism. In general, the problem is very difficult; just to study the modifications of the Bloch wave functions by a uniform magnetic field[6] is an extremely difficult task. For the purpose of gaining some insight into the problem, it should be useful to study the effect of a strong magnetic field on the scattering of free electrons by phonons and impurities. The advantage of studying such cases is that the wave functions and the energy eigenvalues of an electron in a uniform magnetic field are known. Thus the magnetic field can in principle be taken into account exactly, while the various scattering processes can be treated as perturbations.

The purpose of this work is to determine the effect of collisions on the magnetic susceptibility of an electron gas without assuming the existence of a relaxation time and at the same time to examine the influence of a magnetic field on the collision process itself. A very simple model is considered; it consists of a collection of noninteracting electrons obeying Fermi-Dirac statistics in the presence of a strong uniform magnetic field. The collision mechanism is provided by a set of fixed impurity centers distributed at random throughout the volume occupied by the electrons. The electrons are

[1] L. Landau, Z. Physik **64**, 629 (1930).
[2] See, for example, A. H. Wilson, *The Theory of Metals* (Cambridge University Press, London, 1953), 2nd ed., Chap. 6, p. 160.
[3] R. E. Peierls, Z. Physik **80**, 763 (1933).
[4] R. E. Peierls, *Quantum Theory of Solids* (Oxford University Press, London, 1955), Chap. 7, p. 155.
[5] R. B. Dingle, Proc. Roy. Soc. (London) **A211**, 517 (1952).
[6] G. H. Wannier and D. R. Fredkin, Phys. Rev. **125**, 1910 (1962).

treated as completely free except for their interaction with the impurities and the externally applied magnetic field. It is assumed that the collisions take place elastically and that their effect on the electrons is small enough so that it can be treated as a perturbation.

In Sec. II an expansion of the Helmholtz free energy in powers of the scattering potential is obtained using as a representation the exact eigenfunctions of an electron in a uniform magnetic field. The free energy is evaluated in Sec. III for a set of impurities represented by a screened Coulomb potential. Here we limit ourselves to terms of second order in the scattering potential; this is sufficient to show the effect of collisions on the oscillatory part of the susceptibility. The result is in agreement with that obtained by Dingle to the order considered and provides an explicit expression for the collision relaxation time and the corresponding Dingle temperature.

In order to obtain collision corrections to the constant part of the susceptibility, the expansion of the free energy must be carried to terms of the fourth order in the scattering potential. The results of this further investigation, which will appear in a subsequent paper, indicate that the effect of collisions on the constant part of the susceptibility is negligible when the inequality (1.2) is satisfied in agreement with the prediction of Peierls.

An estimate is made in Appendix A of certain second-order contributions to the free energy which turn out to be very small. These terms result from our requirement that the impurity potential contain no constant term. In Appendix B an inequality needed in Sec. III is established.

II. MATHEMATICAL FORMULATION

The magnetic susceptibility χ of a system in terms of its Helmholtz free energy F is given by

$$\chi=-\frac{1}{VB}\left(\frac{\partial F}{\partial B}\right)_{VTN}, \tag{2.1}$$

where V is the volume of the system containing N electrons. For a system obeying Fermi-Dirac statistics, the free energy can be written[7]

$$F=N\eta-KT\sum_{\nu}\ln[e^{\beta(\eta-E_\nu)}+1], \tag{2.2}$$

where η is the Fermi energy, $\beta=1/KT$, and the summation is to be taken over all states ν having the energy E_ν. The Fermi energy η is determined by the relation

$$\left(\frac{\partial F}{\partial \eta}\right)=0 \tag{2.3}$$

which is equivalent to

$$N=\sum_{\nu}f_\nu=\sum_{\nu}[e^{\beta(E_\nu-\eta)}+1]^{-1}, \tag{2.4}$$

where f_ν is just the Fermi-Dirac distribution function. The problem is to calculate the energy eigenvalues E_ν and perform the sum over states required to obtain the free energy; the susceptibility is then easily found by performing a simple differentiation according to Eq. (2.1).

Consider a collection of electrons in the presence of a strong uniform magnetic field; the electrons are elastically scattered by a set of fixed impurity centers distributed at random throughout the volume occupied by the electrons. Except for the effects of the Pauli exclusion principle, the dynamical interaction of the electrons is completely neglected. Then the total Hamiltonian H_T for each electron may be written

$$H_T=H_0+H', \tag{2.5}$$

where H_0 is the Hamiltonian of a free electron in the presence of a uniform magnetic field and H' is the interaction of the electrons with the impurity centers. We have

$$H_0=\frac{1}{2m}\left(\mathbf{p}-\frac{e}{c}\mathbf{A}\right)^2, \tag{2.6}$$

$$H'=\sum_{i=1}^{N'}\phi(\mathbf{r}-\mathbf{r}_i), \tag{2.7}$$

where $\mathbf{A}$ is the vector potential, $\phi(\mathbf{r})$ is the interaction energy with a single impurity, and $\mathbf{r}_i$ are the locations of the N' impurity centers.

It is assumed that the effect of the impurities is small enough so that H' can be treated as a perturbation. Then the effects of the magnetic field can be included exactly since the exact wave functions of H_0, φ_ν are known; they satisfy the lowest-order Schrödinger equation obtained from H_T,

$$H_0\varphi_\nu=E_\nu^{(0)}\varphi_\nu, \tag{2.8}$$

where $E_\nu^{(0)}$ is the corresponding energy eigenvalue. Taking the magnetic field in the z direction and choosing a Landau gauge, $\mathbf{A}=(0,xB,0)$, the eigenfunctions of H_0 can be written

$$\varphi_\nu=\frac{1}{(L_yL_z)^{1/2}}u_n(x+x_0)e^{ik_yy}e^{ik_zz}, \tag{2.9}$$

where $x_0=\hbar k_y/m\omega_0$. Here $u_n(x)$ is the normalized harmonic-oscillator wave function

$$u_n(x)=N_nH_n(\alpha x)e^{-(1/2)\alpha^2x^2}. \tag{2.10}$$

$H_n(x)$ is the Hermite polynomial of order n, $\alpha^2=m\omega_0/\hbar$, and

$$N_n=\left(\frac{\alpha}{\pi^{1/2}2^nn!}\right)^{1/2}. \tag{2.11}$$

[7] See Ref. 2, Appendix 2A, p. 329

The energy eigenvalues of H_0 are

$$E_\nu^{(0)}=\hbar\omega_0(n+\tfrac{1}{2})+\hbar^2k_z^2/2m, \tag{2.12}$$

where ν now stands for the set of quantum numbers (nk_yk_z).

Treating H' as a perturbation, the energy eigenvalues of H_T, E_ν can be developed as a power series in H'. If we limit ourselves to terms no higher than second order in H', E_ν can be written

$$E_\nu=E_\nu^{(0)}+E_\nu^{(1)}+E_\nu^{(2)}, \tag{2.13}$$

where the order of each term in the scattering potential is indicated by a superscript. In order to proceed further, the corresponding development of F is also needed. This can be found by making use of a generalized thermodynamic perturbation expansion for the case of degenerate statistics.[8] In general, the Fermi energy as well as the free energy depends on the scattering potential so that one can write

$$F=F^{(0)}+F^{(1)}+F^{(2)}, \tag{2.14}$$

$$\eta=\eta^{(0)}+\eta^{(1)}+\eta^{(2)} \tag{2.15}$$

to the order now being considered. Then, performing a Taylor series expansion of the free energy (2.2), one finds that

$$F^{(0)}=N\eta^{(0)}-KT\sum_\nu \ln[e^{\beta(\eta^{(0)}-E_\nu^{(0)})}+1], \tag{2.16}$$

$$F^{(1)}=\sum_\nu f_\nu^{(0)}E_\nu^{(1)}, \tag{2.17}$$

$$F^{(2)}=\sum_\nu f_\nu^{(0)}E_\nu^{(2)}+\tfrac{1}{2}\sum_\nu \frac{\partial f_\nu^{(0)}}{\partial E_\nu^{(0)}}(E_\nu^{(1)}-\eta^{(1)})^2, \tag{2.18}$$

where use has been made of Eq. (2.3) to eliminate the first-order correction to F depending on $\eta^{(1)}$. In a similar way, the corrections to the Fermi energy can be found from Eq. (2.4):

$$N=\sum_\nu f_\nu^{(0)}=\sum_\nu[e^{\beta(E_\nu^{(0)}-\eta^{(0)})}+1]^{-1}, \tag{2.19}$$

$$\eta^{(1)}=\left(\sum_\nu \frac{\partial f_\nu^{(0)}}{\partial E_\nu^{(0)}}E_\nu^{(1)}\right)\Big/\left(\sum_\nu \frac{\partial f_\nu^{(0)}}{\partial E_\nu^{(0)}}\right), \tag{2.20}$$

$$\eta^{(2)}=\left[\sum_\nu \frac{\partial f_\nu^{(0)}}{\partial E_\nu^{(0)}}E_\nu^{(2)}+\tfrac{1}{2}\sum_\nu \frac{\partial^2 f_\nu^{(0)}}{\partial (E_\nu^{(0)})^2}(E_\nu^{(1)}-\eta_\nu^{(1)})^2\right]\times\left(\sum_\nu \frac{\partial f_\nu^{(0)}}{\partial E_\nu^{(0)}}\right)^{-1}. \tag{2.21}$$

The principal contribution to the susceptibility of a collection of free electrons comes from $F^{(0)}$ and was first correctly obtained by Landau.[1] Here we are interested in finding the contributions made by $F^{(1)}$ and $F^{(2)}$ resulting from collisions of the electrons with impurities. First, expand the potential of an impurity located at the origin in a Fourier series;

$$\phi(\mathbf{r})=\frac{1}{V}\sum_{\mathbf{q}} W(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}}. \tag{2.22}$$

Here periodic boundary conditions are chosen so that the components of $\mathbf{q}$ satisfy

$$q_\alpha=(2\pi/L_\alpha)m, \quad \alpha=1,2,3 \tag{2.23}$$

where m is any positive or negative integer including zero. By inversion of (2.22), we find that

$$W(\mathbf{q})=\int_{-\infty}^{\infty} e^{-i\mathbf{q}\cdot\mathbf{r}}\phi(\mathbf{r})d\mathbf{r}. \tag{2.24}$$

To make the problem as simple as possible, we exclude the possibility of including a constant term in the impurity potential by subtracting the contribution from the $\mathbf{q}=0$ term:

$$H'(\mathbf{r})=\frac{1}{V}\sum_{\mathbf{q}}\sum_{i=1}^{N'} W(\mathbf{q})e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}_i)}-\frac{N'}{V}W(\mathbf{0})$$
$$=\frac{1}{V}\sum_{i=1}^{N'}\sum_{\mathbf{q}} W(\mathbf{q})(1-\delta_{\mathbf{q}0})e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}_i)}. \tag{2.25}$$

It will be assumed that any constant potential associated with the impurities has been included in the zero-order Hamiltonian where it would appear as an added term in $E_\nu^{(0)}$. By resetting the zero of energy this constant can be removed, and for simplicity it will be imagined that this has been done.

First consider the terms $F^{(1)}$ and $\eta^{(1)}$; to calculate these the first-order energy correction $E_\nu^{(1)}$ is required. Applying ordinary Rayleigh-Schrödinger perturbation theory we find

$$E_\nu^{(1)}=\langle\nu|H'(\mathbf{r})|\nu\rangle=\frac{1}{V}\sum_{q_x} W'(q_x,0,0)\times\int_{-\infty}^{\infty} dx\, u_n^2(x+x_0)e^{iq_xx}\sum_{i=1}^{N'} e^{-iq_xx_i}, \tag{2.26}$$

where we have let

$$W'(\mathbf{q})=W(\mathbf{q})(1-\delta_{\mathbf{q}0}). \tag{2.27}$$

Place this expression for $E_\nu^{(1)}$ in Eq. (2.17) and rewrite the sum over k_y as an integral according to the transformation

$$\sum_{k_\alpha}=\frac{L_\alpha}{2\pi}\int dk_\alpha, \quad \alpha=x,y,z. \tag{2.28}$$

[8] L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Addison-Wesley Publishing Company, Reading, Massachusetts, 1958), p. 93.

This gives

$$F^{(1)}=\frac{L_y}{2\pi V}\sum_n\sum_{kz} f_\nu^{(0)}\sum_{qx} W'(q_x,0,0)\int_{-\infty}^{\infty}dk_y\int_{-\infty}^{\infty}dx\, u_n^2(x+\hbar k_y/m\omega_0)e^{iq_x x}\sum_{i=1}^{N'}e^{-iq_x x_i}$$

$$=\frac{L_y}{2\pi V}\frac{m\omega_0}{\hbar}\sum_n\sum_{kz} f_\nu^{(0)}\sum_{qx} W'(q_x,0,0)\int_{-\infty}^{\infty}dx\, e^{iq_x x}\sum_{i=1}^{N'}e^{-iq_x x_i}$$

$$=\frac{m\omega_0 N'}{2\pi L_z\hbar}\sum_n\sum_{kz} f_\nu^{(0)}W'(\mathbf{0})$$

$$=0, \tag{2.29}$$

since $W'(\mathbf{0})=0$ according to (2.27). In the same way it can also be shown that $\eta^{(1)}$ vanishes. Thus the elimination of the constant part of the impurity potential ensures that no first-order corrections to either the free energy or the Fermi energy exist. These results are independent of the arrangement of the scattering centers.

Now consider the second order. Contributions to the free energy are given by (2.18). $\eta^{(2)}$ will not be needed since it does not appear in $F^{(2)}$. Let

$$F^{(2)}=F_a{}^{(2)}+F_b{}^{(2)}, \tag{2.30}$$

where

$$F_a{}^{(2)}=\sum_\nu f_\nu^{(0)}E_\nu^{(2)} \tag{2.31}$$

and

$$F_b{}^{(2)}=\frac{1}{2}\sum_\nu\frac{\partial f_\nu^{(0)}}{\partial E_\nu^{(0)}}[E_\nu^{(1)}]^2 \tag{2.32}$$

since $\eta^{(1)}=0$. The principal correction to the susceptibility comes from $F_a{}^{(2)}$. From second-order perturbation theory

$$E_\nu^{(0)}=\sum_{\nu'}\frac{|\langle\nu|H'|\nu'\rangle|^2}{E_\nu^{(0)}-E_{\nu'}{}^{(0)}}$$

$$=\frac{1}{V^2}\sum_{\nu'}\sum_{\mathbf{q}}\sum_{\mathbf{q}'}\frac{W'(\mathbf{q})W'(\mathbf{q}')}{E_\nu^{(0)}-E_{\nu'}{}^{(0)}}\langle\nu|e^{i\mathbf{q}\cdot\mathbf{r}}|\nu'\rangle\langle\nu'|e^{i\mathbf{q}'\cdot\mathbf{r}}|\nu\rangle\sum_{i=1}^{N'}\sum_{j=1}^{N'}e^{-i(\mathbf{q}\cdot\mathbf{r}_i+\mathbf{q}'\cdot\mathbf{r}_j)}. \tag{2.33}$$

Place this expression for the energy in Eq. (2.31) and take the ensemble average over all the different arrangements of the impurities without any correlation between the impurities.[9] (In assuming that the impurities are truly independent, we are allowing two or more to occupy the same position. In the present case where the impurity concentration is low, this assumption should not seriously affect the results.) A large contribution is obtained only when $i=j$ and $\mathbf{q}+\mathbf{q}'=0$. The final result can be written

$$F_a{}^{(2)}=\frac{1}{2}\frac{N'}{V^2}\sum_\nu\sum_{\nu'}D(E_\nu^{(0)},E_{\nu'}{}^{(0)})$$

$$\times\sum_{qx}|W(q_x,k_y-k_y',k_z-k_z')|^2$$

$$\times(1-\delta_{qx0}\delta_{k_yk_y'}\delta_{k_zk_y'})|F_{\nu\nu'}(q_x)|^2, \tag{2.34}$$

where

$$D(E_\nu^{(0)},E_{\nu'}{}^{(0)})=\frac{f_\nu^{(0)}-f_{\nu'}{}^{(0)}}{E_\nu^{(0)}-E_{\nu'}{}^{(0)}} \tag{2.35}$$

and

$$F_{\nu\nu'}(q_x)=\int_{-\infty}^{\infty}u_n(x+x_0)e^{iq_xx}u_n'(x+x_0')dx. \tag{2.36}$$

In order to simplify $F_b{}^{(2)}$, replace $E_\nu^{(1)}$ using (2.26) and again take the ensemble average over all possible arrangements of the impurities. This gives

$$F_b{}^{(2)}=\frac{1}{2}\frac{N'}{V^2}\sum_\nu\frac{\partial f_\nu^{(0)}}{\partial E_\nu^{(0)}}\sum_{qx}|W(q_x,0,0)|^2$$

$$\times(1-\delta_{qx0})|F_{\nu\nu}(q_x)|^2 \tag{2.37}$$

which turns out to be very small compared with $F_a{}^{(2)}$.

III. COLLISION RELAXATION TIME

As a simple but interesting application of the results obtained in Sec. II we consider the scattering of free electrons by a set of randomly distributed ionized impurities. This model might be used to describe a substitutional metal alloy, where breaks in the periodic potential caused by the minority atoms result in electron scattering. According to the Thomas-Fermi

[9] W. Kohn and J. M. Luttinger, Phys. Rev. **108**, 590 (1957); see Appendix B.

theory applied to metal alloys,[10] the effective potential about each impurity ion can be represented approximately by a spherically symmetric screened Coulomb potential

$$\phi(\mathbf{r})=-Ze^2e^{-r/a}/r, \tag{3.1a}$$

where Ze is the excess charge of the minority ions over that of the host ions and a is the effective range of the potential given by

$$a^2=\pi\hbar^2/4me^2(3N\pi^2/V)^{1/3}. \tag{3.1b}$$

For most metals, a is of the order of 10^{-8} cm, as might be expected from the fact that the metal is electrically neutral. This choice of potential enables us to carry out most of the required integrations analytically and finally obtain the periodic part of the susceptibility in terms of an explicit expression for the relaxation time. Substituting the expression (3.1a) into Eq. (2.24), we find that the Fourier transform of the impurity potential is just

$$W(\mathbf{q})=\tilde{\phi}\frac{1}{(1+a^2\mathbf{q}^2)}, \tag{3.2a}$$

where

$$\tilde{\phi}=-4\pi Ze^2a^2 \tag{3.2b}$$

is the integral of $\phi(\mathbf{r})$ over all space.

In the presence of a magnetic field the screening must actually be calculated using the dielectric constant in a magnetic field.[11] The effective potential is then no longer spherically symmetric and the screening depends on the magnetic field.[12] However, even for quite high field strengths the magnetic corrections to the effective potential turn out to be rather small for metals and Eqs. (3.1) can still be used to a very good approximation. Since the motion of charged particles along the magnetic field is unaffected by the field, the effective screening in this direction remains the same as in the absence of a field. Now consider electrons moving perpendicular to the direction of the magnetic field and neglect for the moment the effects of ordinary screening. It can then be shown that the Fourier transform of the effective potential of an ion in the presence of a magnetic field is just[13]

$$W_B(\mathbf{q}_\perp,0)=\frac{4\pi Ze^2}{2\alpha^2}\times\left\{x+e^{-x}\left[x_0+x_1\sum_{n=1}^{\infty}\frac{x^n}{n(n!)}\right]\right\}^{-1}, \tag{3.2a'}$$

where

$$\begin{aligned}x&=\mathbf{q}_\perp^2/2\alpha^2,\\ x^0&=2mZe^2/\pi\hbar p,\\ x_1&=4Ze^2p/\pi\hbar^2\omega_0,\end{aligned} \tag{3.2b'}$$

and p is the electron momentum. In order to obtain an estimate of the magnetic screening distance in a direction perpendicular to the magnetic field, say $a_B(q_\perp)$, which will in general depend on $q_\perp$ as indicated, we set $q_\perp=0$ and take $p\approx[(6/5)m\eta]^{1/2}$, just the average value of the electron momentum in a Fermi distribution at $T=0$. Then comparing $W_B(0)$ obtained in this way from Eqs. (3.2′) with $W(0)$ given by Eqs. (3.2), we find that

$$a_B^2(0)\approx(\hbar/Ze^2\alpha^2)(\eta/m)^{1/2}.$$

For a magnetic field as high as 10^5 G we find that $a_B(0)\approx10^2a$ and the effective screening distance is still given by a to a very good approximation. More generally it can be shown that $a_B(q_\perp)\gg a$, provided that $\eta\gg\hbar\omega_0$. Therefore, $a_B(a_\perp)$ is quite ineffective in providing screening compared with a at ordinary field strengths. If many Landau levels are occupied, the screening should be quite close to its value in the absence of a magnetic field; in the case in which only a few Landau levels are occupied it would be necessary to take into account the magnetic dependence of the screening.

The principal contribution to $F^{(2)}$ comes from the first term on the right-hand side of Eq. (2.34) and its evaluation is carried out in this section. The remaining terms in $F^{(2)}$ are quite negligible and an estimate of their size is made in Appendix A. Using (3.2), the first term in $F_a^{(2)}$, say $F_{a1}^{(2)}$, can be written

$$F_{a1}^{(2)}=-\frac{1}{2}\frac{N'\tilde{\phi}^2}{(2\pi)^2V^2a^4}\sum_\nu\sum_{\nu'}D(E_\nu^{(0)},E_{\nu'}^{(0)})\times\sum_{q_x}[a^{-2}+q_x^2+(k_y-k'_y)^2+(k_z-k'_z)^2]^{-2}\times\left|\int_{-\infty}^{\infty}u_n(x+\xi)e^{iq_xx}u_{n'}(x)dx\right|^2, \tag{3.3}$$

where

$$\xi=(x_0-x_0')=\alpha^{-2}(k_y-k_y'). \tag{3.4}$$

First, perform the sum over q_x by replacing it with an integral according to (2.28). A simple contour integration then gives

$$F_{a1}^{(2)}=-\frac{1}{2}\frac{N'\tilde{\phi}^2L_x}{(8\pi)^2V^2a^4}\sum_\nu\sum_{\nu'}D(E_\nu^{(0)},E_{\nu'}^{(0)})\times\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dx'\,u_n(x+\xi)u_{n'}(x)u_{n'}(x')u_n(x'+\xi)\times s^{-3}(1+s|x-x'|)e^{-s|x-x'|}, \tag{3.5}$$

where we have let

$$s^2=a^{-2}+(k_y-k_y')^2+(k_z-k_z')^2. \tag{3.6}$$

To proceed further, some approximation is necessary. Assume that the average range of the potential is small compared with the length α^{-1} characterizing the magnetic field; then

$$a\alpha\ll1. \tag{3.7}$$

[10] N. F. Mott and H. Jones, *The Theory of the Properties of Metals and Alloys* (Oxford University Press, London, 1936), Chap. II, Sec. 5, p. 86.
[11] M. J. Stephen, Phys. Rev. **129**, 997 (1963).
[12] N. D. Mermin and E. Canel, Am. J. Phys. (N. Y.) **26**, 247 (1964).
[13] V. Celli and N. D. Mermin, Phys. Rev. **140**, A839 (1965).

This condition is well satisfied for an interesting range of potentials and magnetic field strengths. For a field as high as 10^5 G, $\alpha \approx 10^6$ cm^{-1}. Then for metals where a typical value of a is about 0.5 Å, we have $a\alpha \approx 10^{-2}$. When the condition (3.7) is satisfied the final exponential factor in (3.5) is a rapidly decreasing function of $|x-x'|$ compared with $u_n(x-x')$, as is evident from the form of (2.10) and the dependence of s on the potential range a. A good approximation of (3.5) can then be obtained by expanding the product of harmonic-oscillator functions in powers of $(x-x')$; this is equivalent to an expansion in powers of $a\alpha$ or α/s since $a\alpha \geq a/s$. To lowest order this amounts to taking

$$u_n(x+\xi)u_{n'}(x)u_{n'}(x')u_n(x'+\xi) \approx u_n^2(x'+\xi)u_{n'}^2(x'), \quad (3.8)$$

if higher-order terms are neglected. This is just what might be expected since the contribution to the integral over q_x is small except where $|x-x'|$ is sufficiently small; the integral over q_x would give a delta function $\delta(x-x')$ if the dependence of $W(\mathbf{q})$ on q_x were neglected. This can be done when the potential range is small, since then s is very large according to Eq. (3.6). By making the replacement (3.8) in Eq. (3.5), the integration over x can be readily carried out. Then

$$F_{a1}^{(2)} = \frac{1}{4\pi}\frac{\bar{\phi}^2 N'\alpha^2}{L_z V}\sum_{\nu'}\sum_{n}\sum_{k_z} D(E_\nu^{(0)}, E_{\nu'}^{(0)}) \times \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} d\xi \frac{u_n^2(x'+\xi)u_{n'}^2(x')}{[1+(a\alpha)^2(\alpha\xi)^2+a^2(k_z-k_z')^2]^2} \quad (3.9)$$

after finally replacing the sum over k_y by an integral over ξ using Eqs. (2.28) and (3.4). Since we are already working to zero order in $a\alpha$, it now appears appropriate to expand the denominator of the double integral in powers of $a\alpha$ and retain only the zero-order term. This is equivalent to setting the ξ-dependent term in the denominator equal to zero. The double integration over ξ and x' can then be carried out, and Eq. (3.9) becomes

$$F_{a1}^{(2)} = \frac{1}{4\pi}\frac{\bar{\phi}^2 N'\alpha^2}{L_z V}\sum_{\nu'}\sum_{n}\sum_{k_z} D(E_\nu^{(0)}, E_{\nu'}^{(0)}) \times (1+a^2(k_z-k_z')^2)^{-2}. \quad (3.10)$$

However, for large n, n' the right-hand side of Eq. (3.10) contains as a factor the harmonic series which is known to diverge logarithmically. A more careful examination of the double integral in (3.9) reveals that it is very small unless

$$n \approx n' \lesssim 1/(2a\alpha)^2; \quad (3.11)$$

this is shown in Appendix B. Consequently, the further evaluation of (3.10) is considered subject to the limitation (3.11). It turns out, however, that the lowest-order contribution to the susceptibility is very small unless $E_\nu^{(0)}$, $E_{\nu'}^{(0)}$ is close to the Fermi energy; this at once places an upper limit on n, n' and turns out to be approximately equivalent to condition (3.11). However, (3.11) is still necessary to obtain a finite value of the field-independent part of $F_{a1}^{(2)}$, but this of course does not contribute to the susceptibility.

The integrand of (3.10) is now completely independent of k_y'. If the electrons are restricted to lie within the volume V, it can be shown that the number of states N_y for a given energy is just[14]

$$N_y = \frac{\alpha^2}{2\pi} L_x L_y. \quad (3.12)$$

At this point it is advantageous to change from a sum over k_z to an integral over the energy. From Eq. (2.12) we find

$$k_z = \left\{\frac{2m}{\hbar^2}[E_\nu^{(0)} - \hbar\omega_0(n+\tfrac{1}{2})]\right\}^{1/2}, \quad (3.13a)$$

$$dk_z = \frac{1}{2}\left(\frac{2m}{\hbar^2}\right)^{1/2}[E_\nu^{(0)} - \hbar\omega_0(n+\tfrac{1}{2})]^{-1/2} dE_\nu^{(0)}, \quad (3.13b)$$

where n must satisfy the inequality

$$E_\nu^{(0)} - \hbar\omega_0(n+\tfrac{1}{2}) > 0.$$

Now use (3.12) to replace the sum over k_y' in (3.10) and rewrite the result using Eqs. (3.13). This gives

$$F_{a1}^{(2)} = \frac{1}{32}\frac{\bar{\phi}^2 N'\alpha^4 m}{\pi^4\hbar^2}\sum_{n}\sum_{n'}\int_0^\infty dE_\nu^{(0)}\int_0^\infty dE_{\nu'}^{(0)} \times D(E_\nu^{(0)}, E_{\nu'}^{(0)})\,[1+\gamma\{[E_\nu^{(0)} - \hbar\omega_0(n+\tfrac{1}{2})]^{1/2} \pm [E_{\nu'}^{(0)} - \hbar\omega_0(n'+\tfrac{1}{2})]^{1/2}\}^2]^{-2} \times [E_\nu^{(0)} - \hbar\omega_0(n+\tfrac{1}{2})]^{-1/2}[E_{\nu'}^{(0)} - \hbar\omega_0(n'+\tfrac{1}{2})]^{-1/2}, \quad (3.14)$$

where both signs are to be included and $\gamma = 2ma^2/\hbar^2$.

It is well known that the susceptibility of a system of free electrons depends on the "bunching" of electronic energy levels caused by a magnetic field and represented by a sum over the integral quantum number n. If both sums over n in Eq. (3.14) are replaced by integrals, the resulting expression is independent of the magnetic field and the system has zero susceptibility. An approximation sufficiently good to retain the essential magnetic field dependence can be obtained by means of Poisson's summation formula,[15]

$$\sum_n F[E-(n+\tfrac{1}{2})\hbar\omega_0] = \frac{1}{\hbar\omega_0}\sum_{l=-\infty}^{\infty}(-1)^l \times \int_0^E F(E-x)e^{2\pi i l x/\hbar\omega_0}dx, \quad (3.15)$$

[14] F. Seitz, *Modern Theory of Solids* (McGraw-Hill Book Company, Inc., New York, 1940), p. 585.

[15] E. C. Titchmarsh, *Introduction to the Theory of Fourier Integrals* (Oxford University Press, London, 1937), p. 60.

where l is an integer. Replace the sums over n, n' in Eq. (3.14) using this expression. In the resulting sum over l, l' the largest contribution to $F_{a1}{}^{(2)}$ comes from the $l=l'=0$ term; this is just the integral approximation already mentioned and does not contribute to the susceptibility. The largest contribution to $F_{a1}{}^{(2)}$ involving the magnetic field, say $F(B)$, comes from the sum of the two identical cross terms $l=0$, $l'\neq 0$; $l\neq 0$, $l'=0$ and can be written

$$F(B)=\frac{1}{16}\frac{\bar{\phi}^2N'm^3}{\pi^3\hbar^6}\sum_{\substack{l=-\infty\\ l\neq 0}}^{\infty}(-1)^l\int_0^\infty dE'\,e^{2\pi ilE'/\hbar\omega_0}$$
$$\times\int_0^\infty dE\,D(E,E')e^{2\pi il(E-E')/\hbar\omega_0}I(E,E'), \quad (3.16)$$

where

$$I(E,E')=\int_0^E dy\,e^{-2\pi ily/\hbar\omega_0}y^{-1/2}\int_0^{E'}dx'$$
$$\times\{1+\gamma[(E'-x')^{1/2}\pm y^{1/2}]^2\}^{-2}(E'-x')^{-1/2}. \quad (3.17)$$

According to Eq. (3.11), x' is now subject to the condition

$$x'\lesssim\frac{\hbar\omega_0}{(2a\alpha)^2}=\frac{1}{2\gamma} \quad (3.18)$$

and this is sufficient to ensure the convergence of $F(B)$.

The remaining integrations cannot in general be carried out analytically; however, the principal contribution to $F(B)$ can still be found by first carefully examining the dependence of the integrand in Eq. (3.16) on the energy. It is assumed that

$$\eta^{(0)}\gg\hbar\omega_0, KT. \quad (3.19)$$

Then $D(E,E')\approx 0$ when $E,E'<\eta^{(0)}$ or $E,E'>\eta^{(0)}$; this follows from the properties of the Fermi-Dirac distribution function. Now consider the region where $E\leq\eta^{(0)}\leq E'$ or $E'\leq\eta^{(0)}\leq E$. If $|E-E'|\gtrsim\eta^{(0)}$ then $D(E,E')\lesssim(\eta^{(0)})^{-1}$, a very small factor. On the other hand, if $|E-E'|\ll\eta^{(0)}$, then $D(E,E')$ becomes a highly peaked function centered at $\eta^{(0)}$ and approaches the delta function $-\delta(E-\eta^{(0)})$ as E approaches E'. This peaked function is multiplied by the oscillatory function $\exp[2\pi il(E-E')/\hbar\omega_0]$ which means that the value of the integral depends critically on the ratio $\hbar\omega_0/lKT$. Assume that $I(E,E')$ is a comparatively smooth function of $(E-E')$ for energies near $\eta^{(0)}$ and first consider the case where $\hbar\omega_0/|l|\ll KT$ for a given l. Since $D(E,E')$ can never have a width less than KT, the contribution to $F(B)$ must vanish and the susceptibility is unaffected by impurity scattering when $\hbar\omega_0\ll KT$, in agreement with Dingle's result. Next consider the case where $\hbar\omega_0/|l|\gtrsim KT$; this gives a nonvanishing result. In order to estimate the contribution to $F(B)$, rewrite integrals (3.16) and (3.17) in terms of E' and the energy difference $(E-E')$. Next divide the range of $(E-E')$ into two regions: $|E-E'|\leq\frac{1}{2}KT$ and $|E-E'|>\frac{1}{2}KT$. When $|E-E'|\leq\frac{1}{2}KT$, $D(E,E')$ can be expanded in powers of $(E-E')/KT$ and replaced by $-\delta(E-\eta^{(0)})$ if terms of order $KT/\eta^{(0)}$ and higher are neglected. In the range $|E-E'|>\frac{1}{2}KT$, $D(E,E')$ is approximately equal to $-|E-E'|^{-1}$. The principal contribution to $F(B)$ must then be given by replacing $\exp(2\pi il(E-E')/\hbar\omega_0)$ by unity and integrating over E,E' subject to the conditions $E<\eta^{(0)}<E'$, $E'<\eta^{(0)}<E$, and $|E-E'|\lesssim\hbar\omega_0/2|l|$. Here l must be limited to those values for which $\hbar\omega_0/|l|\gtrsim KT$, otherwise the corresponding term in $F(B)$ vanishes. With these approximations it can be shown that

$$F(B)\approx-\frac{\bar{\phi}^2N'm^3}{16\pi^4\hbar^6}\sum_{l\neq 0}{}'(-1)^le^{2\pi il\eta^0/\hbar\omega_0}\frac{\hbar\omega_0}{2|l|}$$
$$\times\left[1+\left(1-\frac{|l|KT}{\hbar\omega_0}\right)\ln\frac{\hbar\omega_0}{|l|KT}\right]I(\eta^{(0)},\eta^{(0)}) \quad (3.20)$$

if terms of order $KT/\eta^{(0)}$ and $\hbar\omega_0/\eta^{(0)}$ are neglected. The prime on the summation sign is to remind us that l is an integer such that $|l|\lesssim\hbar\omega_0/KT$. The first term in the bracket comes from integrating over the region $|E-E'|\leq\frac{1}{2}KT$ while the logarithmic term arises from the region $\frac{1}{2}KT<|E-E'|\leq\hbar\omega_0/2|l|$.

From (3.17) it is seen that the factor $I(\eta^{(0)},\eta^{(0)})$ depends on the range of the impurity potential through γ which also appears in the restrictive condition (3.11). For an impurity potential range $a=0.5\times10^{-8}$ cm, γ^{-1} is found to have a value of 10 eV, which exceeds the Fermi energy of most metals. The condition (3.18) is then satisfied for $I(\eta^{(0)},\eta^{(0)})$, and one finds

$$I(\eta^{(0)},\eta^{(0)})=\int_0^{\eta^{(0)}}dy\,e^{-2\pi ily/\hbar\omega_0}y^{-1/2}$$
$$\times\left\{\frac{(\eta^{(0)})^{1/2}\pm y^{1/2}}{1+\gamma[(\eta^{(0)})^{1/2}\pm y^{1/2}]^2}\right.$$
$$\left.+\frac{1}{\gamma^{1/2}}\tan^{-1}\gamma^{1/2}[(\eta^{(0)})^{1/2}\pm y^{1/2}]\right\} \quad (3.21)$$

after carrying out a simple integration. In order to simplify the final integration over y, the further assumption is made that $\gamma\eta^{(0)}<1$. This should be reasonably well satisfied for most metals in vew of our estimate of γ^{-1}. Then $I(\eta^{(0)},\eta^{(0)})$ can be obtained as a power series in $\gamma\eta^{(0)}$. To first order one finds

$$I(\eta^{(0)},\eta^{(0)})=\int_0^{\eta^{(0)}}dy\,e^{-2\pi ily/\hbar\omega_0}y^{-1/2}$$
$$\times\{4(\eta^{(0)})^{1/2}(1-\tfrac{2}{3}\eta^{(0)}\gamma)-8\gamma(\eta^{(0)})^{1/2}y\}$$
$$=4\pi^{1/2}\left(\frac{\hbar\omega_0}{2\pi il}\right)^{1/2}(\eta^{(0)})^{1/2}(1-\tfrac{2}{3}\gamma\eta^{(0)}) \quad (3.22)$$

if terms of order $\hbar\omega_0/\eta^{(0)}$ are neglected. Using this result, Eq. (3.20) can be written

$$F(B)=-\frac{Vm^{3/2}(\hbar\omega_0)^{3/2}}{2\pi^3\hbar^2}\sum_{\substack{l=1\\(l\geq 1)}}{}'\frac{(-1)^l}{l^{3/2}}\tau(l,\gamma)^{-1}\times\cos\left(\frac{2\pi l\eta^{(0)}}{\hbar\omega_0}-\frac{\pi}{4}\right),\quad\frac{\hbar\omega_0}{KT}\gtrsim 1,\tag{3.23}$$

where $\tau(l,\gamma)$ is the collision relaxation time given by

$$\tau(l,\gamma)^{-1}\approx\tau_0^{-1}(1-\tfrac{2}{3}\eta^{(0)}\gamma)\times\left[1+\left(1-\frac{lKT}{\hbar\omega_0}\right)\ln\left(\frac{\hbar\omega_0}{lKT}\right)\right]\tag{3.24}$$

with

$$\tau_0^{-1}=\frac{n'\bar{\phi}^2m^{3/2}(\eta^{(0)})^{1/2}}{4\pi^{1/2}\hbar^4}.\tag{3.25}$$

Here n' is the density of impurities. When $\hbar\omega_0/lKT<1$, $F(B)\approx 0$ and the susceptibility vanishes.

If Eq. (3.23) is to be valid as a perturbation result, one must require that $\hbar\omega_0>\hbar/\tau$ since the perturbing energy associated with the impurities must be small compared with the magnetic energy-level separation. To obtain a nonvanishing result for $F(B)$ we must have $\hbar\omega_0\gtrsim KT$, and the effect of collisions on the susceptibility is small if $\hbar\omega_0\gg\hbar/\tau$. Then the susceptibility is unaffected by collisions if $KT\gg\hbar/\tau$, which is just Peierls's inequality (1.1). In the limit where the influence of collisions on the susceptibility can be considered small, these results are in complete agreement with those obtained by Dingle if (3.24) is taken to be the collision relaxation time. However, not too much significance should be attached to the logarithmic dependence of $\tau(l,\gamma)$ on the ratio $\hbar\omega_0/lKT$ because of the approximate way in which the energy integrals in (3.16) are evaluated.

It is interesting to examine the dependence of the relaxation time and the susceptibility on the range of the impurity potential. To terms of order $KT/\eta^{(0)}$, the Fermi energy of free electrons is given by

$$\eta^{(0)}=\frac{\hbar}{2m}\left(\frac{3\pi^2N}{V}\right)^{2/3}.\tag{3.26a}$$

Combining this with Eq. (3.1b), we find that the dependence of the free energy on the potential range is just

$$\eta^{(0)}=\frac{\hbar^6\pi^2}{32m^3e^4}\frac{1}{a^4}.\tag{3.26b}$$

Then the dimensionless expansion parameter $\eta^{(0)}\gamma$ is given by

$$\eta^{(0)}\gamma=\frac{\pi^2\hbar^2}{16m^2e^4}\frac{1}{a^2}.\tag{3.27}$$

In order for the expansion (3.22) to be valid, one must require that

$$a>\pi\hbar^2/4me^2=0.35\times10^{-8}\text{ cm}.\tag{3.28}$$

This condition is just satisfied in most metals. Since $\bar{\phi}^2(\eta^{(0)})^{1/2}$ is proportional to a^2, it is seen that an increase in the range of the potential causes a decrease in the relaxation time and an increase in the susceptibility according to Eqs. (3.24) and (3.25). In cases where the inequality (3.29) is not satisfied, a more exact evaluation than (3.22) of the integral (3.21) is required to determine the dependence of the susceptibility on the scattering potential.

IV. SUMMARY

In the present work the effect of collisions on the diamagnetic susceptibility of a system of free electrons is determined. Here we limit ourselves to terms of second order in the scattering potential; this is sufficient to determine the effect of collisions on the oscillatory part of the susceptibility. No assumption is made about the existence of a relaxation time. Neglecting terms of order $KT/\eta^{(0)}$ and $\hbar\omega_0/\eta^{(0)}$ it is shown that collisions do not influence the oscillatory part of the susceptibility provided $\hbar\omega_0\gg\hbar/\tau$, where τ is the relaxation time. The result is in agreement with the work of Dingle to the order considered. An explicit expression for the relaxation time is found, and its dependence on the scattering potential is discussed.

In order to obtain collision corrections to the constant part of the susceptibility, terms of fourth order in the scattering potential must be included. In a subsequent paper the expansion of the free energy begun here will be extended to this order and it will be shown that the effect of collisions on the constant part of the susceptibility is small when $\eta^{(0)}\gg\hbar/\tau$, in agreement with the prediction of Peierls.

APPENDIX A

The principal contribution to $F^{(2)}$ comes from the first term in Eq. (2.34); its evaluation is carried out in Sec. III. Here an estimate is made of the remaining terms in $F^{(2)}$. The contribution of these terms to the susceptibility turns out to be very small compared with that of $F(B)$.

First consider the second term in Eq. (2.34), say $F_{a2}{}^{(2)}$. This can be written

$$\begin{aligned}F_{a2}{}^{(2)}&=-\frac{n'\bar{\phi}^2}{2}\frac{1}{V}\sum_\nu\sum_{n'}D(E_{nk_z}{}^{(0)},E_{n'k_z}{}^{(0)})\,|F_{nk_yn'k_y}(0)|^2\\&=-\frac{n'\bar{\phi}^2}{2}\frac{1}{V}\sum_\nu\sum_{n'}D(E_{nk_z}{}^{(0)},E_{n'k_z}{}^{(0)})\delta_{nn'}\\&=\frac{n'\bar{\phi}^2}{2}\frac{1}{V}\sum_\nu\delta(E_\nu{}^{(0)}-\eta^{(0)})\end{aligned}\tag{A1}$$

after carrying out the indicated sums and using (3.2). Now perform the sum over k_y using Eq. (3.12) and rewrite the result as an integral over the energy. This gives

$$F_{a2}{}^{(2)}=-\frac{1}{4}\frac{n'\tilde{\phi}^2}{(2\pi)^2}\frac{\omega_0(2m)^{3/2}}{\hbar^2}\sum_n[\eta^{(0)}-\hbar\omega_0(n+\tfrac{1}{2})]^{-1/2}. \tag{A2}$$

The magnetic-field-dependent part of this expression, say $F_{a2}(B)$, can be obtained using Poisson's summation formula (3.15). Then

$$F_{a2}(B)=\frac{\hbar}{\pi^{3/2}\tau_0}\left(\frac{\hbar\omega_0}{\eta^{(0)}}\right)^{1/2}\sum_{l=1}{}'\frac{(-1)^l}{l^{1/2}}\times\cos\left(\frac{2\pi l\eta^{(0)}}{\hbar\omega_0}-\frac{\pi}{4}\right). \tag{A3}$$

Comparing the coefficient of this series with that of Eq. (3.23), we find that

$$\frac{F_{a2}(B)}{F(B)}\approx-\frac{\hbar^2}{Vm^{3/2}\omega_0(\eta^{(0)})^{1/2}}. \tag{A4}$$

For a field of 10^4 G the absolute value of this ratio is approximately 10^{-18} which shows that the contribution of $F_{a2}(B)$ to the susceptibility is quite negligible compared with that of $F(B)$.

Next consider $F_b{}^2$ given by Eq. (2.37). The first term in this expression, say $F_{b1}{}^{(2)}$, can be reduced to the form

$$F_{b1}{}^{(2)}=-\frac{n'}{2}\frac{\tilde{\phi}^2}{V}\sum_\nu\delta(\eta^{(0)}-E_\nu{}^{(0)})L_z\int_{-\infty}^{\infty}u_n{}^4(x)dx \tag{A5}$$

by making use of the same methods and approximations employed in Sec. III. Except for the last two factors, the right-hand side of (A5) is the same as $F_{a2}{}^{(2)}$. Since

$$\int_{-\infty}^{\infty}u_n{}^4(x)dx\approx\frac{|\alpha|}{[2\pi(n+1)]^{1/2}}\lesssim\frac{|\alpha|}{(2\pi)^{1/2}} \tag{A6}$$

the oscillatory part of $F_{b1}{}^{(2)}$, say $F_{b1}(B)\lesssim\alpha F_{a2}(B)/(2\pi)^{1/2}$. Then for a field of 10^4 G, $F_{b1}(B)/F(B)\lesssim10^{-8}$ according to (A4). Actually since the integral (A6) is proportional to $|B|^{1/2}$, $F_{b1}{}^{(2)}$ also makes a contribution to the nonoscillatory part of the susceptibility but this again is negligible compared with that of $F(B)$ as well as with the principal term contributing to the constant part of the susceptibility. This will be shown in a subsequent paper where the influence of collisions on the constant part of the susceptibility is treated.

Finally the second term in $F_b{}^{(2)}$ turns out to be identical with $F_{a2}{}^{(2)}$ since it can be put in the form (A1) and is therefore negligible.

APPENDIX B

For large values of x the Hermite polynomial of order n, $H_n(x)$, approaches the value 2^nx^n. Then according to Eq. (2.10), the asymptotic behavior of the harmonic-oscillator function is given by

$$u_n(x)\underset{x\to\infty}{\longrightarrow}N_n2^nx^ne^{-(1/2)\alpha^2y^2}. \tag{B1}$$

If the range of $u_n(x)$, R_n, is defined to be twice the value of x at the point where the expression on the right-hand side of (B1) has its maximum value, then

$$R_n=2n^{1/2}/\alpha. \tag{B2}$$

Now consider the integrals over x' and ξ contained in Eq. (3.9). Since $u_n(x)$ is normalized to unity, the integration over x' will produce a very small factor unless $R_n\approx R_n'$ for otherwise there will be very little overlap of the two harmonic-oscillator functions. At the same time the integrand will certainly decrease very rapidly for $\xi>1/a\alpha^2$. Because of the factor $u_n{}^2(x'+\xi)$, the entire integral will be small unless $R_n\lesssim1/a\alpha^2$. Using (B2) we conclude that most of the contribution to $F_{a1}{}^{(2)}$ must come from values of n, n' for which

$$n\approx n'\lesssim1/(2a\alpha)^2. \tag{B3}$$