The General Motion of Conduction Electrons in a Uniform Magnetic Field, with Application to the Diamagnetism of Metals

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The General Motion of Conduction Electrons in a Uniform Magnetic Field, with Application to the Diamagnetism of Metals

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Abstract. Using translational properties of the Hamiltonian, a standard form is derived for the wave functions describing conduction electrons moving in a uniform magnetic field. This is used to obtain a solution of the Schrödinger equation in order to examine the magnetic energy levels. For non-overlapping bands the notion of effective mass is shown adequate (neglecting level broadening) but in an overlap region neighbouring bands interact strongly and distort the single band levels. A brief application to the diamagnetism of metals is considered.

Introduction

The large diamagnetism of metals has long been understood to be due in some way to the 'free' conduction electrons. It is also well known that it is entirely quantum-mechanical in origin, since classically a mechanical system can possess no magnetic moment at all. To get a first understanding, therefore, one neglects entirely the effect of the crystal lattice and solves the Schrödinger equation for a free electron moving in a uniform magnetic field. For the alkali metals, where the electrons are very nearly free, the approximation is, in fact, likely to be a good one. The energy eigenvalues (including magnetic energy due to spin) are simple to obtain and may be used to calculate the free energy F from which the total magnetic moment is obtained as $M = -\partial F/\partial H$. Fermi–Dirac statistics are used, otherwise the electrons are treated as independent. That this is permissible is to some extent justified by the success of the model.

The susceptibility is thus obtained as a function of the field and temperature. Measurements of the constant susceptibility (weak fields, high temperature) of the alkali metals demand the variation of some parameter, however, and of the universal constants available the electronic mass is the only one permissible. The notion of 'effective mass' is, of course, also supported by the band theory of metals, and its use in the magnetic problem is already plausible. Further support comes from the (low temperature, strong field) susceptibility where it was pointed out by Peierls that if the electronic mass is sufficiently small and the electron density low, an oscillatory behaviour might be expected. Such an effect was indeed observed by de Haas and van Alphen in bismuth.

More direct support was provided by Peierls (1933) when he obtained an expression for the constant susceptibility for conduction electrons, of which the greatest contribution appeared essentially as an average of the effective Bohr magneton over the Fermi surface. For free electrons this reduced to the form obtained by Landau. There remained a contribution analogous to atomic diamagnetism (and thus small) and a third part having no simple interpretation but again apparently small.

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These results were obtained, not by considering directly the energy eigenvalues but by application of the interesting theorem that an equivalent energy operator is found (at least approximately) by replacing $E(\mathbf{k})$ by $E(\boldsymbol{\varkappa})$, $[\varkappa_x, \varkappa_y] = i(e/\hbar c)H_z$ etc. All results were obtained for the limiting case of tight binding but have since been shown to be of more general application (Wilson 1936, Luttinger 1951).

For electrons lying near the top or bottom of a band, $E(\mathbf{k})$ may be taken as quadratic in $\mathbf{k}$ (not necessarily isotropic) and the replacement of $\mathbf{k}$ by $\boldsymbol{\varkappa}$ then introduces the effective mass in a natural way. Blackman (1938) was thus able to extend the expression for the low-temperature susceptibility to allow for anisotropy of the metal. That is, by considering combinations of ellipsoids of suitable eccentricities to represent the Fermi surface (for holes and overflowing electrons), effective mass parameters are introduced and used to interpret the complicated modulations, phases, etc., of the susceptibility oscillations (Shoenberg 1952).

However, some doubt was thrown on the simple use of an effective mass when Adams (1953) showed that, at least in the case of the constant susceptibility, the previously neglected third contribution mentioned above could become very important in just those situations for which the effective mass approximation is most useful, that is, when the energy gap is small and consequently the effective mass small. Briefly, his argument was that in such a case there is a degeneracy of Bloch states, and that the magnetic field mixes them considerably.

The main purpose of the present paper is to examine this and other difficulties by means of a direct solution of the Schrödinger equation for a conduction electron moving in a uniform magnetic field. An exact solution in closed form is not, of course, to be expected since, even without the field, that does not exist. What is meant is a treatment analogous to the solution for nearly free electrons which establishes the existence of energy gaps, etc. A brief application of some of the results to the magnetic susceptibility is given though much more remains to be done.

§ 1. Translational Properties of the State Function

If an electron moves in the periodic field of a crystal lattice, and an external uniform magnetic field $\mathbf{H}$ is imposed, the electron stationary states are determined by the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\left(\nabla - \frac{ie}{\hbar c}\mathbf{A}\right)^2 + V(\mathbf{r}) - W\right]\psi = 0, \qquad \ldots\ldots(1.1)$$

where $\mathbf{H} = \operatorname{curl}\mathbf{A}$, and the vector potential $\mathbf{A}$ is linear in coordinates $\mathbf{r}$. $V(\mathbf{r})$ represents the lattice potential and therefore $V(\mathbf{r}+\boldsymbol{\tau}_i) = V(\mathbf{r})$, where $\boldsymbol{\tau}_i$, $i = 1, 2, 3$ are basic lattice vectors. Consider a displacement $\boldsymbol{\tau}_i$ of $\mathbf{r}$; then from the linearity of (1.1),

$$\psi_\lambda(\mathbf{r}+\boldsymbol{\tau}_i) = \exp\left[i\epsilon\mathbf{A}(\boldsymbol{\tau}_i).\mathbf{r}\right]\sum_{\lambda'} C^i_{\lambda'\lambda}\psi_{\lambda'}, \qquad \ldots\ldots(1.2)$$

where $\epsilon = e/\hbar c$ and the index λ enumerates all states of energy W. The matrices $C^i_{\lambda'\lambda}$, together with the phase factors $\exp\left[i\epsilon\mathbf{A}(\boldsymbol{\tau}_i).\mathbf{r}\right]$ (which simply effect a change of gauge) form representations of the elementary translations. Such operations commute and therefore

$$C^jC^i = C^iC^j \exp i\epsilon[\mathbf{A}(\boldsymbol{\tau}_j).\boldsymbol{\tau}_i - \mathbf{A}(\boldsymbol{\tau}_i).\boldsymbol{\tau}_j], \qquad \ldots\ldots(1.3)$$

matrix multiplication being understood. Thus C^i do not in general commute

and cannot be simultaneously diagonalized. For example, taking a cubic lattice of lattice constant a, and $\mathbf{A}=(0, Hx, 0)$

$$C^yC^x = C^xC^y \exp(-i\epsilon Ha^2)$$
$$C^zC^x = C^xC^z$$
$$C^zC^y = C^yC^z.$$

In this case C^z commutes with C^x, C^y and may be treated as diagonal. Since C^x, C^y do not commute, if C^x is diagonal, C^y is not, and vice versa.

It is interesting to note that symbolically C^l could be represented by $C^l=\exp(i\boldsymbol{\kappa}\cdot\boldsymbol{\tau}_l)$, where $[\kappa_x, \kappa_y]=i\epsilon H_z$ etc. (for the case $\mathbf{A}=\frac{1}{2}\mathbf{H}\times\mathbf{r}$). A more useful representation is obtained by introducing a vector $\mathbf{k}$ and writing

$$(\mathbf{k}'\,|\,C^l\,|\,\mathbf{k}) = \exp(i\mathbf{k}\cdot\boldsymbol{\tau}_l)\delta[\mathbf{k}'-\mathbf{k}+\epsilon\mathbf{A}(\boldsymbol{\tau}_l)]. \qquad \ldots\ldots(1.4)$$

(In the above example this makes C^x and C^z diagonal.) Thus, taking $\mathbf{A}=0$, (1.4) reduces to the diagonal Bloch representation. In the magnetic case however, the vector $\mathbf{k}$ is not to be identified as a momentum vector since the motion is not that of plane waves.

That (1.4) satisfies (1.3) is clear since

$$(\mathbf{k}'\,|\,C^jC^l\,|\,\mathbf{k}) = \exp[-i\epsilon\mathbf{A}(\boldsymbol{\tau}_l)\cdot\boldsymbol{\tau}_j]\exp(i\mathbf{k}\cdot\boldsymbol{\tau}_l+\boldsymbol{\tau}_j)\delta[\mathbf{k}'-\mathbf{k}+\epsilon\mathbf{A}(\boldsymbol{\tau}_l+\boldsymbol{\tau}_j)].$$

Interchanging i, j the result follows.

Choosing this representation then and using (1.2) and (1.4),

$$\psi_{\mathbf{k}}(\mathbf{r}+\boldsymbol{\tau}_l) = \exp(i\mathbf{k}\cdot\boldsymbol{\tau}_l)\exp[i\epsilon\mathbf{A}(\boldsymbol{\tau}_l)\cdot\mathbf{r}]\psi_{\mathbf{k}-\epsilon\mathbf{A}(\boldsymbol{\tau}_l)}(\mathbf{r}). \qquad \ldots\ldots(1.5)$$

It should be noted that since the summation over $\mathbf{k}$ is restricted to the surface $W(\mathbf{k})=W$, if the only surviving term that the δ-function permits is to be included, it must follow that

$$W[\mathbf{k}-\epsilon\mathbf{A}(\boldsymbol{\tau}_l)] = W(\mathbf{k}),$$

i.e. that W be periodic in $\mathbf{k}$ with the (vector) period $\mathbf{A}(\boldsymbol{\tau}_l)$. For the case $\mathbf{A}=0$, (1.5) reduces to the familiar Bloch relation

$$\psi_{\mathbf{k}}(\mathbf{r}+\boldsymbol{\tau}_l) = \exp(i\mathbf{k}\cdot\boldsymbol{\tau}_l)\psi_{\mathbf{k}}(\mathbf{r}).$$

A formal solution to the functional equation (1.5) is

$$\psi_{\mathbf{k}}(\mathbf{r}) = \exp(i\mathbf{k}\cdot\mathbf{r})U[\mathbf{k}-\epsilon\mathbf{A}(\mathbf{r})\,;\,\mathbf{r}\,;\,\mathbf{k}], \qquad \ldots\ldots(1.6)$$

where U is understood to be formed from a unique function of three variables by replacing the first written by a linear combination of $\mathbf{r}$ and $\mathbf{k}$. Furthermore the dependence of U upon $\mathbf{r}$ is periodic, of lattice periodicity, the dependence of U upon $\mathbf{k}$ periodic with (vector) period $\mathbf{A}(\boldsymbol{\tau}_l)$. If such a function be constructed, it will be seen to be the most general function satisfying equation (1.5). That it is unique will presently appear when explicit representations are introduced.

By using the functional form (1.6) in the Schrödinger equation and taking the gradient with respect to $\mathbf{k}$, matrix relations analogous to those holding for Bloch functions may be obtained.

Thus,

$$\left.\begin{aligned}
&\int\psi^*_{\mathbf{k}\alpha}\left(\mathbf{p}-\frac{e}{c}\mathbf{A}\right)\psi_{\mathbf{k}\alpha}d^3\mathbf{r} = \frac{m}{\hbar}\nabla_{\mathbf{k}}W_\alpha(\mathbf{k}),\\
&\int\psi^*_{\mathbf{k}\alpha}\left(\mathbf{p}-\frac{e}{c}\mathbf{A}\right)\psi_{\mathbf{k}\alpha}d^3\mathbf{r}+\frac{m}{\hbar}(W_{\alpha'}-W_\alpha)\int U_{\mathbf{k}\alpha'}\nabla_{\mathbf{k}}U_{\mathbf{k}\alpha}d^3\mathbf{r}=0,\\
&\frac{2}{m}\sum_{\alpha'}\frac{|(p_x-(e/c)A_x)_{\alpha\alpha'}|^2}{W_{\alpha'}-W_\alpha} = 1-\frac{m}{\hbar^2}\frac{\partial^2W_\alpha}{\partial k_x{}^2}\text{ etc.},
\end{aligned}\right\} \qquad \ldots\ldots(1.7)$$

where α denotes any other quantum variables necessary for a complete description.

For the particular case of free electrons, i.e. $V(\mathbf{r})=0$, and using $\mathbf{A}=(0, Hx, 0)$ say, all results obtained so far may be verified provided one is careful to choose the proper linear combinations of the degenerate states, W then being degenerate in k_x, k_y.

§ 2. Representations for the Schrödinger Equation

To avoid unnecessary complication, take $\mathbf{A}=\frac{1}{2}\mathbf{H}\times\mathbf{r}$. Then from (1.6)

$$\psi_{\mathbf{k}}=\exp(i\boldsymbol{\varkappa}\,.\,\mathbf{r})U(\boldsymbol{\varkappa},\mathbf{r}), \qquad \text{where} \qquad \boldsymbol{\varkappa}=\mathbf{k}-\epsilon\mathbf{A}(\mathbf{r}).$$

(The separate dependence of U upon $\mathbf{k}$ is now understood to be present and will not be written in explicitly.)

In this form it resembles a Bloch function though it must be remembered that $\boldsymbol{\varkappa}$ is a linear combination of $\mathbf{k}$ and $\mathbf{r}$.

The Schrödinger equation (1.1) becomes therefore,

$$\left[\frac{1}{2m}\left(\mathbf{p}-\frac{e}{c}\mathbf{A}\right)^2+V(\mathbf{r})-W\right]\exp(i\boldsymbol{\varkappa}\,.\,\mathbf{r})U(\boldsymbol{\varkappa},\mathbf{r})=0. \quad \ldots\ldots(2.1)$$

$\mathbf{p}$, in the kinetic term, is a total differential operator; it acts on the explicit $\mathbf{r}$ (in which U, keeping $\boldsymbol{\varkappa}$ constant, is periodic) and on the $\mathbf{r}$ contained implicitly in $\boldsymbol{\varkappa}$. If $\partial/\partial x^\mu$ therefore be replaced by

$$\frac{\partial}{\partial x^\mu}+\frac{\partial\kappa^\nu}{\partial x^\mu}\frac{\partial}{\partial\kappa^\nu},$$

i.e. $\mathbf{p}\to\mathbf{p}-\frac{1}{2}\mathbf{H}\times i\nabla_{\boldsymbol{\varkappa}}$ the two operations are separated and $\boldsymbol{\varkappa}$ and $\mathbf{r}$ may be regarded as independent variables. This is nothing more than elementary implicit differentiation, but one should note that since the square of $\mathbf{p}$ occurs, it is important that $\boldsymbol{\varkappa}$ be linear in $\mathbf{r}$.

Then (2.1) becomes a differential equation in the two independent vector variables, $\mathbf{r}$ and $\boldsymbol{\varkappa}$, thus:

$$\left\{\frac{1}{2m}\left[\mathbf{p}-\frac{e}{c}\mathbf{A}(\mathbf{r})-\frac{e}{c}\mathbf{A}(i\nabla_{\boldsymbol{\varkappa}})\right]^2+V(\mathbf{r})-W\right\}\exp(i\boldsymbol{\varkappa}\,.\,\mathbf{r})U(\boldsymbol{\varkappa},\mathbf{r})=0 \quad \ldots.(2.2)$$

($\nabla_{\boldsymbol{\varkappa}}$ means gradient with respect to $\boldsymbol{\varkappa}$).

There are now two different representations possible:

(i) $\exp(i\boldsymbol{\varkappa}\,.\,\mathbf{r})U(\boldsymbol{\varkappa},\mathbf{r})$ having the translational symmetry of the lattice, may be expanded into the ordinary Bloch functions $\phi_{\boldsymbol{\varkappa},l}(\mathbf{r})$ where

$$\left[\frac{p^2}{2m}+V(\mathbf{r})-E_l(\boldsymbol{\varkappa})\right]\phi_{\boldsymbol{\varkappa},l}(\mathbf{r})=0.$$

Thus,
$$\exp(i\boldsymbol{\varkappa}\,.\,\mathbf{r})U(\boldsymbol{\varkappa},\mathbf{r})=\sum_l v_l(\boldsymbol{\varkappa})\phi_{\boldsymbol{\varkappa},l}(\mathbf{r}),$$

the summation over l extending over all bands.

(ii) $U(\boldsymbol{\varkappa},\mathbf{r})$ being periodic in $\mathbf{r}$, may be expanded into Fourier plane waves thus

$$\exp(i\boldsymbol{\varkappa}\,.\,\mathbf{r})U(\boldsymbol{\varkappa},\mathbf{r})=\sum u_l(\boldsymbol{\varkappa})\exp[i(\boldsymbol{\varkappa}_l+\boldsymbol{\varkappa})\,.\,\mathbf{r}],$$

where $\boldsymbol{\varkappa}_l$ are the lattice vectors of the inverse lattice, i.e. $\exp(i\boldsymbol{\varkappa}_l\,.\,\boldsymbol{\tau}_{l'})=1$ for all l,l'.

Considering (i), it is a matter of algebra to verify that it leads to a set of simultaneous differential equations in $\boldsymbol{\varkappa}$ which may be written as follows:

$$\left.\begin{aligned}E_n v_n-\frac{e}{mc}\sum_{n'}[\mathbf{p}\,.\,\mathbf{A}+\mathbf{A}(i\nabla_{\boldsymbol{\varkappa}})]_{nn'}v_{n'}\\+\frac{e^2}{2mc^2}\sum_{n'}[\mathbf{A}^2+2\mathbf{A}\,.\,\mathbf{A}(i\nabla_{\boldsymbol{\varkappa}})+\mathbf{A}^2(i\nabla_{\boldsymbol{\varkappa}})]_{nn'}v_{n'}\\-Wv_n=0\end{aligned}\right\} \quad \ldots\ldots(2.3)$$

where $(\mathbf{p}\cdot\mathbf{A})_{nn'}$, $\mathbf{A}_{nn'}{}^2$ etc. are the matrix elements

$$\int \phi^*_{\kappa,n}(\mathbf{p}\cdot\mathbf{A})\phi_{\kappa,n'}d^3\mathbf{r}, \qquad \int \phi^*_{\kappa,n}\mathbf{A}^2\phi_{\kappa,n'}d^3\mathbf{r} \text{ etc.},$$

and $\mathbf{A}(i\nabla_\kappa)_{nn'}$ means $\mathbf{A}(i\nabla_\kappa)\delta_{nn'}$.

Equation (2.3) might be written more elegantly as

$$\sum_{n'}\left[E-\frac{e}{mc}\,\mathbf{p}\cdot\mathfrak{A}+\frac{e^2}{2mc^2}\,\mathfrak{A}^2\right]_{nn'} v_{n'}=Wv_n, \qquad \ldots\ldots(2.4)$$

where $\mathfrak{A}_{nn'}\equiv\mathbf{A}(\mathbf{r}+i\nabla_\kappa)_{nn'}$ and $\mathfrak{A}^2$ is defined to mean the last term in (2.3) so that $\mathbf{A}i(\nabla_\kappa)\cdot\mathbf{A}$ does *not* occur.

An equation similar to (2.4) has been derived by Wilson (1936) though from quite different principles. It differed in being an equation for the density matrix rather than for eigenvalues.

Adams (1953) has also considered a somewhat similar equation though he used the formalism of Wannier functions to derive it. Both these authors were intent on calculating the constant magnetic susceptibility to which purpose the equation is well suited. For eigenvalues it is more convenient to use (ii).

With less trouble it is seen to produce

$$\frac{\hbar^2}{2m}\,[\boldsymbol{\varkappa}+\boldsymbol{\varkappa}_l-\epsilon\mathbf{A}(i\nabla_\kappa)]^2u_l(\boldsymbol{\varkappa})+\sum_{l'l''}V_{l'}u_{l''}(\boldsymbol{\varkappa})=Wu_l(\boldsymbol{\varkappa}) \qquad \ldots\ldots(2.5)$$

where V_l are the Fourier components of $V(\mathbf{r})$ and $\Sigma_{l',l''}$ is restricted to l', l'' for which $\boldsymbol{\varkappa}_{l'}+\boldsymbol{\varkappa}_{l''}=\boldsymbol{\varkappa}_l$.

Equation (2.5) is again a set of coupled second-order differential equations which are simpler than (2.4) in that the coupling occurs only through the numbers V_l and that no complicated matrix elements appear. The equations are an evident generalization of those holding in the absence of a magnetic field for the Fourier components of Bloch functions: $\mathbf{k}$ is replaced by $\boldsymbol{\pi}=\boldsymbol{\varkappa}-\epsilon\mathbf{A}(\nabla_\kappa)$ so that $[\pi_x, \pi_y]=i\epsilon H_z$ etc.

It may be remarked that the unambiguous derivations of equations (2.4), (2.5) are further demonstrations, if such were needed, of the uniqueness of $U(\boldsymbol{\varkappa}, \mathbf{r})$ as a function of the two independent variables, $\mathbf{r}$, $\boldsymbol{\varkappa}$.

§ 3. Discussion and Solution of the Schrödinger Equation

Since Adams has extensively discussed what is probably the only useful application of equation (2.4), nothing more will be said about it in this paper. In any case, (2.5), besides being simpler to treat, gives some useful insight into the origins of the non-diagonal contributions which Adams regarded as important.

In analogy with the non-magnetic case, $\mathbf{A}=0$, $V(\mathbf{r})$ is restricted for the sake of simplicity to be sinusoidal; it is not pretended that this is at all realistic but it may be expected to lead to results of qualitative importance and suggest extensions to more general potentials. An immediate consequence (which would not be generally true) is that motion in the field direction is separable and is simply the unperturbed Bloch motion. If this is removed there remains the motion in a plane normal to the field $\mathbf{H}$, which will be taken to be in the z direction.

A second simplification involving no loss of generality is to take $\mathbf{A}=(0,Hx,0)$. Since the equations were derived using $\mathbf{A}=\frac{1}{2}\mathbf{H}\times\mathbf{r}$, the necessary corrections are discussed in the Appendix and it is seen that $\mathbf{A}(i\nabla_\kappa)$ must be replaced by

$(-iH\partial/\partial\kappa_y, 0, 0)$. Supposing **H** to coincide with a crystallographic axis equation (2.5) may be simplified to

$$\left\{\frac{\hbar^2}{2m}\left[\left(\kappa_x+\frac{2\pi m}{a}+i\epsilon H\frac{\partial}{\partial\kappa_y}\right)^2+\left(\kappa_y+\frac{2\pi n}{a}\right)^2\right]-W\right\}u_{m,n}$$
$$+V(u_{m+1,n}+u_{m-1,n})+V'(u_{m,n+1}+u_{m,n-1})=0 \quad \ldots\ldots(3.1)$$

where the metal is supposed to have cubic symmetry of lattice constant a, and V, V' (taken as different for convenience) are the Fourier components of $V(x, y)$ in the x, y directions.

In (3.1), κ_x is a constant of the motion and, in fact, is equal to k_x since $A_x=0$. First suppose $V=0$, i.e. a periodic field in one dimension only (though the motion is, of course, two-dimensional). This is not physically interesting, but serves to illustrate simply how the calculation proceeds. Then the index m is redundant and (3.1) becomes

$$\left\{\frac{\hbar^2}{2m}\left[\left(k_x+i\epsilon H\frac{\partial}{\partial\kappa}\right)^2+\left(\kappa+\frac{2\pi n}{a}\right)^2\right]-W\right\}u_n+V'(u_{n+1}+u_{n-1})=0 \quad \ldots.(3.2)$$

where κ_y is abbreviated to κ.

Suppose the last term is small (the precise condition for this will appear shortly), then the effect of a lattice may be treated as a perturbation to the free magnetic motion, the zero-order wave function being

$$u_n(\kappa)=\exp\left[i\left(k_x+\frac{2\pi n}{a}\right)\Big/\epsilon H\right]\text{. oscillator function of }\left(\kappa+\frac{2\pi n}{a}\right)$$

and
$$W_j=(j+\tfrac{1}{2})\hbar\omega_L, \qquad \omega_L=\frac{eH}{mc}.$$

The perturbed energy then becomes

$$2V'\cos\frac{2\pi k_x}{\epsilon aH}\int u_j(\kappa)u_j\left(\kappa+\frac{2\pi}{a}\right)d\kappa.$$

Provided the overlap integral is sufficiently small, the level W_j is thus broadened since k_x can take a continuous range of values. That the lattice forces might produce such broadening was earlier suggested by Dingle and Shoenberg (1950), Dingle (1952 a) and Shoenberg (1952). Remembering the definition of u_n, it is seen that $\psi_{\mathbf{k}}$ extends throughout the lattice, this representing the proper linear combination of (localized) Landau solutions. These simple results are also obtainable more directly by treating $V(x, y)$ as a perturbation to such free-electron solutions and one then obtains the useful results $-\frac{1}{2}\epsilon aH<k_x<\frac{1}{2}\epsilon aH$, $k_x=2\pi t/L_x$, t an integer and L_x the x-dimension of the metal.

However, the requirement

$$V\int u_j(\kappa)u_j\left(\kappa+\frac{2\pi}{a}\right)d\kappa\ll\mu H,$$

necessary for the success of perturbation treatment, is satisfied only for $W\ll\epsilon_0=(\hbar^2/2m)(\pi/a)^2$, this being the energy at which $u(\kappa)$, $u(\kappa+2\pi/a)$ begin to overlap appreciably. An asymptotic expansion of the integral is given by

$$\int_{-\infty}^{\infty}u_j(\kappa)u_j\left(\kappa-\frac{2\pi}{a}\right)d\kappa\simeq\left(\frac{2\pi^4}{a^2\epsilon H}\right)^{-1/4}(j-j_0)^{-1/4}\cos\Theta, \quad W_j>\epsilon_0$$

Θ being a slowly varying function of j. The approximation is poor near $W\gtrsim\epsilon_0$, but improves with increasing W. Taking $H\sim10^4$ oersted, $V\sim1$ ev its order of

magnitude is 0·02 ev, compared with $\mu H \sim 10^{-4}$ ev. Thus, perturbation methods fail for energies close to and beyond ϵ_0, that is, beyond the first energy gap region.

Returning to equation (3.2), an inspection of the non-magnetic solution (nearly-free electrons) suggests that a better method is to neglect all but two adjacent components, say u_0, u_1 and regard these as strongly coupled. Symmetry considerations will then show how to allow for a true solution.

Then (3.2) becomes,

$$\left.\begin{aligned}\left\{\frac{\hbar^2}{2m}\left[\left(k_x+i\epsilon H\frac{d}{d\kappa}\right)^2+\kappa^2\right]-W\right\}u_0+V'u_1=0,\\ \left\{\frac{\hbar^2}{2m}\left[\left(k_x+i\epsilon H\frac{d}{d\kappa}\right)^2+\left(\kappa+\frac{2\pi}{a}\right)^2\right]-W\right\}u_1+V'u_0=0.\end{aligned}\right\} \quad \ldots\ldots(3.3)$$

From the first,

$$u_1=-\frac{1}{V'}\left\{\frac{\hbar^2}{2m}\left[\left(k_x+i\epsilon H\frac{d}{d\kappa}\right)^2+\kappa^2\right]-W\right\}u_0. \quad \ldots\ldots(3.4)$$

Inserting (3.4) into the second of (3.3)

$$\left\{\left[\frac{\hbar^2}{2m}\left(D^2+\left\{\kappa+\frac{2\pi}{a}\right\}^2\right)-W\right]\left[\frac{\hbar^2}{2m}(D^2+\kappa^2)-W\right]-V'^2\right\}u_0=0, \quad \ldots.(3.5)$$

abbreviating $k_x+i\epsilon Hd/d\kappa$ to D. Define now $\vartheta_a'(\kappa)$, $\vartheta_b'(\kappa)$ to be the roots of

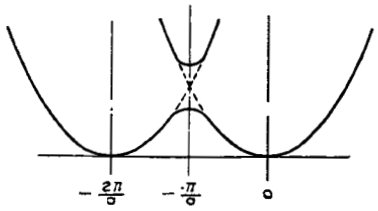
$$\left(\vartheta-\frac{\hbar^2\kappa^2}{2m}\right)\left[\vartheta-\frac{\hbar^2}{2m}\left(\kappa+\frac{2\pi}{a}\right)^2\right]-V'^2=0; \quad \ldots\ldots(3.6)$$

then (3.5) may be re-written as

$$\left\{\left[\frac{\hbar^2D^2}{2m}+\vartheta_b'(\kappa)-W\right]\left[\frac{\hbar^2D^2}{2m}+\vartheta_a'(\kappa)-W\right]+\left[\frac{\hbar^2D^2}{2m},\frac{\hbar^2\kappa^2}{2m}-\vartheta_a'(\kappa)\right]\right\}u_0=0, \quad \ldots\ldots(3.7)$$

the last (commutator) term arising from the necessary re-ordering of the operator D^2.

The potentials ϑ_a', ϑ_b' are illustrated below; the broken curve corresponds to the 'free electron' potentials.



Consider first the region $\kappa > -\pi/a$. If $\vartheta_a'(\kappa)$ is chosen as the lower branch then $\hbar^2\kappa^2/2m - \vartheta_a'(\kappa)$ is slowly varying except near $\kappa = -\pi/a$. In zero order therefore, the commutator in (3.7) may be neglected, and $u_0(\kappa > -\pi/a)$ may be taken to satisfy

$$\left[\frac{\hbar^2D^2}{2m}+\vartheta_a'(\kappa)-W\right]u_0=0,$$

and consequently from (3.4)

$$u_1=-\frac{1}{V'}\left(\frac{\hbar^2\kappa^2}{2m}-\vartheta_a'\right)u_0; \quad \ldots\ldots(3.8)$$

Equation (3.8) is incomplete since boundary conditions are necessary to determine W. Considering now the region $\kappa < -\pi/a$, it is evident that (to a similar degree of approximation) a solution is

$$\left.\begin{aligned} &\left(\frac{\hbar^2 D^2}{2m} + \vartheta_a' - W\right) u_1 = 0, \\ &u_0 = -\frac{1}{V'}\left[\frac{\hbar^2}{2m}\left(\kappa + \frac{2\pi}{a}\right)^2 - \vartheta_a'\right] u_1. \end{aligned}\right\} \quad \ldots\ldots (3.9)$$

The boundary condition adopted is that $u_0(\kappa > -\pi/a)$ (determined from equation (3·8)) join smoothly to $u_1(\kappa < -\pi/a)$ (determined from the first of (3.9)). Note that choosing ϑ_b' requires interchanging u_0, u_1.

One might at first object to such boundary conditions since from (3.8), for example, $u_1(\pi/a) = -u_0(-\pi/a)$ and therefore both u_0 and u_1 are discontinuous at $\kappa = -\pi/a$. There need be no discontinuity in $\psi_{\mathbf{k}}$ however; it is merely necessary to re-label the u_l such that the greatest is denoted by u_0 and simultaneously change the origin of k_y by an inverse lattice vector, $2\pi/a$. This corresponds in the non-magnetic problem, to adopting the convention of regarding all functions of $\mathbf{k}$ as periodic with the periodicity of the inverse lattice.

It should be remarked that, owing to the neglect of commutators, these solutions are only approximate, and choosing the largest component to be continuous (along with its derivative) means that in general the smaller one will not be. In fact there is a slight discontinuity in slope at $\kappa = -\pi/a$. It is of no special consequence however, and may be ignored.

It is now evident from symmetry how to include all components u_l: ϑ_a', ϑ_b' are to be replaced by $E_y^{(1)}(\kappa)$ and $E_y^{(2)}(\kappa)$, the latter being the first and second band energies (in κ) relating to a sinusoidal potential in the y direction. Equation (3.6) is the usual secular equation determining $E(\kappa)$ in the simple one-dimensional problem of nearly free electrons.

Thus u_0 satisfies the equation

$$\left[\frac{\hbar^2}{2m}\left(k_x + i\epsilon H\frac{d}{d\kappa}\right)^2 + E_y^{(1)}(\kappa) - W\right] u_0 = 0, \quad \ldots\ldots (3.10)$$

with the boundary condition that $u_0'(\kappa)$ should be zero at a maximum of $E^{(1)}(\kappa)$. The generalization to more complicated potentials is obvious and will not be elaborated upon. The remaining components are provided (approximately) by equations like (3.8) and are evidently small compared with u_0 except in the immediate vicinity of maximum $E(\kappa)$. Note that a knowledge of such components is not necessary for a determination of W.

Since $E_y^{(l)}(\kappa)$ is periodic in κ, (3.10) is a Bloch-like equation whose eigenvalues are therefore bands. Considering dimensions however, one sees that far from an energy gap, the width of the potential barrier is so great that the bands must be very narrow; they are in fact, nothing but the broadened levels mentioned earlier.

The effect of a periodic potential in the x direction may also be considered, it now being necessary to factorize (approximately) the expression

$$\left\{\frac{\hbar^2}{2m}\left[\left(k_x + \frac{2\pi}{a} + i\epsilon H\frac{d}{d\kappa}\right)^2 + \kappa^2\right] - W\right\}\left\{\frac{\hbar^2}{2m}\left[\left(k_x + i\epsilon H\frac{d}{d\kappa}\right)^2 + \kappa^2\right] - W\right\} - \eta^4$$

Using the Fourier transform of u_0

$$u_0(\kappa)=\int \bar{u}(q)\exp\left[-i(q-k_x)(\kappa-k_y)/\epsilon H\right]dq,$$

then $k_x+i\epsilon Hd/d\kappa\to q$, $\kappa\to k_y+i\epsilon Hd/dq$, and the equations reduce to the previous form, κ being replaced by q and k_x by k_y. The solutions for $\bar{u}_0(q)$, $\bar{u}_1(q)$ may be discussed as before and lead to similar conclusions, the broadening now being described by k_y.

The analogue of (3.10) is

$$\left[E_x^{(l)}\left(k_x+i\epsilon H\frac{d}{d\kappa}\right)+\frac{\hbar^2\kappa^2}{2m}-W\right]u_0=0, \qquad \ldots\ldots(3.11)$$

where the boundary conditions are now applied to $u_0(q)$, thus introducing the absent k_y. k_x in (3.11) is of course redundant, just as k_y is for (3.10); these degeneracies are removed when both V and V' are present.

One might guess that using a two-dimensional potential, i.e. including V, V', (3.10) and (3.11) would be combined in an obvious manner. In fact, a fresh difficulty arises which may be loosely described as a band coupling. To discuss this it is sufficient to consider the equations (3.1) retaining only u_{00}, u_{01}, u_{10}, u_{11}.

Then the equations run,

$$\left.\begin{aligned} H_{00}u_{00}+Vu_{10}+V'u_{01}&=0,\\ H_{01}u_{01}+Vu_{11}+V'u_{00}&=0,\\ H_{10}u_{10}+Vu_{00}+V'u_{11}&=0,\\ H_{11}u_{11}+Vu_{01}+V'u_{10}&=0,\end{aligned}\right\} \qquad \ldots\ldots(3.12)$$

where $H_{l,m}$ are abbreviations for the differential operators (including W) which appear in (3.1).

From the first and second equations of (3.12),

$$\left.\begin{aligned} u_{10}&=-\frac{1}{V}(H_{00}u_{00}+V'u_{01}),\\ u_{11}&=-\frac{1}{V}(H_{01}u_{01}+V'u_{00}).\end{aligned}\right\} \qquad \ldots\ldots(3.13)$$

Substitution in the third and fourth gives

$$(H_{10}H_{00}-V^2+V'^2)u_{00}+V'(H_{10}+H_{01})u_{01}=0,$$
$$V'(H_{11}+H_{00})u_{00}+(H_{11}H_{01}-V^2+V'^2)u_{01}=0.$$

These are conveniently written in the following form:

$$\left(\vartheta_b+\frac{\hbar^2\kappa^2}{2m}-W\right)\chi_1+V'\chi_2-\left[\frac{\hbar^2D^2}{2m}-\vartheta_a,\ \frac{\hbar^2\kappa^2}{2m}\right]u_{00}=0 \qquad \ldots\ldots(3.14)$$

$$V'\chi_1+\left[\vartheta_b+\frac{\hbar^2}{2m}\left(\kappa+\frac{2\pi}{a}\right)^2-W\right]\chi_2-\left[\frac{\hbar^2D^2}{2m}-\vartheta_a,\ \frac{\hbar^2}{2m}\left(\kappa+\frac{2\pi}{a}\right)^2\right]u_{01}=0$$

where

$$\left.\begin{aligned} \chi_1&=\left(\vartheta_a+\frac{\hbar^2\kappa^2}{2m}-W\right)u_{00}+V'u_{01}\\ \chi_2&=V'u_{00}+\left[\vartheta_a+\frac{\hbar^2}{2m}\left(\kappa+\frac{2\pi}{a}\right)^2-W\right]u_{01}\end{aligned}\right\} \qquad \ldots\ldots(3.15)$$

(the argument of ϑ_a, ϑ_b being $D\equiv k_x+i\epsilon Hd/d\kappa$).

If the final commutators in (3.14) are omitted then a solution is $\chi_1=\chi_2=0$.

This, from (3.15), leads to

$$\left[(\vartheta_a+\vartheta_b'-W)(\vartheta_a+\vartheta_a'-W)+\vartheta_a,\left[\frac{\hbar^2\kappa^2}{2m}-\vartheta_a'\right]\right]u_{00}=0.$$

Neglecting the final commutator, an approximate solution is

$$(\vartheta_a+\vartheta_a'-W)u_{00}=0. \qquad \ldots\ldots(3.16)$$

This is the form expected to appear from a combination of the two cases already discussed. From (3.15) the other components are given by

$$\left.\begin{aligned} u_{01}&=-\frac{1}{V'}\left(\frac{\hbar^2\kappa^2}{2m}-\vartheta_a'\right)u_{00}\\ u_{10}&=-\frac{1}{V}\left(\frac{\hbar^2D^2}{2m}-\vartheta_a\right)u_{00}\\ u_{11}&=\frac{1}{VV'}\left(\frac{\hbar^2D^2}{2m}-\vartheta_a\right)\left(\frac{\hbar^2\kappa^2}{2m}-\vartheta_a'\right)u_{00}. \end{aligned}\right\} \qquad \ldots\ldots(3.17)$$

Equation (3.16) may be discussed along similar lines as before except that no boundary conditions are to be applied to both $u_{00}(\kappa)$ and $\bar{u}_{00}(q)$. By choosing appropriate combinations of ϑ_a, ϑ_b, ϑ_a', ϑ_b', three other bands are obtainable, two of which, for $V'=V$, are degenerate.

Symmetry considerations again permit the immediate generalization of equations like (3.16) to

$$\left[E_x^{(n)}\left(k_x+i\epsilon H\frac{d}{d\kappa}\right)+E_y^{(m)}(\kappa)-W\right]u_{00}=0 \qquad \ldots\ldots(3.18)$$

with appropriate boundary conditions at the maxima of E_x, E_y.

Equation (3.18) is a particular instance of Peierls' theorem stated more exactly, namely, that replacing $E(\mathbf{k})$ by $E(\boldsymbol{\pi})$, $[\kappa_x,\kappa_y]=i\epsilon H_z$ etc., provides an approximate energy operator for the conduction electrons in a uniform magnetic field. $\boldsymbol{\pi}$ in this case, is $\mathbf{k}-\epsilon\mathbf{A}^0(i\nabla_{\mathbf{k}})$, $\mathbf{A}^0=\mathbf{H}\times\mathbf{r}-\mathbf{A}$ (see Appendix). Luttinger (1951) has also given a general demonstration of this theorem using the Wannier representation. An advantage of the present treatment is that the theorem is presented quite naturally as a zero-order approximation, the validity conditions of which are easy to obtain. To this end, consider again equations (3.14), (3.15). By eliminating χ_2, u_{01}, there results a pair of simultaneous equations u_{00}, χ_1 which may be written as:

$$\left.\begin{aligned} &\left[(\vartheta_a+\vartheta_b'-W)(\vartheta_a+\vartheta_a'-W)+\left[\frac{\hbar^2\kappa^2}{2m},\frac{\hbar^2D^2}{2m}-\vartheta_a\right]\right.\\ &\qquad\left.+\left[\vartheta_a,\frac{\hbar^2\kappa^2}{2m}-\vartheta_a'\right]\right]u_{00}\\ &\quad=\left[\vartheta_a-\vartheta_b+\frac{\hbar^2}{2m}\left\{\left(\kappa+\frac{2\pi}{a}\right)^2-\kappa^2\right\}\right]\chi_1,\\ &\left[(\vartheta_b+\vartheta_b'-W)(\vartheta_b+\vartheta_a'-W)+\left[\vartheta_b,\frac{\hbar^2\kappa^2}{2m}-\vartheta_a'\right]\right.\\ &\qquad\left.+\left[\frac{\hbar^2}{2m}\left(\kappa+\frac{2\pi}{a}\right)^2,\frac{\hbar^2D^2}{2m}-\vartheta_a\right]\right]\chi_1\\ &\quad=\left[\left\{\vartheta_b+\frac{\hbar^2}{2m}\left(\kappa+\frac{2\pi}{a}\right)^2-W\right\}\left[\frac{\hbar^2D^2}{2m}-\vartheta_a,\frac{\hbar^2\kappa^2}{2m}\right]\right.\\ &\qquad\left.+\left[\frac{\hbar^2}{2m}\left(\kappa+\frac{2\pi}{a}\right)^2,\frac{\hbar^2D^2}{2m}-\vartheta_a\right]\left(\vartheta_a+\frac{\hbar^2\kappa^2}{2m}-W\right)\right]u_{00}. \end{aligned}\right\} \qquad \ldots\ldots(3.19)$$

Considering the left-hand sides of these equations, it is clear (from previous arguments) that in both the leading term is the first one written. For u_{00} the first operating factor represents (approximately) the first band; for χ_1, the second band. Their eigenvalues (or more properly, the eigenvalues of their generalizations to forms like equation (3.18)) themselves form bands of broadened levels lying between the same energy limits as those found in the non-magnetic problem (Harper 1955). Thus, in the present case of nearly free electrons, these bands will certainly overlap, though the equations might be regarded as including the less interesting situation that arises when they do not.

The commutator terms (still on the left-hand side) will modify these eigenvalues. Treating them as a perturbation, the first-order correction η to a level W will be given by

$$\eta \int \phi^*(\vartheta_a' - \vartheta_b')\phi \, d\kappa = \int \phi^* U \phi \, d\kappa$$

where U is the sum of the two commutators appropriately defined on both sides of κ, $q = -\pi/a$, and ϕ is an eigenfunction of $\vartheta_a + \vartheta_a'$. A typical term in U is

$$\left[\vartheta_a, \frac{\hbar^2\kappa^2}{2m} - \vartheta_a'\right] \sim \left[\frac{\hbar^2 D^2}{2m}, \frac{\hbar^2\kappa^2}{2m} - \vartheta_a'\right]$$

$$= \frac{\hbar^2}{2m}\left[2i\epsilon H \frac{d}{d\kappa}\left(\frac{\hbar^2\kappa^2}{2m} - \vartheta_a'\right)\left(k_x - i\epsilon H \frac{d}{d\kappa}\right) - (\epsilon H)^2 \left(\frac{d}{d\kappa}\right)^2 \left(\frac{\hbar^2\kappa^2}{2m} - \vartheta_a'\right)\right].$$

Now $\langle \vartheta_a' - \vartheta_b' \rangle$ is least when the electron is largely confined to the vicinity of $\kappa = -\pi/a$. This happens when $W \sim 2(\epsilon_0 - V)$, i.e. near the top of the first band. $\langle \vartheta_a' - \vartheta_b' \rangle$ is then of order $2V$ and the electron behaviour is described by the use of an effective mass m^*. The final term in the above expression is then approximately

$$-(\epsilon H)^2 \left(\frac{\hbar^2}{2m}\right)^2 \left(\frac{d}{d\kappa}\right)^2 \left(\kappa^2 - \frac{m}{m^*}\kappa^2\right) = -2(\mu H)^2 \left(1 - \frac{m}{m^*}\right)$$

where $\mu = e\hbar/2mc$.

Thus it contributes $(\mu H/V)(1 - m/m^*)\mu H$ to η which is a small correction even though $1 - m/m^*$ might be of the order of 10, since $\mu H/V \ll 1$. The first term is not constant and therefore more difficult to estimate, but on dimensional grounds it is probably of the same order of magnitude.

These commutator terms then are likely to be small and are conjectured to correspond, in the limiting case of tight binding, to perturbation of atomic levels, though this has not been verified directly.

The discussion so far applies, for example, to the case $\chi_1 = 0$ and neglects coupling between first and second band. Suppose now, as a better approximation χ_1 is determined from the second of (3.19) using u_{00} from the first (but with $\chi_1 = 0$). Then this contribution to η is given by

$$\eta \int \phi^*(\vartheta_a' - \vartheta_b')\phi d\kappa = \int \phi^* \left[\vartheta_a - \vartheta_b + \frac{\hbar^2}{2m}\left\{\left(\kappa + \frac{2\pi}{a}\right)^2 - \kappa^2\right\}\right] \chi_1 \, d\kappa.$$

But in the case when the eigenvalues $W^{a,a}$ of $\vartheta_a + \vartheta_a'$ overlap with $W^{b,a}$ of $\vartheta_b + \vartheta_a'$, it will frequently happen that a pair of them nearly coincide (periodically so, in fact, when the two effective masses in this region are constant) and consequently χ_1 becomes large since it contains components of the order $(W^{a,a} - W^{b,a})^{-1}$. The complexity of the coupled equations (3.19) makes any quantitative examination of their solution an unattractive programme. In any

case they represent the situation only approximately since all but adjace components were neglected. It is not difficult however to obtain the follow dimensional estimate for η:

$$\eta \sim \frac{(\mu H)^2}{W^{a,a} - W^{b,a}} \qquad \text{provided} \qquad W^{a,a} \neq W^{b,a}, \qquad \ldots\ldots (3.20)$$

$W^{b,a}$ being the closest eigenvalue of $\vartheta_b + \vartheta_a'$ to $W^{a,a}$. (The resemblance this result to perturbation theory seems fortuitous since, for example, there shou be a factor $V(W^{a,a} - W^{b,a} + V)^{-1}$ which is supposed of order unity.)

If now the bands do overlap, $\eta \sim \mu H$ in the overlap region, i.e. of the order the level spacing itself, which means that the coupling is strong and cannot regarded as a weak perturbation to single band levels. However, an inspecti of the matrix elements concerned shows that in the overlap region (where general the use of effective masses for the separate bands is permissible) they a slowly varying and, since near coincidences of $W^{b,a}$ with $W^{a,a}$ will occur (almos periodically, the actual level spectrum should still exhibit great regularity, eve periodicity. Whether this situation can be represented by the use of effecti mass parameters is not clear from such simple arguments. The success obtain in fitting experimental curves by such means suggests that it can, though th interpretation of such masses is then uncertain.

For non-overlapping bands, or far from an overlap region, (3.20) giv $\eta \sim (\mu H)^2/\Delta E$, ΔE being the energy gap, and thus, $\eta \ll \mu H$. The correction this situation is thus comparable with the perturbation first considered, though origin is different.

§ 4. Summary and Conclusions

Apart from some initial generalities concerning properties of the state functio most results refer to a simplified model chosen in order to avoid purely math matical difficulties. Firstly, the periodic potential describing the effect of th lattice was restricted to be sinusoidal. It is evident however, that results co cerning single-band motion are immediately extendible to include all $V(\mathbf{r})$ the form $V_1(x) + V_2(y) + V_2(z)$ using, of course, any convenient set of ax (x, y, z). Secondly, the magnetic field $\mathbf{H}$ was supposed to lie along such an ax (not necessarily a crystallographic axis). In consequence of this, and the fa that $E(\mathbf{k})$ is separable into $E_x(k_x) + E_y(k_y) + E_z(k_z)$, no ordering ambiguities ar in applying Peierls' theorem concerning $\mathbf{k} \to \boldsymbol{\varkappa} - \epsilon \mathbf{A}(i\nabla_{\boldsymbol{\varkappa}})$.

The magnetic wave functions depend of course upon choice of gauge $\mathbf{A}(\mathbf{r})$. Comparison with those for free electrons (in a magnetic field) show th in the particular case $\mathbf{A} = (0, Hx, 0)$ the wave functions are of the extended so being (for low energies at least) approximately linear combinations of t degenerate Landau functions. Application of the first of formulae (1.7) sho that there is a very slow linear motion of the electron in the x direction, this bei a translation of the 'orbit' due to Bragg collisions with the lattice.

Of more interest are the magnetic energy levels. Neglecting field direct motion, the highly degenerate discrete levels of free electrons are broadened a result of lattice forces. In the preceding paper (Harper 1955) the case tight binding was discussed and some of the results are quite general. The le spacing is also affected, since it is no longer uniform. When there is no ba overlap the variation in spacing is slow and the concept of effective mass certai

valid. For overlapping bands however, there appears to be a strong coupling which, while distorting the level structure in that vicinity, may still leave great regularity. It is not certain whether a description in terms of effective mass is applicable.

Knowing something of the magnetic level density what can one say of its effect on the magnetic susceptibility? Consider first the level broadening. Dingle has shown that the effect of collision broadening is to damp the low temperature susceptibility oscillation or what proves to be equivalent, raise the effective temperature by a degree or so. Lattice broadening has the same effect. Taking the spacing as uniform, simple perturbation theory indicates that the broadening might be well described by

$$\epsilon = b\left(\cos\frac{2\pi k_x}{\epsilon a H} + \cos\frac{2\pi k_y}{\epsilon a H}\right)$$

for each level, where $2b < \mu^* H$. If one now corrects the classical partition function by a factor

$$\sum_{k_x}\sum_{k_y} \exp\{-\beta\epsilon(k_x, k_y)\}$$

and uses the analytical method of Sondheimer and Wilson (1951), the vth Fourier component of the level density is seen to be diminished by a factor $J[_0(bv\pi/\mu^* H)]^2$ J_0 being the zero-order Bessel function regular at the origin. Consequently the magnetic moment is damped by the same factor. Dingle (1951) also examined this question and arrived at a similar result to the one given above, namely, that a periodic perturbation in one direction (perpendicular to the field) reduces the susceptibility amplitude by the factor $J_0(bv\pi/\mu^* H)$, b being given by the overlap integral of two Landau wave functions. Taking $2b \lesssim \mu^* H$, i.e. extreme broadening, the first (and greatest component) is heavily damped. Since in the monovalent metals the Fermi surface may be supposed to lie in the centre of the band and since the broadening is greatest there (see Harper 1955), it suggests a possible explanation of the absence of any observed oscillations in these metals.

For $b \ll \mu^* H$, the broadening factor may be written approximately $\exp[-(bv\pi/\mu^* H)^2]$ and the broadening effect becomes additive to that due to collision as described by Dingle (1952 b).

The level structure in the vicinity of an energy gap near a zone boundary is all-important for the de Haas–van Alphen effect. Unfortunately, this seems very difficult to determine in detail, even for a sinusoidal potential. Apart from the regularity already mentioned there seems little one can say. It is likely, however, that if periodicity exists, the period will give rise to effective mass parameters much smaller than one would otherwise expect. This is because the level structure will consist of irregular groups, regularly repeated. Since the period is large, the oscillatory period will also be large and the effective mass correspondingly smaller.

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APPENDIX

With an arbitrary gauge $\mathbf{A}(\mathbf{r})$, the Schrödinger equation becomes

$$\left[-\frac{\hbar^2}{2m}\left(\nabla-\frac{ie}{\hbar c}A\right)^2+V(r)-W\right]\exp\left[i\epsilon\mathbf{A}(\mathbf{r})\,.\,\mathbf{r}\right]U(\boldsymbol{\varkappa},\mathbf{r})\exp\left(i\boldsymbol{\varkappa}\,.\,\mathbf{r}\right)=0$$

or

$$\left\{-\frac{\hbar^2}{2m}\left[\nabla-i\epsilon\mathbf{A}+i\epsilon\nabla(\mathbf{A}\{\mathbf{r}\}\,.\,\mathbf{r})\right]^2+V(\mathbf{r})+\frac{\hbar^2\nabla^2}{2m}(\mathbf{A}\,.\,\mathbf{r})i\epsilon\right\}\exp\left(i\boldsymbol{\varkappa}\,.\,\mathbf{r}\right)U(\boldsymbol{\varkappa},\mathbf{r})$$

Now $$\nabla^2(\mathbf{A}\,.\,\mathbf{r})=0, \qquad \nabla(\mathbf{A}\,.\,\mathbf{r})=2\mathbf{A}-\mathbf{H}\times\mathbf{r},$$

consequently, $+\mathbf{A}-\nabla(\mathbf{A}\,.\,\mathbf{r})=\mathbf{H}\times\mathbf{r}-\mathbf{A}$ replaces $\mathbf{A}(\mathbf{r})$ in the kinetic term. Considering now the implicit differentiation on $\boldsymbol{\varkappa}$,

$$\frac{\partial}{\partial x^\mu}\rightarrow\frac{\partial}{\partial x^\mu}-\epsilon\left(\frac{\partial A^\nu}{\partial x^\mu}\frac{\partial}{\partial\kappa^\nu}\right).$$

Writing curl $\mathbf{A}=\mathbf{H}$ and remembering that $\partial A^\nu/\partial x^\mu$ are constants,

$$\begin{aligned}\frac{\partial A^\nu}{\partial x^\mu}\frac{\partial}{\partial\kappa^\nu}&=-\mathbf{H}\times\nabla_\kappa+(\nabla_\kappa\,.\,\nabla)\mathbf{A}(\mathbf{r})\\&=-\mathbf{H}\times\nabla_\kappa+\mathbf{A}(\nabla_\kappa).\end{aligned}$$

Therefore in the kinetic term,

$$\nabla\rightarrow\nabla+\epsilon[\mathbf{H}\times\nabla_\kappa-\mathbf{A}(\nabla_\kappa)].$$

Then the whole term may be written

$$\left[\mathbf{p}-\frac{e}{c}\mathbf{A}^0(\mathbf{r}+i\nabla_\kappa)\right]^2$$

where $$\mathbf{A}^0(\mathbf{r})=\mathbf{H}\times\mathbf{r}-\mathbf{A}(\mathbf{r}).$$

For the case $\mathbf{A}=\frac{1}{2}\mathbf{H}\times\mathbf{r}$, $\mathbf{A}^0=\mathbf{A}$. For $\mathbf{A}=(0, Hx, 0)$, $\mathbf{A}^0=(-Hy, 0, 0)$ and vice versa. Note however, that the definition of $\boldsymbol{\varkappa}$ is unaltered, i.e. $\boldsymbol{\varkappa}=\mathbf{k}-\epsilon\mathbf{A}(\mathbf{r})$.

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