Quasiclassical quantization in a magnetic field for matrix Hamiltonians

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The Keller-Rubinow method is used to examine the form of wave functions. Equations for the g-factor are found in the quasiclassical approximation. An expression is obtained for the electron magnetic moment operator. Quantization in a complex valence band of cubic semiconductors is discussed as an example.

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1. There are many problems in quantum mechanics that involve a matrix Hamiltonian. In particular, this includes problems on the behavior of charge carriers in semiconductors and metals in complex bands or in those cases where the coupling between a number of bands must be taken into account. In this paper, we examine quasiclassical quantization in magnetic fields in such cases. A similar problem was previously solved by Falkovskiĭ,[1] who calculated the effective g-factor for bismuth. However, in this particular case, the set of equations that is satisfied by the wave functions for the Kramers-degenerate (without the magnetic field) states is separable, which does not occur in other cases. To some extent, the present work is a generalization of work reported in Ref. 1.

The form of the eigenfunctions turns out to be a nontrivial question, especially when the particle orbit has concave segments. We shall use the Keller-Rubinow method,[2–4] which will enable us to solve this problem in a simple form that is easy to interpret.

Quantization in a complex valence band of a cubic semiconductor described by the Luttinger Hamiltonian is discussed as an example.

2. Let the Schrödinger equation be

$$[\hat{\mathscr{H}}(\mathbf{P}_\perp, p_z) - \mathbf{H}\times\hat{\mathbf{M}}_1]\psi = E\psi, \tag{1}$$

where $\hat{\mathscr{H}}$ is a matrix that depends on the operators $\mathbf{P}_\perp = -i\hbar\nabla_\perp - (e/c)\mathbf{A}$; $\mathbf{P}_\perp$ is the two-dimensional vector (P_x, P_y), ψ is the wave column function describing the motion of the particle across the magnetic field H, $H \| z$, and $\hat{M}_1$ is the matrix describing the direct coupling between the intrinsic magnetic moment of the electron and the magnetic field. If we substitute

$$\psi = e^{iS/\hbar}\chi, \tag{2}$$

where χ is a new column function, we obtain the following set of algebraic equations in the zeroth approximation in $\hbar$:

$$\hat{\mathscr{H}}(\mathbf{p})\chi = E\chi. \tag{3}$$

(We are assuming that $\hat{M}$ is of first order in $\hbar$.) In these expressions, the kinematic momentum is given by

$$\mathbf{p} = \nabla S - (e/c)\mathbf{A}. \tag{4}$$

The set of equations given by (3) determines the energy spectrum and the wave functions in the absence of the magnetic field, namely, $E = \varepsilon(\mathbf{p})$ and $\chi(\mathbf{p})$, respectively. We shall suppose that the matrix $\hat{\mathscr{H}}(\mathbf{p})$ is invariant under time reversal, so that each branch of the spectrum $\varepsilon(\mathbf{p})$ is doubly degenerate and the corresponding two wave functions χ_1 and χ_2 can be obtained from one another by the time reversal transformation:

$$\chi_1 = T\chi_2; \quad \chi_2 = -T\chi_1. \tag{5}$$

Consider one branch of the spectrum

$$E = \varepsilon(p_x, p_y, p_z). \tag{6}$$

Substituting the kinematic momenta (4) in (6), we obtain the Hamilton-Jacobi equation, and the corresponding Hamilton equations yield

$$\frac{d\mathbf{p}}{dt} = \frac{e}{c}[\mathbf{v}\times\mathbf{H}], \quad v_\alpha = \frac{dx_\alpha}{dt} = \frac{\partial\varepsilon}{\partial p_\alpha}, \quad \frac{dS}{dt} = \left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)\mathbf{v}, \tag{7}$$

where $\mathbf{H} = \operatorname{curl}\mathbf{A}$ is the magnetic field. The shape of the trajectory in momentum space is given by (6) for $p_z = \text{const}$.

The discussion given so far is well known, and the equations given by (7) determine the dynamics in the magnetic field of a classical electron with a complicated dispersion law.[5] The solution of (7) enables us to determine the magnitude of p at any point on the trajectory from initial values and, hence, the gradient of the action at all points on the trajectory. Integration along the trajectory then enables us to find the action S itself. However, if we are to determine the wave function, we must find the action as a function of the coordinates x and y. To ensure that the action is a single-valued function of x and y, we must construct a family of trajectories for which there is only one definite trajectory for each point (x, y). It is readily seen that this type of family cannot be constructed from closed trajectories. For each point (x, y) there are therefore several (at least) trajectories, i.e., several values of the action. The true eigenfunction must therefore consist of several (at least two) terms of the form given by (2).

3. The Keller-Rubinow method[2,3] enables us to examine this situation. In this method, the (x, y) plane is represented by a superposition of sheets, attached to one another along the caustics of a certain family of trajectories. On each sheet, each coordinate pair (x, y) has a uniquely corresponding trajectory. The wave function in a classically accessible region contains several terms whose number is equal to the number of sheets containing the point (x, y). It relation to our case, this can be done as follows. Figure 1a shows a simple convex trajectory and a family of trajectories obtained from it by translation along the axis.

The two straight lines $y = a$ and $y = b$ parallel to the x axis are the caustics. Two trajectories correspond to each point in the band. Figure 1b shows two sheets attached to

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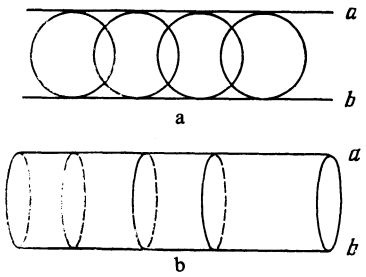

FIG. 1. (a) Family obtained by translation of convex trajectories along the x axis (horizontally); (b) splitting of the band ab into two sheets joined along caustic curves.

one another along the caustic. Left-hand portions of the trajectories lie on the upper sheet and right-hand portions on the lower sheet. The wave function consists of two terms at each point on the band. A somewhat more complicated situation is illustrated in Fig. 2. The trajectory has a concave segment, and the family is constructed by translation along the axis. There are four sheets lying one above the other in the sequence I, II, III, and IV, and the lines of attachment are shown by the same numbers on the four sheets. In the band ac, the wave function consists of four terms, and in the band bc it consists of two.

From these trajectories we can also construct a family of translations along the y axis. In the entire classically accessible band, there will then be two sheets, and the wave function will consist of two terms. It is also possible to choose the family of trajectories in a different way (see Fig. 3). All that is important is to ensure that the classically accessible region can be split into two sheets that are attached to one another along caustics in such a way that, on each sheet, segments of the trajectories will occupy the entire sheet without crossing.

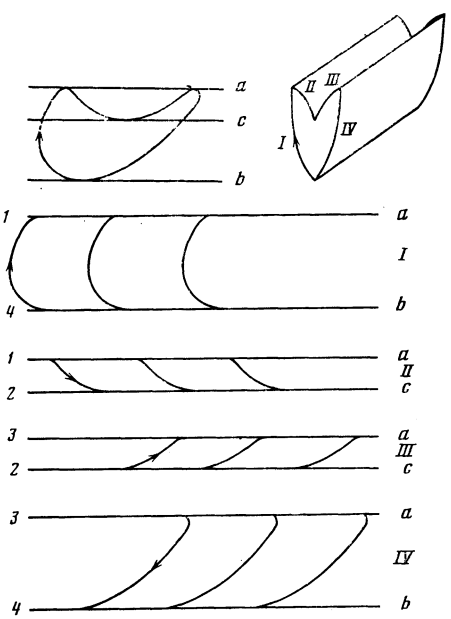

FIG. 2. Splitting of bands ab into sheets when the trajectory has a concave segment.

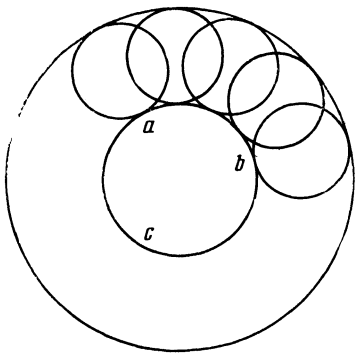

FIG. 3. Family of trajectories obtained by rotating the centers on a circle.

It is not surprising that, for given E and p_z, one can obtain wave functions of different form, depending on the method used to construct the family of trajectories. The levels are infinitely degenerate for fixed E and p_z and, under these conditions, the eigenfunctions can be chosen in different ways.

In general, the family of trajectories can be constructed as follows. Integrating (7), we obtain

$$\mathbf{p}=\frac{e}{c}[\mathbf{r}\times\mathbf{H}]-\frac{e}{c}[\mathbf{r}_0\times\mathbf{H}]. \tag{8}$$

The vector $\mathbf{r}_0$ defines a trajectory. A one-parameter family of trajectories is obtained by assuming that $\mathbf{r}_0$ is a function of some continuous parameter α. For example, for the family shown in Fig. 2, we have $y_0=\text{const}$, $x_0=\alpha$.

The essential point is that, on each sheet, $\mathbf{p}$ (and hence the gradient of action) are single-valued functions of position. In fact, if we specify $\mathbf{r}$ and the family, i.e., $\mathbf{r}_0(\alpha)$, Eqs. (6) and (8) yield a set of three equations for α, p_x, p_y. The subdivision into sheets is constructed precisely in a manner that ensures that this set has a unique solution on each sheet.

4. Let us now write χ as an expansion in powers of $\hbar$: $\chi=\chi_{(0)}-i\hbar\chi_{(1)}+\ldots$. In the first approximation in $\hbar$, we then have from (1)

$$\frac{\partial\hat{\mathscr{H}}}{\partial p_j}\frac{\partial\chi_{(0)}}{\partial x_j}+\frac{1}{2}\frac{\partial^2\hat{\mathscr{H}}}{\partial p_j\partial p_k}\frac{\partial p_k}{\partial x_j}\chi_{(0)}-\frac{i}{\hbar}\hat{\mathbf{H}}\mathbf{M}_1\chi_{(0)}=(E-\hat{\mathscr{H}})\chi_{(1)}. \tag{9}$$

Here and henceforth, $\hat{\mathscr{H}}$ is a matrix that depends on the components of the kinematic momentum given by (4).

The condition for the consistency of (9) demands that its left-hand side must be orthogonal to the column functions χ_1 and χ_2, which are two linearly independent solutions of (3). This condition leads to the following transfer equation:

$$(\chi_j,\operatorname{div}\hat{\mathbf{V}}\chi)+(\chi_j,\hat{\mathbf{V}}\nabla\chi)-\frac{2i}{\hbar}(\chi_j,\hat{H}\hat{M}_1\chi)=0\qquad(j=1,2), \tag{10}$$

where the subscript (0) of χ is omitted and we have introduced the two-dimensional velocity vector-matrix

$$\hat{\mathbf{V}}=\nabla_{\mathbf{p}}\hat{\mathscr{H}}.$$

Since χ satisfies (3), let us write it as a linear combination of χ_1 and χ_2: $\chi=c_1\chi_1+c_2\chi_2$. The coefficients can then be shown to be given by

$$\mathbf{v}\nabla c_1+{}^1/_2 c_1 \operatorname{div}\mathbf{v}+{}^1/_2[(\chi_1,\hat{\mathbf{V}}\nabla\chi_1)-(\hat{\mathbf{V}}\nabla\chi_1,\chi_1)]c_1$$
$$+(\chi_1,\hat{\mathbf{V}}\nabla\chi_2)c_2-i\hbar^{-1}[c_1(\chi_1,\mathbf{H}\hat{M}_1\chi_1)+c_2(\chi_1,\mathbf{H}\hat{M}_1\chi_2)] \quad (11)$$

and there are analogous equations obtained by interchanging the subscripts 1 and 2. In deriving the equation, we use the relations

$$(\chi_1,\hat{\mathbf{V}}\chi_1)=(\chi_2,\hat{\mathbf{V}}\chi_2)=\mathbf{v}\equiv\nabla_p\varepsilon,\quad (\chi_1,\hat{\mathbf{V}}\chi_2)=0.$$

Next, it is readily shown by analogy with what was done in Ref. 3 that $\operatorname{div}\mathbf{v}=\sigma^{-1}d\sigma/dt$, where $\sigma d\alpha dt$ is an infinitesimal area bounded by the trajectories and the $t=$ const surfaces. When the parameter α defining the trajectory and the time t are taken as ray coordinates, the quantity σ can be expressed as the Jacobian for the transformation from Cartesian to ray coordinates:

$$\sigma=\left|\left[\frac{d\mathbf{r}}{dt}\times\frac{d\mathbf{r}}{d\alpha}\right]\right|. \quad (12)$$

Since $\mathbf{v}\nabla=d/dt$, and replacing c_1, c_2 by new coefficients b_1, b_2, in accordance with the formulas $b_i=\sigma^{1/2}c_i$, we can reduce (11) to the form (see Appendix)

$$i\hbar\frac{db_1}{dt}=-H[M_{11}b_1+M_{12}b_2],\quad i\hbar\frac{db_2}{dt}=-H[M_{21}b_1+M_{22}b_2], \quad (13)$$

where $M_{ik}=(\chi_i,\hat{M}\chi_k)$ and the operator $\hat{M}$ is given by

$$\hat{M}=\frac{i\hbar e}{2c}\left\{(\hat{V}_y+v_y)\frac{\partial}{\partial p_x}-(\hat{V}_x+v_x)\frac{\partial}{\partial p_y}\right\}+\hat{M}_{1z} \quad (14)$$

and has the properties $M_{11}=-M_{22}$, $M_{12}=M_{21}^*$. We then have on each sheet

$$\psi=e^{iS/\hbar}\sigma^{-1/2}[b_1\chi_1+b_2\chi_2]. \quad (15)$$

The operator $\hat{M}$ may be looked upon as the z-component of the intrinsic magnetic moment operator for the particle.

The coefficients M_{ik} in (13) depend only on p_x and p_y, i.e., they are periodic functions of time. Consequently, the solution can be written in the form

$$b^{\pm}=e^{i\mu Ht/\hbar}u^{\pm}(t), \quad (16)$$

where $u^{\pm}(t)$ is a periodic function of time, and $\mu_+=-\mu_-\equiv\mu$. The quantities $b^{\pm}$ and $u^{\pm}$ in (16) are two-component columns. Two "correct" functions ψ corresponding to states in which the magnetic moment is, respectively, parallel and antiparallel to the field can therefore be written in the form

$$\psi_{\pm}=\exp[i(S\pm\mu Ht)/\hbar]\sigma^{-1/2}\varphi_{\pm},\quad \varphi_{\pm}=u_1^{\pm}\chi_1+u_2^{\pm}\chi_2,$$

where the spin column functions $\varphi_{\pm}$ satisfy the equation

$$\hat{M}\varphi_{\pm}=\pm\mu\varphi_{\pm}, \quad (17)$$

projected onto the space of the functions χ_1 and χ_2.

5. Since ∇S is single-valued on each sheet, the action S is also single-valued. We can therefore specify the action at any given point on the sheet, and this will ensure that, at any other point, it will be given by an integral of ∇S over a contour passing through these points. The integral will, of course, be independent of the shape of the contour.[1)]

The caustic curve must be crossed as we pass from one sheet to another. It is well known that each such crossing results in the multiplication of the wave function by $\exp(-i\pi/2)$, i.e., there is a loss of phase of $\pi/2$.[3,6] However, this occurs only in the usual case, when $\partial v_y/\partial p_y=\partial^2\varepsilon/p_y^2$ is positive at the crossing point (the y axis is perpendicular to the caustic curve). When, on the other hand, this quantity is negative, the crossing of the caustic curve produces a phase gain of $\pi/2$. The derivation of the change in phase across the caustic curve can be performed by displacement into the complex plane of y, in which case the important point is that $\sigma\sim y^{1/2}$ near the caustic curve.[7] The usual phase-change rule is obtained from the condition that the wave incident on the caustic curve is the wave obtained from the damped solution (appearing in the classically forbidden region) when the circuit is completed in the lower half-plane. When $\partial n_y/\partial p_y<0$, the completion of this circuit results in a wave that departs from the caustic curve rather than being incident upon it. The change in the sign of the phase change depends on this fact. It is readily shown that, in Fig. 2, there is a phase loss on the caustic curves $y=a, y=b$, but a phase gain on $y=c$. We note that there is always a phase loss of π when a circuit is completed along a trajectory (independently of the choice of the family and, hence, of the caustic curves).

The quantization conditions are obtained from the requirement that the phase of the wave function changes by $2n\pi$, where n is an integer, over any closed contour on a surface formed by the sheets. However, the phase change is the same for all equivalent contours, i.e., contours that can be superimposed on one another by continuous deformation. It is therefore sufficient to consider only one contour in each set of equivalent contours.[2-4] In Figs. 1 and 2, the surface formed by the sheet is topologically equivalent to a cylinder, whereas, in Fig. 3, to a torus. Energy quantization is obtained by circuiting along a contour drawn around a cylinder or torus, and the contour can simply be a trajectory (since, in our case, this will be closed). In Fig. 3, there is a second independent contour *abca*, the circuiting along which gives quantization of angular momentum.

According to (15) and (16), energy quantization can be written in the form

$$\frac{c}{eH\hbar}S(E,p_z)\pm\frac{2\pi\mu H}{\hbar\omega}=2\pi\left(n+\frac{1}{2}\right), \quad (18)$$

where $S(E,p_z)$ is the area encompassed by the trajectory in momentum space, and ω_c is the cyclotron frequency. Here, we have taken into account the fact that there is a loss of phase of π when the circuit is completed along a closed trajectory. It is clear from (18) that[1,5] the quantity

$$g(E,p_z)=4\mu H/\hbar\omega_c, \quad (19)$$

plays the role of the g-factor that governs the "spin" splitting of the levels.

The spin splitting itself is then $\Delta E=g\hbar H/2m_c c$, where m_c is the cyclotron mass.[2)]

The determination of the g-factor is thus reduced to the solution of (13), in which the right-hand sides depend on p_x and p_y. The time dependence of p_x and p_y must be determined from the equations of motion, given by (7).

However, it is possible to avoid the solution of (7) in an explicit form by transforming in (13) from the variable t to

the variable φ, where φ is the polar angle of the vector $\mathbf{p}_\perp$. Since, in momentum space, we then have $p_x = p_\perp \cos\varphi$, $p_y = p_\perp \sin\varphi$, Eq. (7) yields

$$d\varphi = -\frac{e}{c}\frac{H}{p_\perp}\frac{\partial\varepsilon}{\partial p_\perp}dt,$$

so that (13) can be rewritten in the form

$$i\hbar\frac{db_k}{d\varphi} = \frac{c}{e}p_\perp\left(\frac{\partial\varepsilon}{\partial p_\perp}\right)^{-1}\sum_{l=1,2}M_{kl}b_l, \qquad k=1,2. \qquad (20)$$

The momentum $p_\perp$ can be expressed in terms of φ by using the dispersion relation (6) in such a way that all the coefficients on the right-hand side of (19) are expressed in terms of φ. If we write the solution of (19) in the form $b^{(k)} = e^{i\lambda\varphi}v^{(k)}(\varphi)$ ($b^{(k)}$ and $n^{(k)}$ are two-component columns and $v^{(k)}$ is a function that is periodic in φ with period 2π, $\lambda_1 = -\lambda_2 \equiv \lambda$), we find that $g = -4\lambda$.

6. Let us now apply these results to magnetic quantization in the valence band of cubic semiconductors described by the Hamiltonian[8,9]

$$\hat{\mathscr{H}}(\mathbf{p}) = \frac{1}{2m_0}\{(\gamma_1+4\gamma)p^2 - 6\gamma(\mathbf{p}\hat{\mathbf{I}})^2\} + \frac{1}{3}\Delta(\hat{\boldsymbol{\sigma}}\hat{\mathbf{I}}) - \frac{1}{3}\Delta,$$

$$\hat{\mathbf{M}}_1 = -\mu_0\{(3k+1)\hat{\mathbf{I}} - \hat{\boldsymbol{\sigma}}\},$$

where μ_0 is the Bohr magneton, Δ is the spin-orbit coupling constant, γ_1, γ, k are the Luttinger constants (we are using the spherical model in which $\gamma_2 = \gamma_3 \equiv \gamma$), $\hat{\mathbf{I}}$ are the angular momentum matrices, and $\hat{\boldsymbol{\sigma}}$ are the Pauli matrices.

The energy is measured from the top of the valence band in the downward direction. The Hamiltonian is a 6×6 matrix and the wave function a six-component column.

We shall use the representation in which the total angular momentum $\hat{\mathbf{J}} = \hat{\mathbf{I}} + \hat{\boldsymbol{\sigma}}/2$ and its z component are diagonal. The components of the column function χ in this representation will be denoted by $\chi_{j\mu}$. The six components correspond to $j = 3/2$, $\mu = \pm 3/2$, $\pm 1/2$ and $j = 1/2$, $\mu = \pm 1/2$. The operator $\hat{\mathscr{H}}(\mathbf{p})$ commutes with the operator $(\hat{\mathbf{J}}\mathbf{p})$, so that the component of the total angular momentum along the linear momentum is a quantum number. Let us denote it by M. The values $M = \pm 3/2$ correspond to the heavy-hole band, and to each of the two values $M = \pm 1/2$ there correspond two states, one in the light-hole band and one in the split band. We now equip the components $\chi_{j\mu}$ with superscripts nM (n is the band number), so that, in view of the spherical symmetry of the Hamiltonian $\hat{\mathscr{H}}(\mathbf{p})$, we can write these components

$$(\chi^{nM})_{j\mu} = a_{nM}{}^{j}D^{j}_{\mu,M}(\varphi,\theta,\psi),$$

where θ,φ are the polar angles of the momentum $\mathbf{p}$. The angle ψ, which defines the phase of the wave function, can be chosen arbitrarily (in particular, we can set $\psi = 0$). For the heavy-hole band, ($n = 1$, $M = \pm 3/2$) $a^{3/2}_{1,\pm 3/2} = 1$, $a^{1/2}_{1,\pm 3/2} = 0$. For the light-hole band ($n = 2$) and the split band ($n = 3$), we have[9]

$$\left(\frac{\gamma_1+2\gamma_2}{2m_0}p^2 - \varepsilon\right)a^{3/2}_{n,\pm 1/2} \mp \frac{2^{1/2}\gamma_2}{m_0}p^2 a^{1/2}_{n,\pm 1/2} = 0,$$

$$\pm\frac{2^{1/2}\gamma_2}{m_0}p^2 a^{3/2}_{n,\pm 1/2} + \left(\frac{\gamma_1 p^2}{2m_0} + \Delta - \varepsilon\right)a^{1/2}_{n,\pm 1/2} = 0,$$

$$|a^{3/2}_{n,\pm 1/2}|^2 + |a^{1/2}_{n,\pm 1/2}|^2 = 1,$$

$$\varepsilon_n = \frac{\gamma_1+\gamma_2}{2m_0}p^2 + \frac{\Delta}{2} \mp \left[\frac{\Delta^2}{4} - \frac{\gamma_2\Delta p^2}{2m_0} + \frac{9\gamma_2^2 p^4}{4m_0^2}\right]^{1/2}.$$

We now consider the extremal section $p_z = 0$ ($\theta = \pi/2$). It is convenient to take the functions χ_1 and χ_2 in the form

$$\chi_1 = \exp(-i3\varphi/2)\chi^{1,-3/2}, \quad \chi_2 = \exp(i3\varphi/2)\chi^{1,3/2},$$

for the heavy-hole band and

$$\chi_1 = 2^{-1/2}(\chi^{n,1/2} + \chi^{n,-1/2})\exp(i\varphi/2),$$

$$\chi_2 = 2^{-1/2}(\chi^{n,1/2} - \chi^{n,-1/2})\exp(-i\varphi/2),$$

for the light-hole and split bands. Using (1) and (14), we find for the heavy-hole band

$$M_{11} = -M_{22} = \frac{3}{2}\frac{e\hbar}{m_0 c}(\gamma_1 - 2\gamma_2); \qquad M_{12} = 0;$$

and, for the light-hole and split bands,

$$M_{11} = -M_{22}$$

$$= \frac{e}{c}\left\{3\hbar(a^{3/2}_{n,1/2})^2\frac{\varepsilon_n}{p^2} - \frac{\hbar}{2m_0}[2k(a^{3/2}_{n,1/2})^2 - (2k+1)(a^{1/2}_{n,1/2})^2 + 2^{1/2}(k+1)a^{3/2}_{n,1/2}a^{1/2}_{n,1/2}]\right\}, \qquad M_{12} = 0.$$

Since, in this case, the matrix $\hat{M}$ is diagonal and time-independent, we find from (17) that $\mu = M_{11}$ and, using (19), we have $g = 4M_{11}H/\hbar\omega_c$, $\omega_c = (eH/cp)(d\varepsilon/dp)$. For heavy holes $g = 6$, i.e., there is no spin splitting for $p_z = 0$. Figure 4 shows the g-factors in the light-hole band and in the split band for germanium as functions of $\gamma_2 p^2/m_0\Delta$. It is clear that the g-factor for light holes has a maximum when this parameter is equal to 0.3. As $p \to \infty$, we have $g \to 2$, for the light-hole band and $g \to 4 + 2/(\gamma_1 + 4\gamma_2)$ for the split band.

The expression for the g-factor when $p_z \neq 0$ can also be readily obtained. In particular, for heavy holes,

$$g_h = 6\frac{m_h}{m_0}|\gamma_1 - \gamma_2 - k|\frac{|p_z|}{p} + 6.$$

This result is identical with that reported by Bir *et al.*,[11] who obtained it from the exact Luttinger solution for the Landau levels with $n \gg 1$.

It is interesting to consider the extent to which these results are affected by the corrugation of the equal-energy

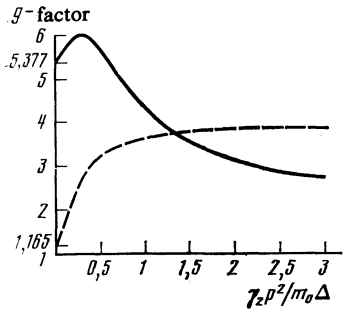

FIG. 4. Quasiclassical g-factors of germanium for $p_z = 0$ as functions of momentum for light-hole bands (solid curve) and the split band (dashed curve).

surfaces. When corrugation is taken into account, the set of equations given by (13) cannot, in general, be solved. However, the solution can be found for certain special cases. Consider the situation where the magnetic field lies along the [001] axis of a crystal. When $p_z = 0$, and the energies are much greater than Δ, the set of equations given by (13) can be solved exactly because $M_{12} = M_{21} = 0$. The g-factors for heavy and light holes are given by

$$g = \frac{4}{\pi}\int_0^{\pi/2}\left[\frac{3\gamma_3}{(2\eta\mp1)\gamma_2} + k\frac{\eta\mp1}{\gamma_1\mp2\gamma_2\eta}\right]\frac{d\psi}{\eta}, \qquad (21)$$

where the upper signs refer to heavy holes and the lower to light holes: $\eta = (1+\alpha\sin^2\psi)^{1/2}$; $\alpha = 3(\gamma_3^2-\gamma_2^2)/4\gamma_2^2$. The integral in (21) can be expressed in terms of tabulated elliptic integrals.

Thus, spin splitting of the levels occurs in the heavy-hole band even for $p_z = 0$. As p_z increases, the g-factor acquires an increment that is quadratic in p_z (rather than linear as in the spherical approximation). However, the evaluation of g_h for germanium (for $p_z = 0$) on the basis of (21), using known values of γ_1, γ_2, γ_3, k in the Luttinger Hamiltonian,[12] shows that the precision of these values is insufficient to determine the departure of g_h from (6).

7. The equations given by (7) and (13) are readily generalized to the case where, in addition to the magnetic field, there is also an electric field **E**, and the fields are time-independent. Here are the results:

$$\frac{d\mathbf{p}}{dt} = \frac{e}{c}[\mathbf{v}\times\mathbf{H}] + e\mathbf{E},$$

$$i\hbar\frac{db_i}{dt} = -\sum_k (\mathbf{H}\mathbf{M}_{ik} + \mathbf{E}\mathbf{D}_{ik})\, b_k,$$

where the operators $\hat{\mathbf{M}}$ and $\hat{\mathbf{D}}$ are given by

$$\hat{\mathbf{M}} = -\frac{i\hbar e}{2c}\left[\hat{\mathbf{V}}+\mathbf{v}\times, \frac{\partial}{\partial\mathbf{p}}\right] + \hat{\mathbf{M}}_1, \qquad \hat{\mathbf{D}} = i\hbar e\frac{\partial}{\partial\mathbf{p}}.$$

When the vector product is evaluated, it must be remembered that the operator d/dp_α is always on the right side and does not act on $\hat{\mathbf{V}} + \mathbf{v}$.

APPENDIX

After transformation to the ray coordinates, it is convenient to transform (11) so that the partial derivatives with respect to the coordinates in the last two terms are replaced with partial derivatives with respect to momenta.

Let us first consider the last term $(\chi_1, \hat{\mathbf{V}}\nabla\chi_2)$. The column function χ_2 satisfies (3). Differentiating this first with respect to p_x and then with respect to x, we obtain

$$\left(\frac{\partial}{\partial x}\frac{\partial\hat{\mathscr{H}}}{\partial p_x}\right)\chi_2 + \frac{\partial\hat{\mathscr{H}}}{\partial p_x}\frac{\partial\chi_2}{\partial x} + \frac{\partial\mathscr{H}}{\partial x}\frac{\partial\chi_2}{\partial p_x} + \hat{\mathscr{H}}\frac{\partial^2\chi_2}{\partial x\,\partial p_x}$$
$$= \left(\frac{\partial}{\partial x}\frac{\partial E}{\partial p_x}\right)\chi_2 + \frac{\partial E}{\partial p_x}\frac{\partial\chi_2}{\partial x} + \frac{\partial E}{\partial x}\frac{\partial\chi_2}{\partial p_x} + E\frac{\partial^2\chi_2}{\partial x\,\partial p_x}.$$

The last terms on the two sides cancel out, and the first term on the left side is zero because $\hat{\mathscr{H}}(\mathbf{p})$ commutes with the time-reversal operator, and the first term on the right-hand side is zero because χ_1 and χ_2 are orthogonal. Since

$$\frac{\partial\hat{\mathscr{H}}}{\partial x}\frac{\partial}{\partial p_x} = \hat{V}_\alpha\frac{\partial p_\alpha}{\partial x}\frac{\partial}{\partial p_x} = \hat{V}_x\frac{\partial}{\partial x} + \hat{V}_y\frac{\partial p_y}{\partial x}\frac{\partial}{\partial p_x} - \hat{V}_x\frac{\partial p_y}{\partial x}\frac{\partial}{\partial p_y},$$

we have the identity

$$2\left(\chi_1, \hat{V}_x\frac{\partial\chi_2}{\partial x}\right) + \left(\chi_1, \hat{V}_y\frac{\partial p_y}{\partial x}\frac{\partial\chi_2}{\partial p_x}\right) - \left(\chi_1, \hat{V}_x\frac{\partial p_y}{\partial x}\frac{\partial\chi_2}{\partial p_y}\right)$$
$$= 2\left(\chi_1, \frac{\partial\chi_2}{\partial x}\right)v_x + \left(\chi_1, \frac{\partial\chi_2}{\partial p_x}\right)v_y\frac{\partial p_y}{\partial x} - \left(\chi_1, \frac{\partial\chi_2}{\partial p_y}\right)v_x\frac{\partial p_y}{\partial x}.$$

A similar identity is obtained by replacing x with y and p_x with p_y. Adding the two identities and recognizing that

$$\mathbf{v}_\perp\nabla_\perp\chi_2 = \frac{d\chi_2}{dt} = \frac{\partial\chi_2}{\partial p_{\perp\alpha}}\frac{dp_{\perp\alpha}}{dt} = \frac{e}{c}H\left(v_y\frac{\partial}{\partial p_x} - v_x\frac{\partial}{\partial p_y}\right)\chi_2$$

and $\partial p_x/\partial y - \partial p_y/\partial x = He/c$, since $H\|z$, we find that

$$(\chi_1, \hat{V}\nabla\chi_2) = \frac{eH}{2c}\left[\chi_1, \left((\hat{V}_y+v_y)\frac{\partial}{\partial p_x} - (\hat{V}_x+v_x)\frac{\partial}{\partial p_y}\right)\chi_2\right].$$

The penultimate term in (11) can be transformed in an analogous fashion.

Replacing c_i with b_i, as indicated in the text [see (11) and the discussion following it], we obtain (13) and (14).

[1)] However, it is frequently convenient to specify S at a particular point on the caustic curve, and take the contour at first along the caustic curve and then along the trajectory.

[2)] This definition of the g-factor is identical with that given in Refs. 1–5. However, it differs from the usual definition of $\tilde{g}$ in which $\Delta E = \tilde{g}\mu_0 H_r$, where μ_0 is the Bohr magneton. Obviously, $\tilde{g} = gm_0/m_c$, where m_0 is the mass of the free electron.

[3)] We are using the notation introduced in Ref. 10.

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