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[1]M. S. Khaikin, Zh. Eksperim. i Teor. Fiz. 39, 212 (1960) [Sov. Phys. JETP 12, 152 (1961)].

[2]J. F. Koch and A. F. Kip, in *Low Temperature Physics LT9* (Plenum, New York, 1965), p. B818.

[3]T. W. Nee and R. E. Prange, Phys. Letters 25A, 582 (1969).

[4]R. E. Prange and T. W. Nee, Phys. Rev. 168, 779 (1968).

[5]T. W. Nee, J. F. Koch, and R. E. Prange, Phys. Rev. 174, 758 (1968).

[6]J. F. Koch and J. D. Jensen, Phys. Rev. 184, 643 (1969).

[7]J. F. Koch (private communication).

[8]J. F. Koch and R. E. Doezema, Phys. Rev. Letters 24, 507 (1970).

[9]J. F. Koch and T. E. Murray, Phys. Rev. 186, 722 (1969).

[10]R. E. Prange, Phys. Rev. 187, 894 (1969).

[11]S. P. Singhal, Nuovo Cimento (to be published).

[12]H. J. Fischbeck and J. Mertsching, Phys. Status Solidi 27, 345 (1968); and to be published.

[13]R. E. Prange, Phys. Rev. 171, 737 (1968); also M. S. Khaikin, Zh. Eksperim. i Teor. Fiz. 55, 1696 (1969) [Sov. Phys. JETP 28, 892 (1969)].

[14]R. E. Doezema, J. F. Koch, and U. Strom, Phys. Rev. 182, 7171 (1969).

[15]J. F. Koch (private communication).

[16]This is a somewhat oversimplified criterion. In the last section, a corrected statement will be made. We have assumed the field to be in the y direction.

[17]E. A. Kaner, N. M. Makarov, and I. M. Fuks, Zh. Eksperim. i Teor. Fiz. 55, 931 (1969) [Sov. Phys. JETP 28, 483 (1969)].

[18]S. P. Singhal, Ph. D. thesis (unpublished).

[19]R. E. Doezema (unpublished); J. F. Koch and C. C. Kuo, Phys. Rev. 143, 470 (1966).

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Energy Levels of Bloch Electrons in Magnetic Fields*

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From the calculation of the energy levels of conduction electrons in a simple model of a metal in a magnetic field three interesting results emerge. (a) Quantum corrections to Onsager's semiclassical quantization formula are found to be sufficiently small that the usual interpretation of the de Haas–van Alphen effect should provide an accurate measure of Fermi-surface cross sections in potassium. (b) The undetermined constant appearing in Onsager's formula is found to be $\frac{3}{4}$ for effects due to "lens" orbits in hexagonal metals when the magnetic field lies in the basal plane. (c) The quantization of energy levels in a variety of periodic open orbits is predicted to be observable in principle through cyclotron-resonance experiments in a suitable geometry in the intermediate magnetic-breakdown regime.

I. INTRODUCTION

One of the most useful concepts in the theory of metals is that of the quantization of the orbits of conduction electrons in a magnetic field. A semiclassical treatment due to Onsager[1] predicts that in the presence of a uniform magnetic field $\vec{B}$ the area $\vec{\mathfrak{a}}(\mathcal{E})$ in wave-number space of an allowed orbit is given by

$$\vec{\mathfrak{a}}(\mathcal{E}) = (n+\sigma)(2\pi e/\hbar c)\vec{B}\ , \qquad (1)$$

where n is an integer and σ is an unspecified constant. These orbits are intersections of surfaces of constant energy with planes perpendicular to $\vec{B}$.

More recently it has been found[2] that if $\vec{B}$ is large enough, the phenomenon known as magnetic breakdown can occur, resulting in tunneling of electrons from one of the semiclassically allowed orbits to another such orbit. Although calculations using this tunneling concept have provided results consistent with most observations of the de Haas–van Alphen and similar effects, such work does not provide an entirely satisfying description from a theoretical point of view. The phenomena involved depend upon the energy-level structure of electrons in a constant lattice potential and a constant magnetic field, and hence are describable in terms of the eigenstates of a time-independent Hamiltonian. It accordingly is of interest to investigate the energy-level structure that corresponds in the time-independent picture to the interpretation in terms of tunneling between orbits in the time-dependent description.

The difficulty of solving the Schrödinger equation for this problem makes it convenient for us to consider what we will call the "sandwich" model,[3] in which the lattice potential takes on the simple form $2V \cos gx$. We assume the magnetic field to be uniform and constant and to be acting in the z direction. There are then two major aspects to the calculation. The first question concerns the qualitative description of the energy-level structure as a function of the strength of the lattice potential. One is interested in the shift and regrouping of the energy levels of the quantized orbits of the free electrons as V is increased from zero to a value at which all magnetic breakdown has ceased. This part of the calculation does not readily yield to perturbation theory, and will be described in detail in a subsequent paper. In the present paper we address ourselves to the second, more delicate, question of the accuracy of the Onsager formula in the regime where the effect of the lattice potential is weak enough that perturbation theory may be used. We shall also determine the magnitude of the constant σ, and investigate the interpretation to be given of the Onsager formula for the case of periodic open orbits. The relevance of the sandwich model rests on two facts. First, in certain divalent metals having the hexagonal-close-packed crystal structure there are groups of electrons whose orbit topology and shape are dominated by a single Fourier component of the lattice potential. The sandwich model, which similarly exhibits lens-shaped and periodic open orbits, thus provides a reasonable model for interpreting some of the properties of a metal such as cadmium. Second, we shall find the quantum corrections to Onsager's formula for states in the first Brillouin zone of the sandwich model to be so small that one can safely predict a similar result for the more complicated lattice potential in potassium.

It is easily shown that for this model the Onsager area-quantization technique yields eigenvalues that may be written to second order in the lattice potential as

$$\mathcal{E}_n = (n+\tfrac{1}{2})\hbar\omega - \frac{V^2}{2\mathcal{E}_g[1-(n+\tfrac{1}{2})\hbar\omega/\mathcal{E}_g]}, \qquad (2)$$

where $\omega = |eB/mc|$ is the cyclotron frequency for an electron in the magnetic field alone, $\mathcal{E}_g \equiv \hbar^2(g/2)^2/2m$, and we have considered only energy levels such that $(n+\frac{1}{2})\hbar\omega/\mathcal{E}_g < 1$. The Onsager prescription is not immediately applicable to all energy levels in this model since the area enclosed by open orbits is not a well defined quantity.

Our purpose in this paper is to obtain an accurate closed-form expression for the energy levels in this simplified model to second order in the lattice potential. This exact expression involves an integral which will be evaluated by an asymptotic expansion technique to yield the energy levels in terms of elementary functions.

Several authors[4–7] have considered various parts of the energy-level structure for this model. Zilberman[4] evaluated the energy-level shift in terms of the overlap integral of two harmonic-oscillator states. The dominant terms in an asymptotic expansion of this integral were evaluated for the case of energy levels far below and far above the breakdown region. Pippard[5] considered this model from the standpoint of a network of coupled orbits; however, his method was designed specifically for evaluation of energy levels in the second zone. Reitz[6] discussed the first-order term, while Langbein[7] discussed both the first- and second-order terms, but only for energy levels far from the zone edge. In this paper we shall find closed-form expressions for the energy levels of this model in terms of elementary functions. These expressions will show clearly how the energy levels vary as we consider energies up to and through the zone edge. In our discussion we shall find the Onsager result, Eq. (2), as a first term in an asymptotic expansion for the energy-level corrections in the first zone. The second terms in this series will be evaluated to provide a measure of the accuracy of the semiclassical Onsager prescription.

II. PERTURBATION THEORY

We choose a gauge such that the vector potential is $A = (0,\ Bx,\ 0)$, in which case the Hamiltonian may be written as

$$\mathcal{H} = (1/2m)[p_x^2 + (p_y + m\omega x)^2 + p_z^2] + 2V\cos gx \ . \qquad (3)$$

In this gauge, p_y and p_z commute with $\mathcal{H}$, and so the problem is to find the eigenvalues $\mathcal{E}_x$ of the reduced Hamiltonian

$$\mathcal{H}_x = (1/2m)[p_x^2 + (\hbar k_y + m\omega x)^2] + 2V\cos gx \ . \qquad (4)$$

The eigenvalues of $\mathcal{H}$ may be written as

$$\mathcal{E} = \mathcal{E}_x + \hbar^2 k_z^2/2m \ . \qquad (5)$$

The eigenfunctions of the unperturbed Hamiltonian $\mathcal{H}_x^{(0)}$ in which V is put equal to zero may be written as

$$\phi_n(x) = (m\omega/\hbar)^{1/4} X_n[(m\omega/\hbar)^{1/2}(x-x_0)], \qquad (6)$$

where $x_0 = -\hbar k_y/m\omega$ and the $X_n(x)$ are dimensionless harmonic-oscillator functions defined in terms of Hermite polynomials H_n as

$$X_n(\rho) = \frac{2^{-n/2}}{(n!)^{1/2}\pi^{1/4}} e^{-\rho^2/2} H_n(\rho) \ . \qquad (7)$$

The eigenvalues of $\mathcal{H}_x^{(0)}$ are $\mathcal{E}_n = (n+\frac{1}{2})\hbar\omega$, the standard harmonic-oscillator energy levels, and are degenerate with respect to k_y.

In this representation we may write the matrix elements of the perturbing potential as convolution integrals of the form

$$V_{nm} = \Re 2 V e^{i[gx_0 + 1/2(m-n)\pi]} \int_{-\infty}^{\infty} X_n(\rho) \times X_m(\rho - (2\gamma)^{1/2})\, d\rho\ , \quad (8)$$

where

$$\gamma \equiv 4\mathcal{E}_g/\hbar\omega\ .$$

Upon integration of (8) we obtain

$$V_{nm} = 2V\cos[gx_0 + \tfrac{1}{2}(m-n)\pi]\,(n!/m!)^{1/2} \times e^{-\gamma/2}\gamma^{1/2(m-n)} L_n^{(m-n)}(\gamma)\ , \quad (9)$$

where $L_n^{(m-n)}(\gamma)$ is the associated Laguerre polynomial defined[8] as

$$L_n^{(\alpha)}(\gamma) = \sum_{m=0}^{n} \binom{n+\alpha}{n-m} \frac{(-\gamma)^m}{m!}\ . \quad (10)$$

It would now be formally possible to evaluate the perturbed energy levels to any order in V. The situations of experimental interest, however, are those where $\mathcal{E}_g$ and $\mathcal{E}_n$ are much greater than either $\hbar\omega$ or the effective lattice strength V. This being the case we shall consider only the first terms in a perturbation-series expansion of the energy. From the expression for the matrix elements in terms of an overlap integral it is clear that the first-order term in V will be exponentially small in the first zone, and so we must retain terms to second order in the lattice potential in order to effect a comparison with the Onsager result, Eq. (2).

Using the standard perturbation-theory formalism we write the energy levels as

$$\mathcal{E}_n = (n+\tfrac{1}{2})\hbar\omega + \Delta\mathcal{E}_1 + \Delta\mathcal{E}_2\ , \quad (11)$$

where

$$\Delta\mathcal{E}_1 = 2V\cos gx_0\, e^{-\gamma/2} L_n(\gamma)\ , \quad (12)$$

$$\Delta\mathcal{E}_2 = \frac{2V^2}{\hbar\omega} \sum_{m(\neq n)} \left(\frac{n!}{m!}\right) e^{-\gamma} \frac{\gamma^{m-n}}{n-m} [L_n^{(m-n)}(\gamma)]^2 \times [1 + (-1)^{m-n}\cos 2gx_0]\ . \quad (13)$$

From Eq. (13) we see that the second-order contribution to the energy may be considered to consist of an energy-shift term and a bandwidth term, the latter coming from the lifting of the k_y degeneracy by the lattice potential. We shall denote the energy-shift term as $\Delta\mathcal{E}_s$ and the bandwidth term as $\Delta\mathcal{E}_b$ and write

$$\Delta\mathcal{E}_2 = \Delta\mathcal{E}_s + \Delta\mathcal{E}_b \cos 2gx_0\ . \quad (14)$$

It will now be convenient to evaluate the various components of $\Delta\mathcal{E}$ as an asymptotic expansion in powers of the small parameter $1/\gamma$ and as functions of the parameter R defined by the equation

$$R = (n+\tfrac{1}{2})\hbar\omega/\mathcal{E}_g\ .$$

It will be found that the Onsager result is the zero-order term in such an expansion for the energy levels in the first Brillouin zone. An asymptotic expansion for $\Delta\mathcal{E}_1$ may be found in any one of several texts[9] and may be summarized in the following equations. For

$$\tfrac{1}{2}\psi = \operatorname{arccosh} R^{-1/2}\ , \quad R < 1$$

we find

$$\Delta\mathcal{E}_1 = \frac{(-1)^n 2V\cos gx_0}{(2\pi\gamma)^{1/2}(1-R)^{1/4}} \times \{\exp[-\tfrac{1}{2}\gamma(\tanh\tfrac{1}{2}\psi - \tfrac{1}{2}R\psi)]\}[1 + O(\gamma^{-1})]; \quad (15a)$$

for

$$\tfrac{1}{2}\phi = \arccos R^{-1/2}\ , \quad R > 1$$

we find

$$\Delta\mathcal{E}_1 = \frac{(-1)^n 4V\cos gx_0}{(2\pi\gamma)^{1/2}(R-1)^{1/4}} \times \left\{\sin[\tfrac{1}{2}\gamma(\tfrac{1}{2}R\phi - \tan\tfrac{1}{2}\phi) + \tfrac{1}{4}\pi] + \frac{1}{\gamma R^{1/2}}\, O(1)\right\}\ ; \quad (15b)$$

for

$$t = \gamma^{2/3}(\tfrac{4}{3}R)^{-1/3}(1-R)\ , \quad R \sim 1$$

we find

$$\Delta\mathcal{E}_1 = \frac{(-1)^n 2V\cos gx_0}{\pi}\left(\frac{6}{R\gamma}\right)^{1/3}[\mathrm{Ai}(t) + O(\gamma^{-2/3})]\ . \quad (15c)$$

Here $\mathrm{Ai}(t)$ is the Airy function.[10]

Since the Onsager result contains no terms of first order in V we expect $\Delta\mathcal{E}_1$ to be negligibly small in the first Brillouin zone. That this is the case is clear from the exponential dependence of $\Delta\mathcal{E}_1$ on the large parameter γ in Eq. (15a). We shall accordingly replace this term by zero in the calculations that follow.

In the second zone, the first-order terms are expressed as oscillatory functions. The physical significance of the argument in (15b) has previously been pointed out.[6] This quantity is directly related to the area $\mathfrak{a}_l$ in k space of the "lens orbit," which is represented as the shaded region in Fig. 1, and which is given by the equation

$$\mathfrak{a}_l = (m\omega/\hbar)\gamma(\tfrac{1}{2}R\phi - \tan\tfrac{1}{2}\phi)\ . \quad (16)$$

The argument of the sine function in Eq. (15b) is thus

$$\hbar\mathfrak{a}_l/2m\omega + \tfrac{1}{4}\pi\ .$$

The region where the unperturbed energy levels approach the zone edge is of considerable interest. In this region the first-order energy correction increases monotonically from essentially zero for

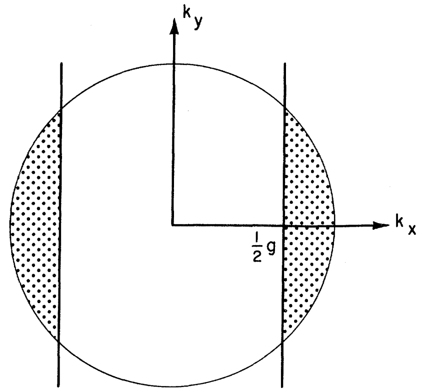

FIG. 1. Shaded areas combine to form "lens orbit" in k space.

$R<1$ to a maximum for R very close to unity, and then oscillates with continuously decreasing amplitude until it merges with the asymptotic form for $R>1$. In this region the convergence of the perturbation series is unfortunately less rapid than elsewhere, as may be seen by comparing the three expressions in Eqs. (15). For energy levels far from the zone edge the magnitude of the matrix elements is dominated by the term $V\gamma^{-1/2}$ while near the band edge the corresponding term is $V\gamma^{-1/3}$.

Asymptotic expansions for $\Delta\mathcal{E}_2$ may be obtained as follows. It is shown in the Appendix that $\Delta\mathcal{E}_s$ and $\Delta\mathcal{E}_b$ may be written in the form

$$\Delta\mathcal{E}_s=\frac{V^2}{\pi\hbar\omega}\,\mathcal{R}\int_0^\pi(\pi-\sigma)\exp[-i\gamma(\cot\sigma+\tfrac{1}{2}R\sigma)]\times\csc\sigma H_0^{(1)}(\gamma\csc\sigma)\,d\sigma\,, \quad (17a)$$

$$\Delta\mathcal{E}_b=\frac{-V^2}{\pi\hbar\omega}\,\mathcal{R}\int_0^\pi\sigma\exp[-i\gamma(\cot\sigma+\tfrac{1}{2}R\sigma)]\times\csc\sigma H_0^{(1)}(\gamma\csc\sigma)\,d\sigma\,, \quad (17b)$$

where $H_0^{(1)}(x)$ is the Hankel function of the first kind. Since the expressions for $\Delta\mathcal{E}_s$ and $\Delta\mathcal{E}_b$ are so similar that the techniques used to evaluate one will suffice to evaluate the other, we will consider only $\Delta\mathcal{E}_s$ in detail. In the region of interest for γ and σ, the Hankel function in the expression for $\Delta\mathcal{E}_s$ may be written[8]

$$H_0^{(1)}(z)=\left(\frac{2}{\pi z}\right)^{1/2}e^{i(z-\pi/4)}\left(\sum_{k=0}^{n-1}\frac{(-1)^k\Gamma(k+\frac{1}{2})}{(2iz)^k\Gamma(-k+\frac{1}{2})}+\theta_1\frac{(-1)^n\Gamma(n+\frac{1}{2})}{(2iz)^n\Gamma(-n+\frac{1}{2})}\right)\,, \quad (18)$$

where θ_1 is a constant of modulus less than unity.

Using Eq. (18) in Eq. (17a) we may write

$$\Delta\mathcal{E}_s=\frac{-4V^2}{(2\pi)^{3/2}\hbar\omega\gamma^{1/2}}\times g\,e^{i\pi/4}\left(I_0-\frac{i}{8\gamma}I_1-\frac{9}{128\gamma^2}I_2+\cdots\right)\,, \quad (19)$$

where the integrals I_m are defined by

$$I_m=\int_0^\pi(\pi-\sigma)\sin^{m-1/2}\sigma\,e^{\gamma f(\sigma)}\,d\sigma \quad (20)$$

with

$$f(\sigma)=i(\tan\tfrac{1}{2}\sigma-\tfrac{1}{2}R\sigma)\,. \quad (21)$$

We note that $f(\sigma)$ has a saddle point at $\sec\frac{1}{2}\sigma=\pm R^{1/2}$ with a corresponding second derivative of $\pm\frac{1}{2}iR\times(R-1)^{1/2}$. As was the situation for the first-order term, one must consider the three cases $R<1$, $R>1$, and $R\sim 1$, with each having a different asymptotic form.

For $R<1$ we observe that along the path C shown in Fig. 2, $f(\sigma)$ decreases monotonically from zero at the origin to $-\infty$ at $\sigma=\pi$. In this case the dominant contribution to I_m comes from the region near the origin and it is not necessary to consider the contribution from the saddle-point region. We find

$$I_m=i^{m+1/2}\left(\frac{2}{\gamma(1-R)}\right)^{m+1/2}\times\left\{\pi\Gamma(m+\tfrac{1}{2})-\frac{2i}{\gamma(1-R)}\left[\Gamma(m+\tfrac{3}{2})+O\left(\frac{1}{\gamma^2}\right)\right]+\frac{1}{\gamma^2}\left(\frac{\Gamma(m+\frac{7}{2})}{3(1-R)^3}-\frac{(1-2m)}{3}\,\frac{(m+\frac{5}{2})}{(1-R)^2}\right)+O\left(\frac{1}{\gamma^4}\right)\right\}\,. \quad (22)$$

Using Eq. (22) in Eq. (19) we have

$$\Delta\mathcal{E}_s=\frac{-2V^2}{\hbar\omega\gamma(1-R)^{1/2}}\left[1+\frac{1}{8\gamma^2(1-R)^3}\times[5-2(1-R)+(1-R)^2]+O\left(\frac{1}{\gamma^4}\right)\right]\,. \quad (23)$$

In Eq. (23) we have calculated the second term in the asymptotic series in order to obtain a correction term to the semiclassical result. For the remaining cases we shall retain only the dominant asymptotic term.

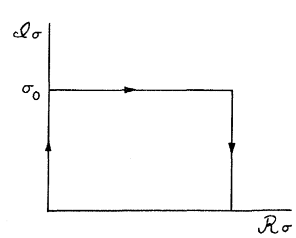

FIG. 2. Contour for integration in Eq. (20) for $R<1$. Here $\sigma_0=2\,\mathrm{arccosh}\,R^{-1/2}$.

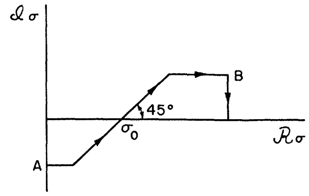

FIG. 3. Contour for integration in Eq. (20) for $R>1$. Now $\sigma_0 = 2\arccos R^{-1/2}$.

For $R>1$ there is a non-negligible contribution from the saddle point on the real axis at $\sec^2 \frac{1}{2}\sigma = R$, as well as from the region near the origin. We choose the path shown in Fig. 3 for this integration and observe that along this path $\Re f(\sigma)$ decreases monotonically from the origin to point A, rises through a maximum at the saddle point, then decreases monotonically from B to π. Denoting the contributions to I_m from the region near the origin as $I_m^{(1)}$ and from the saddle-point region as $I_m^{(2)}$, we find

$$I_m^{(1)} = (-i)^{m+1/2}\left(\frac{2}{\gamma(R-1)}\right)^{m+1/2}\left[\pi\Gamma(m+\tfrac{1}{2}) + O\left(\frac{1}{\gamma}\right)\right], \tag{24}$$

$$I_m^{(2)} = \frac{2\sqrt{\pi}}{(\gamma R)^{1/2}(R-1)^{1/4}}\left(\frac{R}{2(R-1)^{1/2}}\right)^{1/2-m} \times e^{i[\gamma(\tan(\phi/2)-R\phi/2)+\pi/4]}(\pi-\phi)\left[(1+O)\left(\frac{1}{\gamma}\right)\right], \tag{25}$$

where, as before, $\frac{1}{2}\phi = \arccos(R^{-1/2})$. Substituting into Eq. (19) we have

$$\Delta\mathcal{E}_s = \frac{-2V^2}{\hbar\omega\gamma(R-1)^{1/2}} \times\left[\left(\frac{\pi-\phi}{\pi}\right)\cos[\gamma(\tfrac{1}{2}R\phi - \tan\tfrac{1}{2}\phi)] + O\left(\frac{1}{\gamma}\right)\right]. \tag{26}$$

In the region where $R\sim 1$ the above expansions fail. This is indicated by the divergence of Eq. (23) and Eq. (26) as R approaches unity. For this case we choose the path of integration shown in Fig. 4, and express the resulting asymptotic form as an integral,

$$I_m = \pi\left(\frac{24}{\gamma}\right)^{(2m+1)/6} e^{(2m+1)\pi i/12}\left\{\int_0^\infty y^{m-1/2}\left[1-\left(\frac{24}{\gamma}\right)^{1/3}\frac{e^{i\pi/6}}{\pi}y\right]\exp\left[\gamma(1-R)\left(\frac{3}{\gamma}\right)^{1/3} y\, e^{2\pi i/3} - y^3\right]dy + O\left(\frac{1}{\gamma^{1/3}}\right)\right\}. \tag{27}$$

Substituting into Eq. (19) we obtain

$$\Delta\mathcal{E}_s = \frac{-2V^2}{\hbar\omega\gamma^{2/3}}(3)^{1/6} g\,\frac{e^{i\pi/3}}{\sqrt{\pi}}\left\{\int_0^\infty \frac{1}{\sqrt{y}}\left[1-\left(\frac{24}{\gamma}\right)^{1/3}\frac{e^{i\pi/6}}{\pi}y\right]\exp\left[\gamma(1-R)\left(\frac{3}{\gamma}\right)^{1/3} e^{2\pi i/3}y - y^3\right]dy + O\left(\frac{1}{\gamma^{1/3}}\right)\right\}. \tag{28}$$

The remaining integral in Eq. (28) is very similar in form to the Airy function,[10] and it may be shown by standard asymptotic techniques that this integral does approach the dominant terms in Eqs. (23) and (26) for $R<1$ and $R>1$, respectively. For our purposes it will suffice to note that this integral decays monotonically to the dominant term in Eq. (23) for $R<1$ and oscillates with decreasing amplitude for $R>1$. We also note that the value of $\Delta\mathcal{E}_s$ for an energy level just at the band edge, i.e., where $R=1$, is

$$\Delta\mathcal{E}_s = -V^2\Gamma(\tfrac{1}{6})/\sqrt{3}\,\hbar\omega\gamma^{2/3}. \tag{29}$$

The bandwidth terms may be obtained with the same contours in the complex plane as were used for $\Delta\mathcal{E}_s$. The results are

$$\Delta\mathcal{E}_b = 0, \qquad R<1 \tag{30a}$$

$$\Delta\mathcal{E}_b = \frac{2V^2}{\hbar\omega\gamma(R-1)^{1/2}}\left\{\frac{\phi}{\pi}\cos\left[\gamma\left(\frac{R\phi}{2}-\tan\frac{\phi}{2}\right)\right] + O\left(\frac{1}{\gamma}\right)\right\}, \qquad R>1 \tag{30b}$$

$$\Delta\mathcal{E}_b = \frac{4V^2\sqrt{3}}{\hbar\omega\pi\gamma}\left\{\Re\int_0^\infty y^{1/2} \times\exp\left[\gamma(1-R)\left(\frac{3}{\gamma}\right)^{1/3} e^{2\pi i/3} - y^3\right]dy + O(\gamma^{-1/3})\right\}, \qquad R\sim 1. \tag{30c}$$

An important point to note is that the bandwidth term is of the same order of smallness as $\Delta\mathcal{E}_1$ for $R<1$. The integral in (30c) has an exponential decrease for $R<1$ in contrast to the energy-shift term, which drops off only as $(1-R)^{-1/2}$ for $R<1$.

If we retain only the first terms in each series, we have for the second-order contributions to the energy in the three cases

$$\Delta\mathcal{E}_2 = -2V^2/\hbar\omega\gamma(1-R)^{1/2}, \qquad R<1 \tag{31a}$$

$$\Delta\mathcal{E}_2 = -2V^2/\hbar\omega\gamma(R-1)^{1/2} \times\left(1-(1+\cos 2gx_0)\frac{\phi}{\pi}\right)\cos\left[\gamma\left(\frac{R\phi}{2}-\tan\frac{\phi}{2}\right)\right], \qquad R>1 \tag{31b}$$

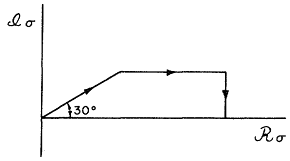

FIG. 4. Contour for integration in Eq. (20) for $R \sim 1$.

$$\Delta\mathcal{E}_2 = \frac{-2V^2}{\hbar\omega\gamma^{2/3}}(3)^{1/6} g \frac{e^{i\pi/3}}{\sqrt{\pi}} \times \left\{ \int_0^\infty \left[1-(1+\cos 2gx_0)\left(\frac{24}{\gamma}\right)^{1/3}\frac{e^{i\pi/6}}{\pi}\, y\right] \times y^{-1/2}\exp\left[\gamma(1-R)\left(\frac{3}{\gamma}\right)^{1/3} y\, e^{2\pi i/3} - y^3\right] dy \right\}, \quad R\sim 1 . \qquad (31c)$$

III. DISCUSSION

From Eqs. (15) and Eqs. (31) we can see clearly just how the energy levels are affected by the lattice perturbation as we consider the three cases corresponding to energies of states in the first zone, near the zone edge, and in the second zone. In the first zone the first-order perturbation term is negligibly small, as is the second-order bandwidth term. The resulting energy levels for this region are

$$\mathcal{E}_n = (n+\tfrac{1}{2})\hbar\omega - 2V^2/\hbar\omega\gamma(1-R)^{1/2}. \qquad (32)$$

We note that the parameter that effectively determines the ratio of energy-level shift to the spacing of the unperturbed levels is $V/(\hbar\omega\mathcal{E}_g)^{1/2}$. This is the same parameter discussed by Blount[11] in connection with the magnetic-breakdown problem. We also notice that the correction term in Eq. (32) that we have obtained as a first term in the asymptotic expansion of the perturbation series is the same as the semiclassical Onsager result, Eq. (2). Referring back to Eq. (23) we see that the corrections to the Onsager relation are smaller by a factor of $1/\gamma^2$ than the corresponding Onsager term. Since γ is large in most practical situations, it is clear that the Onsager prescription is entirely adequate to interpret experiments concerned with energy levels in the first Brillouin zone. It has been speculated that even in situations where one would think the Onsager relation to be quite valid, as is the case in the first Brillouin zone, it may be that deviations from the Onsager result are large enough to affect the interpretation of very precise measurements. One case where this possibility arises is in recent precision measurements of the Fermi surface of potassium,[12] where deviations from the free-electron sphere have been interpreted as a possible indication of a spin- or charge-density wave ground state for the alkali metals rather than the free-electron ground state. For purposes of calculation we have considered the alkali metals Na and K, and assumed that we may use the lowest nonzero Fourier component of the crystal potential for $V(\vec{r})$. The values used for V are those given by Ziman.[13] With these values the corrections to the Onsager relation are calculated to be less than one part in 10^7 in a field of 50 kG.

This result is in qualitative agreement with the conclusions arrived at by Roth[14] from a semiclassical approach. We note, however, that, unlike Roth's treatment of the problem, the present calculation is not a power-series development in the strength of the magnetic field, in that the Landau levels themselves form the unperturbed states.

For a polyvalent metal we are interested in energies equivalent to those of Bloch states in the second Brillouin zone, and so must in that case consider the situation where $R>1$. The energy of the nth state is then given by the expression

$$\mathcal{E}_n = (n+\tfrac{1}{2})\hbar\omega + (-1)^n 2V \times \cos gx_0 \left(\frac{2}{\pi\gamma}\right)^{1/2}\frac{1}{(R-1)^{1/4}}\sin\left(\frac{\hbar\mathcal{A}_l}{2m\omega}+\frac{\pi}{4}\right) - \frac{2V^2}{\hbar\omega\gamma(R-1)^{1/2}}\left(\frac{\pi-\phi}{\pi}-\frac{\phi}{\pi}\cos 2gx_0\right)\cos\left(\frac{\hbar\mathcal{A}_l}{m\omega}\right), \qquad (33)$$

where we have used Eq. (16) for the area $\mathcal{A}_l$ of the "lens" orbit. In order to understand the physical significance of this rather complicated expres-

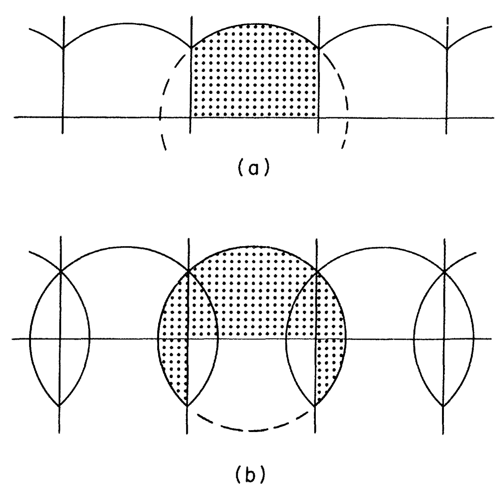

FIG. 5. Two types of periodic open orbit. Shaded area is quantized.

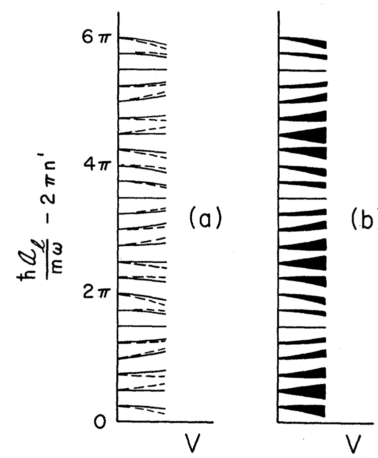

FIG. 6. Energy-level spectrum as a function of strength V of lattice potential. Diagram (a) shows levels for one particular value of k_0, and exhibits periodicities due to periodic open and lens orbits. Total spectrum (b) shows only lens-orbit periodicity.

sion, we first ignore the first- and second-order bandwidth terms (i.e., those containing a factor of $\cos gx_0$ or $\cos 2gx_0$) and concentrate on the energy-shift term $\mathcal{E}_s$. The first point we note is that the energy changes are such as to introduce a new periodicity into the density of states that is in accord with the Onsager formula for the lens orbits. Whereas in the absence of a lattice potential the levels were uniformly spaced with separation $\hbar\omega$, the presence of a nonzero potential induces a clustering of levels around those energies where the maxima of $-d\mathcal{E}/dn$ occur. The condition for such maxima is seen from expression (33) to be that with n' an integer

$$\mathfrak{A}_l = (2\pi m\omega/\hbar)(n' + \tfrac{3}{4}) \ ,$$

which is in accord with the Onsager formula for the quantization of the lens orbit when the constant σ is chosen to be three-quarters. The fact that $\mathfrak{A}_l$ is the area of the lens orbit in a remapped free-electron construction rather than in a nearly free-electron approximation[15] is not significant, since such corrections to $\mathfrak{A}_l$ can only occur in higher terms of the perturbation series.

This value of σ does not appear to have been found in any previous work. Semiclassical treatments[5,14] are inherently incapable of answering such delicate questions, while the exact computations of Butler and Brown[16] involved a tight-binding model in which no lenslike orbits existed.

The first-order bandwidth term introduces some additional periodicities into the energy spectrum. Let us consider, for example, the particular case where $x_0 = 0$. If the lens orbit were very small, so that $\sin(\hbar\mathfrak{A}_l/2m\omega + \frac{1}{4}\pi)$ could be considered a slowly varying function of n, then the factor of $(-1)^n$ would cause alternate terms to have opposite signs; the energy levels would then be drawn together in pairs and a period of $2\hbar\omega$ would appear in the energy spectrum for this value of x_0. More generally this term can be written as proportional to

$$(-1)^n \sin\left(\frac{\hbar\mathfrak{A}_l}{2m\omega} + \frac{\pi}{4}\right) \propto \exp\left(in\pi \pm \frac{in\hbar}{2m\omega}\,\frac{d\mathfrak{A}_l}{dn}\right),$$

from which the period is seen to be

$$\left(\frac{1}{2\hbar\omega} \pm \frac{1}{4\pi m\omega^2}\,\frac{d\mathfrak{A}_l}{dn}\right)^{-1} . \qquad (34)$$

This result represents an extension of the Onsager formula in that it predicts a quantization associated with the periodic open orbits. The two possible forms of expression (34) correspond to the periodic orbits shown in Fig. 5, the negative sign leading to the orbit of Fig. 5(a); here the shaded area is to be quantized following the Onsager prescription. One might now imagine a cyclotron-resonance experiment to be performed in such a geometry that no transitions were possible between states of different k_y (this would be the case if the electric field vector of the incident microwaves were in the x direction). Transitions would then occur only within the family of levels associated with a particular value of x_0, and resonance would be observed at the photon energy given in expression (34).

A de Haas–van Alphen experiment, on the other hand, in which the total energy spectrum for all k_y is investigated, would not be capable of detecting the presence of periodic open orbits,[17] for the factor of $\cos gx_0$ is capable of being negative as well as positive and then contributes a term of the same period but opposite phase to the one considered in the previous paragraph.

This picture of the energy-level structure is summarized in Fig. 6. In the left-hand half of this diagram the energy levels are plotted with neglect of the bandwidth term as solid lines, and for the case where $\cos gx_0 = 1$ as dashed lines, as functions of the strength V of the lattice potential. In Fig. 6(b) the total spectrum is shown, and is seen to differ from Fig. 6(a) in that no period corresponding to open orbits is discernible.

The extension of these results to the case of large V requires methods different from those employed in this paper, and will be described elsewhere.[18] It suffices to say that the sandwich model, whose Schrödinger equation may be reduced to a one-dimensional description, is guilty of only a minimum of the anfractuosity attributed by Pippard[19] to all models of magnetic breakdown.

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APPENDIX

The integral representations (17a) and (17b) will be obtained from Eq. (13) in this appendix. We define the sums

$$S(n,\delta)=\sum_{m\neq n}\delta^{m-n}\,\frac{n!}{m!}\,e^{-\gamma}\gamma^{m-n}\,\frac{[L_n^{(m-n)}(\gamma)]^2}{m-n}\quad,$$

$$T(z,\delta)=\sum_{n=0}^{\infty}S(n,\delta)z^n\,,$$

where δ can be either $+1$ or -1. The quantities $\Delta\mathcal{E}_s$ and $\Delta\mathcal{E}_b$ defined in Eqs. (13) and (14) may then be written as integrals of $T(z,\delta)$ in the form

$$\Delta\mathcal{E}_s=\frac{V^2}{\pi i\hbar\omega}\int_C z^{-n-1}\,T(z,1)\,dz\;, \tag{A1}$$

$$\Delta\mathcal{E}_b=\frac{V^2}{\pi i\hbar\omega}\int_C z^{-n-1}\,T(z,-1)\,dz\;, \tag{A2}$$

where C is a closed contour containing the origin in the z plane. Using standard identities for sums of Laguerre polynomials,[10] $T(z,\delta)$ may be written as

$$T(z,\delta)=\frac{e^{-\gamma(1+z)/(1-z)}}{1-z}\sum_{\alpha=1}^{\infty}\frac{z^{\alpha/2}-z^{-\alpha/2}}{\alpha}\,\delta^{\alpha}I_{\alpha}\!\left(\frac{2\gamma\sqrt{z}}{1-z}\right),$$

with I_α the modified Bessel function[9] of order α. Making use of the Bessel-function identity

$$\sum\nolimits_{\alpha}x^{\alpha}I_{\alpha}(y)=e^{(y/2)(x+1/x)}\;,$$

we express $T(z,\delta)$ as

$$T(z,\delta)=\frac{e^{-\gamma(1+z)/(1-z)}}{1-z}\,\ln\sqrt{z}\times\int_0^1\exp\left(\frac{2\gamma\delta\sqrt{z}}{1-z}\cosh y\,\ln\sqrt{z}\right)dy-I_0\!\left(\frac{2\gamma\sqrt{z}}{1-z}\right)\Bigg]\;.$$

We then need to evaluate the integrals

$$K(\delta)=\int_C z^{-n-1}\,T(z,\delta)\,dz\;.$$

We choose a path in the z plane where $z=e^{i\sigma}$ for $0<\sigma\leq 2\pi$. Then

$$K(\delta)=-i\int_0^{\pi}\csc\sigma\, e^{-i\gamma(\cot\sigma+R\sigma/2)}\times\left[\int_0^{\sigma}e^{i\delta\gamma\csc\sigma\cos y}dy-\sigma J_0(\gamma\csc\sigma)\right]d\sigma\;.$$

We consider first the integral

$$M=\int_0^{\sigma}e^{i\delta\gamma\csc\sigma\cos y}dy\,,$$

let $y=\xi+i\eta$, and choose a path composed of the segments

$$y=i\eta\qquad(0\geq\eta\geq-\infty),$$
$$y=\xi-i\infty\qquad(0\leq\xi\leq\sigma),$$
$$y=\sigma+i\eta\qquad(-\infty\leq\eta\leq 0).$$

Then

$$M=-i\int_0^{\infty}e^{i\delta\gamma\csc\sigma\cosh\eta}d\eta+i\int_0^{\infty}e^{i\delta\gamma\cot\sigma\cosh\eta-\gamma\sinh\eta}d\eta\,. \tag{A3}$$

The contribution of the second term in (A3) to $K(\delta)$ may be shown to vanish as follows. We write this term as

$$M_1=\mathscr{I}\int_0^{\pi/2}\csc\sigma\; e^{-i\gamma(\cot\sigma+R\sigma/2)}\times\int_0^{\infty}e^{i\delta\gamma\cot\sigma\cosh\eta-\gamma\sinh\eta}d\eta\, d\sigma\;. \tag{A4}$$

We choose the path of integration for σ to be composed of the segments

(a) $\sigma=-i\,\delta p\qquad(0\leq p\leq y),$

(b) $\sigma=r-i\,\delta y\qquad(0\leq r\leq\tfrac{1}{2}\pi),$

(c) $\sigma=\tfrac{1}{2}\pi+i\delta p\qquad(y\geq p\geq 0),$

where y is a constant. Along segment (a) the integral in (A4) is real, so there is no contribution to M_1. Along segment (b) we take the limit $y\to\infty$ to obtain the contribution

$$M_1^{(b)}=\frac{e^{\delta\gamma-(1+\gamma R\delta/2)y}}{\pi(\delta+\frac{1}{2}\gamma R)}\,[\sin\tfrac{1}{2}\pi(\delta+\tfrac{1}{2}R\gamma]\times\int_0^{\infty}e^{-\gamma\delta\cosh\eta-\gamma\sinh\eta}d\eta\,.$$

The definitions of R and γ may now be used to show that $\frac{1}{4}R\gamma\pi=(n+\frac{1}{2})\pi$, so that $M_1^{(b)}$ is zero. Along segment (c) the contribution to (A4) is

$$M_1^{(c)}=\frac{-1}{\pi}\cos\left(\frac{\gamma R\pi}{4}\right)\times\int_0^{y}e^{\gamma\delta(-\tanh p+Rp/2)}\int_0^{\infty}e^{\gamma\tanh p\cosh\eta-\gamma\sinh\eta}d\eta\,dp.$$

Again using $\frac{1}{4}R\gamma\pi=(n+\frac{1}{2})\pi$ we find that segment (c) yields no contribution to M_1.

We now return to (A4) and use the results of the above discussion to write

$$K(\delta)=-i\int_0^{\pi}\csc\sigma\, e^{-i\gamma(\cot\sigma+R\sigma/2)}\times\left[-i\int_0^{\infty}e^{i\delta\gamma\csc\sigma\cosh\eta}d\eta-\sigma J_0(\gamma\csc\sigma)\right]d\sigma\,.$$

The Bessel-function integral representation

$$J_0(x) = \frac{-i}{\pi} \int_0^\infty (e^{ix\cosh\eta} - e^{-ix\cosh\eta})\, d\eta$$

may now be used to show

$$K(1) = 2i\mathcal{J} \int_0^\pi \csc\sigma\, e^{-i\gamma(\cot\sigma + R\sigma/2)} \times \left(\frac{\pi-\sigma}{\pi}\right) \int_0^\infty e^{i\gamma\csc\sigma\cosh\eta}\, d\sigma\, d\eta\,,$$

$$K(-1) = -2i\mathcal{J} \int_0^\pi \csc\sigma\, e^{-i\gamma(\cot\sigma + R\sigma/2)} \times \frac{\sigma}{\pi} \int_0^\pi e^{i\gamma\csc\sigma\cosh\eta}\, d\sigma\, d\eta\,.$$

Using[8]

$$\int_0^\infty e^{ix\cosh y}\, dy = \tfrac{1}{2} i\pi H_0^{(1)}(x)$$

with (A1) and (A2) we have

$$\Delta\mathcal{E}_s = \frac{V^2}{\hbar\omega\pi} \mathcal{R} \int_0^\pi \csc\sigma\, e^{-i\gamma(\cot\sigma + R\sigma/2)} \times (\pi - \sigma) H_0^{(1)}(\gamma\csc\sigma)\, d\sigma$$

$$\Delta\mathcal{E}_b = \frac{-V^2}{\hbar\omega\pi} \mathcal{R} \int_0^\pi \csc\sigma\, e^{-i\gamma(\cot\sigma + R\sigma/2)} \times \sigma H_0^{(1)}(\gamma\csc\sigma)\, d\sigma\,.$$

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[1]L. Onsager, Phil. Mag. 43, 1006 (1952).

[2]L. Falicov and M. Cohen, Phys. Rev. Letters 7, 231 (1961).

[3]P. L. Taylor, *A Quantum Approach to the Solid State* (Prentice-Hall, Englewood Cliffs, N. J., 1970), Chap. 4.

[4]G. Zil'berman, Zh. Eksperim. i Teor. Fiz. 30, 1092 (1956) [Sov. Phys. JETP 3, 835 (1957)].

[5]A. B. Pippard, Proc. Roy. Soc. (London) A270, 16 (1962).

[6]J. R. Reitz, J. Phys. Chem. Solids 25, 53 (1964).

[7]D. Langbein, Phys. Rev. 180, 633 (1969).

[8]I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series, and Products* (Academic, New York, 1965).

[9]G. Szego, *Orthagonal Polynomials* (American Mathematical Society Colloquium Publications, New York, 1939), Vol. 33; *Higher Transcendental Functions*, edited by A. Erdelyi (McGraw-Hill, New York, 1953).

[10]G. N. Watson, *A Treatise on the Theory of Bessel Functions* (Cambridge U. P., London, 1944).

[11]E. I. Blount, Phys. Rev. 126, 1636 (1962).

[12]R. L. Thomas and G. Turner, Phys. Rev. 176, 768 (1968); S. A. Werner, E. Gürmen, and A. Arrott, *ibid.* 186, 705 (1969).

[13]J. M. Ziman, Phil. Mag. 6, 1013 (1961).

[14]L. M. Roth, Phys. Rev. 145, 434 (1966).

[15]These terms are defined in such texts as Ref. 3.

[16]F. A. Butler and E. Brown, Phys. Rev. 166, 630 (1968); E. Brown, Solid State Phys. 22, 313 (1968).

[17]A conjecture to this effect was made by Pippard on intuitive grounds in *Low Temperature Physics*, edited by C. DeWitt (Gordon and Breach, New York, 1962).

[18]H. H. Hosack and P. L. Taylor, Bull. Am. Phys. Soc. 14, 366 (1969); and (to be published).

[19]A. B. Pippard, Phil. Trans. Roy. Soc. London A256, 317 (1964).