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STUDIES OF THE MOTION OF AN ELECTRON
IN A MAGNETIC FIELD IN A CRYSTAL LATTICE

BY

ERIC TRENT LANE

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INTRODUCTION

What energy eigenvalues characterize an electron in a uniform magnetic field and in an arbitrary periodic crystal lattice potential? Bloch\(^1\), in 1928, solved the quantum mechanical problem for an electron in a periodic potential. In 1930, Landau\(^2\) did the same for a free electron in a magnetic field. Since that time, most attempts to solve the general problem start with the periodic potential solutions and put on the magnetic field as a perturbation\(^3\). This approach generates the widely held concept of the motion of the crystal momentum vector \(\mathbf{k}\), along a surface on which the band energy normal to the magnetic field is constant\(^4\). This approach culminates in Onsager's\(^5\) identification of the semi-classical phase integral with the area of the electron orbit in \(k\)-space.

To find the representation most suitable to the solution of the problem, the wave functions of a free electron in a uniform magnetic field are found, in section I, in various coordinate systems and in both the coordinate and the momentum or wave-vector representations. The velocity\(^6\) and orbit center\(^7\) variables, of section I.D, turn out to be the most useful. Brown\(^8\), using a group theoretic approach, has shown that solutions of the general problem, in terms of these variables, do exist.

In section II, the opposite of the usual...
approach is taken. We start with the wave functions of a free electron in a magnetic field and then put on a periodic potential as a perturbation. This can be physically justified only for magnetic fields of the order of one-hundred megagauss but the approach gives valuable insight into the problem. To define the important concepts in the approach, a simple periodic cosine potential is treated in section II.A. The first order correction to the energy for an arbitrary periodic potential is found in section II.B.

In section III, the Sommerfeld quantization technique is extended by considering the contour integration in the complex variable plane of the expansion in powers of Planck's constant of the wave function in the coordinate representation. Onsager's phase integral is found to be more precisely expressed in terms of the velocity variables of section I.D.1.

In appendix I, the Fourier transform of shifted Hermite functions is proved. In II, the high field correction to the de Haas-van Alphen effect is found. In Appendix III, the average value of the radius to an arbitrary power of the wave function of a free electron in a magnetic field in cylindrical coordinates is found. In IV, a general set of variables for treating the electron in a magnetic field are defined.
Quantum Mechanical Solutions for a Free Electron in a Uniform Magnetic Field

To gain insight into the problem of the electron in a magnetic field and in a crystal, the wave functions for a free electron in a uniform magnetic field are found in various coordinate systems and in both the coordinate and the wave-vector representations.

I.A Solutions in Rectangular Coordinates

The historically important wave functions in rectangular coordinates are studied in detail to define the basic concepts. The wave functions in terms of the rectangular components of the wave-vector provide a necessary extension of the usual treatments by demonstrating the changes needed to treat an arbitrary set of variables. The Fourier transformation between representations guarantees the accuracy of the normalization factors and shows the correspondence of the various wave functions.

I.A.1 Coordinate Representation

Let us first study the approach used by Landau in his classic paper. The classical Hamiltonian for the free electron in a uniform magnetic field \( \mathbf{B} \) is

\[
\mathcal{H} = \frac{\hbar}{2m} (\mathbf{p} + e \mathbf{A})^2
\]
where the absolute value of the charge of the electron is $e = |e|$ and the negative sign of the electron charge has been explicitly incorporated into the Hamiltonian. The vector potential $\mathbf{A}$, is chosen so as to give a uniform magnetic field $\mathbf{B}$, say in the $z$-direction. If we wish to obtain solutions for the quantum mechanical equation in rectangular coordinates, we may choose the vector potential to be

$$\mathbf{A} = (0, xB, 0).$$

This will give the required uniform magnetic field in the $z$-direction.

$$\mathbf{B} = \nabla \times \mathbf{A} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ 0 & xB & 0 \end{vmatrix} = \hat{z} B$$

The Hamiltonian is then written

$$H = \frac{1}{2m} \left[ p_x^2 + (p_y + eBx)^2 + p_z^2 \right]$$

$$= \frac{1}{2m} \left[ p_x^2 + p_y^2 + p_z^2 \right] + \frac{eB}{mc} x p_y + \frac{eB^2}{2mc^2} x^2.$$

The Schroedinger equation is obtained by replacing the above variables by their quantum mechanical operator equivalents.

$$x \rightarrow x, \ y \rightarrow y, \ z \rightarrow z, \ p_x \rightarrow -i\frac{\partial}{\partial x}, \ p_y \rightarrow -i\frac{\partial}{\partial y}, \ p_z \rightarrow -i\frac{\partial}{\partial z}$$

Thus the time-independent Schroedinger equation is written

$$i\hbar \psi = -\frac{\hbar^2}{2m}(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2}) - i \frac{eB}{mc} x \frac{\partial \psi}{\partial y} + \frac{eB^2}{2mc^2} x^2 \psi = E \psi.$$

Since neither $y$ nor $z$ appears explicitly, we may assume plane wave solutions in those directions.

$$\psi_{k_y,k_z}(x,y,z) = \frac{1}{\sqrt{2\pi}} e^{-ik_y y} e^{-ik_z z} u(x)$$
The equation in the $x$-direction is
\[-\frac{i}{\hbar m} \left( \frac{dU}{dx} - \kappa_x u - \kappa_z u \right) + \frac{e \hbar}{mc} x \kappa_y u + \frac{e^2 \hbar}{mc} \kappa^2 u = E u.
\]
This may be rewritten as
\[\frac{d^2U}{dx^2} + \left[ \frac{2m}{\hbar^2} E - \kappa_x^2 - \left( \frac{e \hbar}{mc} x + \kappa_y \right)^2 \right] U(x) = 0.
\]
This is the simple harmonic oscillator equation, with normalized solutions
\[U_n(x) = \left[ \frac{\gamma}{\pi^{\frac{1}{4}} \kappa y^{\frac{1}{2}} \sqrt{\pi \hbar c/eb}} \right]^{\frac{1}{2}} e^{-\frac{1}{2} \left( \frac{e^2 |x|^2}{2mc} + \kappa_y y^2 \right)} H_n \left( \frac{e^2 |x|^2}{2mc} + \kappa_y y^2 \right)
\]
and with characteristic values
\[\kappa_n = \frac{1}{\kappa y} \left[ \frac{2m}{\hbar^2} E - \kappa_x \right],
\]
provided the following boundary conditions are satisfied:
\[U_n(x) = 0 \quad \text{at} \quad x \sqrt{\frac{e^2}{2mc} + \kappa_y y^2} = \pm \infty.
\]
In section I.D.1, the $y$-component of the velocity of the electron is found to be $v_y = \frac{e}{2mc} x$. Thus the boundary condition is equivalent to the requirement that the square of the absolute value of the wave function integrated over the whole range of the $y$-component of velocity is finite.

The Hermite polynomials are defined by
\[H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} (e^{-x^2}),
\]
\[\int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x) \, dx = \delta_{mn} 2^n n! \sqrt{\pi}.
\]
The complete solution is then
\[\psi_{n, \kappa_x, \kappa_z}(x, y, z) = \left[ 2^n n! 4\pi^2 \sqrt{\pi \hbar c/eb} \right]^{-\frac{1}{2}} e^{i \kappa_y y} e^{i \kappa_z z} e^{-\frac{1}{2} \left( \frac{e^2 |x|^2}{2mc} + \kappa_y y^2 \right)} H_n \left( \frac{e^2 |x|^2}{2mc} + \kappa_y y^2 \right).
\]
This solution has may be interpreted as plane waves in the $y$- and the $z$-directions, modulated by simple harmonic
oscillator functions in the \( x \)-direction, the centers of which are located at the point \( x_{\ast} = -\frac{1}{\kappa_{y}}(\kappa_{x}/c) \). Thus, as the wave-vector \( \kappa_{y} \), changes, the center of the electron orbit shifts in the \( x \)-direction. This property allows one to construct wave packets that, in the time-dependent representation, move in the classically expected circular orbits in the \( x_{\ast}y_{\ast} \)-plane.

I.A.2 Wave-Vector Representation

A slightly different point of view is obtained if we look at the quantum mechanical problem in the wave-vector or momentum representation. The Hamiltonian is the same,

\[
\hat{H} = \frac{1}{2m} \left( \hat{p}_{x}^{2} + \hat{p}_{y}^{2} + \hat{p}_{z}^{2} \right) + \frac{\hbar^{2}}{m c^{2}} \vec{\kappa} \times \hat{p} + \frac{\hbar^{2} \vec{\kappa}^{2}}{2mc^{2}} \hat{x}
\]

but let us now use the following equivalent operators for the variables.\(^{10}\)

\( \hat{p}_{x} \rightarrow i\hbar \kappa_{x}, \hat{p}_{y} \rightarrow i\hbar \kappa_{y}, \hat{p}_{z} \rightarrow i\hbar \kappa_{z}, x \rightarrow i\frac{\partial}{\partial \kappa_{x}} = i\frac{\partial}{\partial \kappa_{x}}, y \rightarrow i\frac{\partial}{\partial \kappa_{y}} = i\frac{\partial}{\partial \kappa_{y}}, z \rightarrow i\frac{\partial}{\partial \kappa_{z}} = i\frac{\partial}{\partial \kappa_{z}} \)

Now the quantum mechanical equation of motion is written as follows\(^{11}\).

\[
\hat{H} \psi = \frac{i}{\hbar} \left( \vec{\kappa} \cdot (\vec{\kappa} \times \vec{p}) + \frac{\hbar^{2} \vec{\kappa}^{2}}{2mc^{2}} \right) \psi + i\frac{\hbar^{2}}{m c^{2}} \vec{\kappa} \cdot \left( \frac{\partial \psi}{\partial \vec{\kappa}} \right) - \frac{\hbar^{2} \vec{\kappa} \cdot \vec{p}}{2mc^{2}} \frac{\partial \psi}{\partial \vec{\kappa}} = E \psi
\]

The energy eigenvalue equation may be rearranged to give

\[
\frac{\hbar^{2}}{\kappa_{c}} \frac{\partial^{2} \psi}{\partial \kappa_{c}^{2}} - 2i \kappa_{y} \frac{\partial \psi}{\partial \kappa_{x}} + \left( \frac{2mc}{\hbar} E - \frac{\kappa_{c}}{\kappa_{x}} \left( \kappa_{x}^{2} + \kappa_{y}^{2} + \kappa_{z}^{2} \right) \right) \psi = 0.
\]

This suggests that we try solutions of the following form.
\[ \Psi(\kappa_x, \kappa_z) = e^{i \frac{2\pi}{\alpha^2} \kappa_x \kappa_z} \ U(\kappa_z) \]

The equation for the electron in the \(\kappa_x\)-direction is
\[
\frac{\hbar}{i} \frac{\partial \psi}{\partial \kappa_x} + \left[ \frac{2m_e}{\hbar^2} F - \frac{\hbar^2}{2m_e} \kappa_z^2 - \frac{\hbar^2}{8a_0^2} \kappa_x^2 \right] \ U(\kappa_z) = 0
\]
which is again the simple harmonic oscillator equation.

Thus the normalized solution is
\[
\psi_n(\kappa_x, \kappa_z) = \left[ 2^n n! \sqrt{\frac{\pi a_0}{\kappa_x}} \right]^{-\frac{1}{4}} e^{i \frac{2\pi}{\alpha^2} \kappa_x \kappa_z} e^{-\frac{\hbar^2}{8a_0^2} \kappa_x^2} H_n(\kappa_z \sqrt{\frac{\pi}{a_0}})
\]
with eigenvalues
\[
E_n, \kappa_z = (2n+1) \frac{\hbar^2}{2m_e} + \frac{\hbar^2 \kappa_z^2}{2m_e}.
\]

Actually the above solution is not complete in the sense that it does not have the other two characteristic quantities needed to specify the solution precisely. Obviously it is characteristic of \(\kappa_z\), the \(z\)-component of the wave-vector and we should thus multiply by \(\delta(\kappa_x - \kappa_x')\) where \(\kappa_x\) is the variable and \(\kappa_x'\) is the eigenvalue. The remaining characteristic quantity may be either the \(x\)- or the \(y\)-component of the orbit center (see section I.D.2).

If the \(x\)-component of the orbit center is specified precisely, then we must multiply by \(\delta(\kappa_x - \kappa_x')\), since \(\kappa_x = -\frac{\hbar}{\alpha^2} \kappa_x'\) with the vector potential that we have chosen. Thus the complete solution is
\[
\psi_{n, \kappa_x, \kappa_z}(\kappa_x, \kappa_y, \kappa_z) = \left[ 2^n n! \sqrt{\frac{\pi a_0}{\kappa_x}} \right]^{-\frac{1}{4}} e^{i \frac{2\pi}{\alpha^2} \kappa_x \kappa_z} e^{-\frac{\hbar^2}{8a_0^2} \kappa_x^2} H_n(\kappa_z \sqrt{\frac{\pi}{a_0}}) \delta(\kappa_y - \kappa_y') \delta(\kappa_z - \kappa_z').
\]

The interpretation of this solution is in terms of plane waves in the \(\kappa_z\)-direction whose wave length varies with \(\kappa_x\). This, with the harmonic oscillator
modulation function, allows wave packets to be built up in k-space that circle the origin as expected classically.

I.A.3 Fourier Transformation

The solution in the coordinate representation can be shown to be equivalent to the solution in the wave-vector representation by taking the Fourier transform over all three coordinates as follows.

\[ \psi_{n,k_x,k_y,k_z}(k_x,k_y,k_z) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{-\infty}^{\infty} e^{-i k_x x} dx \int_{-\infty}^{\infty} e^{-i k_y y} dy \int_{-\infty}^{\infty} e^{-i k_z z} dz \psi_{n,k_x,k_y,k_z}(x,y,z) \]

The integrations over y and z may be performed directly,

\[ \int_{-\infty}^{\infty} e^{-i k_y y} dy = \delta(k_y - k_y) \]
\[ \int_{-\infty}^{\infty} e^{-i k_z z} dz = \delta(k_z - k_z) \]

where \( \delta(k' - k) \) is the Dirac delta function. To transform the x-coordinate, we must use the following Fourier transform\(^\text{12} \).

\[ \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-i \omega t} e^{-\frac{1}{2} \omega^2} H_n(t) dt = (-i)^n e^{-\frac{i}{2} \omega^2} H_n(\omega) \]

Thus we have

\[ \psi_{n,k_x,k_y,k_z}(k_x,k_y,k_z) = (2\pi^{-\frac{3}{2}})^{\frac{1}{4}} \delta(k_y - k_y) \delta(k_z - k_z) \]
\[ \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx e^{-i k_x x} e^{-\frac{1}{2} (x \frac{E_c}{\hbar} + k_y \frac{E_y}{\hbar} + k_z \frac{E_z}{\hbar})^2} H_n(x \frac{E_c}{\hbar} + k_y \frac{E_y}{\hbar} + k_z \frac{E_z}{\hbar}) \].

If we let \( t = x \frac{E_c}{\hbar} + k_y \frac{E_y}{\hbar} + k_z \frac{E_z}{\hbar} \) and \( \omega = k_x \frac{E_c}{\hbar} \) then

\[ \psi_{n,k_x,k_y,k_z}(k_x,k_y,k_z) = (2\pi^{-\frac{3}{2}})^{\frac{1}{4}} \delta(k_y - k_y) \delta(k_z - k_z) \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dt e^{-i \omega t} e^{-\frac{1}{2} t^2} H_n(t) \].

The transformed wave function is thus

\[ \psi_{n,k_x,k_y,k_z}(k_x,k_y,k_z) = (-i)^n (2\pi^{-\frac{3}{2}})^{\frac{1}{4}} e^{i k_x \frac{E_c}{\hbar} - \frac{1}{2} k_x^2 \frac{E_c}{\hbar}} H_n(k_x \frac{E_c}{\hbar}) \delta(k_y - k_y) \delta(k_z - k_z) \]

which agrees with our previous solution to within the
phase factor \((-i)^n\) with an absolute magnitude of unity.

The delta functions indicate that the values of the wave-vectors \(k_y\) and \(k_z\) are specified precisely.

The correspondence of solutions and normalization factors can be checked by making the inverse transformation as follows.

\[
\psi_{n,k_y,k_z}(x,y,z) = [i^n]^{-\frac{1}{2}} \int_{-\infty}^{\infty} e^{ik_y y} dk_y \int_{-\infty}^{\infty} e^{ik_z z} dk_z \psi_{n,k_y,k_z}(x,0,0)
\]

The integrals over \(k_y\) and \(k_z\) may be done immediately\(^{13}\),

\[
\int_{-\infty}^{\infty} e^{ik_y y} dk_y e^{i\frac{2\pi}{L} k_y L_y} \delta(k_y - k_y') = e^{i k_y y} e^{i\frac{2\pi}{L} k_y L_y
}
\]

\[
\int_{-\infty}^{\infty} e^{ik_z z} dk_z \delta(k_z - k_z') = e^{i k_z z}
\]

The transformation on \(k_y\) uses the following Fourier transform\(^{12}\),

\[
\int_{-\infty}^{\infty} e^{i w t} e^{-i \omega \cdot k_y} H_n(\omega) d\omega = (i^n e^{-i t} H_n(t)
\]

Thus we have

\[
\psi_{n,k_y,k_z}(x,y,z) = (-i)^n \left[ 2^n n! \frac{n! \sqrt{\pi e}}{\sqrt{2\pi}} \right]^{-\frac{1}{2}} e^{i k_y y} e^{i k_z z} \int_{-\infty}^{\infty} e^{i w t} e^{-i \omega \cdot k_y} H_n(\omega) d\omega
\]

If we again identify \(\omega = k_y \sqrt{\pi e}/k_y\) and \(t = x \sqrt{\pi e}/k_y = k_y \sqrt{\pi e}/k_y\)
then

\[
\psi_{n,k_y,k_z}(x,y,z) = (-i)^n \left[ 2^n n! \frac{n! \sqrt{\pi e}}{\sqrt{2\pi}} \right]^{-\frac{1}{2}} e^{i k_y y} e^{i k_z z} \int_{-\infty}^{\infty} e^{i w t} e^{-i \omega \cdot k_y} H_n(\omega) d\omega
\]

The final result is therefore

\[
\psi_{n,k_y,k_z}(x,y,z) = \left[ 2^n n! \frac{n! \sqrt{\pi e}}{\sqrt{2\pi}} \right]^{-\frac{1}{2}} e^{i k_y y} e^{i k_z z} e^{-i \left( k_y e k_y + k_z k_z \right)} H_n(x k_y + k_z k_z)
\]

The Fourier transformation between representations provides a valuable check on the normalization factors and on the precise interpretation
of the various components of the process.

I.A.4 Other Solutions in Rectangular Coordinates

The proceeding solutions are characteristic of the $x$-component of the orbit center, $x_0 = -\kappa_\alpha (x_0/\varepsilon_b)$, (see section I.D.2). We may also write solutions characteristic of the $y$-component of the orbit center, $y_0 = y + \kappa_\alpha (x_0/\varepsilon_b)$.

\[
\psi_{y_{0}, y_{0}, \kappa_\alpha} (x, y, z) = \left[ \frac{2^{\kappa_\alpha} \pi^{\frac{1}{2}} \varepsilon_b^{\kappa_\alpha}}{\Gamma\left(1 + \frac{\kappa_\alpha}{2}\right)} \right]^{-\frac{1}{2}} e^{-\frac{i}{\varepsilon_b} y \left( y - y_0 \right) - \frac{1}{2} \varepsilon_b \left( y - y_0 \right)^2} \mathcal{H}_\kappa \left( y - y_0 \right) e^{i\kappa_\alpha z}
\]

\[
\psi_{y_{0}, y_{0}, \kappa_\alpha} (x_0, y_0, z) = \left[ \frac{2^{\kappa_\alpha} \pi^{\frac{1}{2}} \varepsilon_b^{\kappa_\alpha}}{\Gamma\left(1 + \frac{\kappa_\alpha}{2}\right)} \right]^{-\frac{1}{2}} e^{i\kappa_\alpha z} e^{-\frac{i}{\varepsilon_b} y \left( y - y_0 \right) - \frac{1}{2} \varepsilon_b \left( y - y_0 \right)^2} \mathcal{H}_\kappa \left( y - y_0 \right) \delta \left( x_0 + \frac{\varepsilon_b}{\varepsilon_b} (y - y_0) \right)
\]

\[
\psi_{y_{0}, y_{0}, \kappa_\alpha} (x, y, z) = \left[ \frac{2^{\kappa_\alpha} \pi^{\frac{1}{2}} \varepsilon_b^{\kappa_\alpha}}{\Gamma\left(1 + \frac{\kappa_\alpha}{2}\right)} \right]^{-\frac{1}{2}} e^{i\kappa_\alpha z} e^{-i\kappa_\alpha x} e^{-\frac{i}{\varepsilon_b} y \left( y - y_0 \right) - \frac{1}{2} \varepsilon_b \left( y - y_0 \right)^2} \mathcal{H}_\kappa \left( y - y_0 \right) \square \left( x + \frac{\varepsilon_b}{\varepsilon_b} \right)
\]

where the independent variables are as indicated. Each of these solutions is the Fourier transform of each of the others. There are actually four more solutions where $z$ is Fourier transformed to $\kappa_\alpha$.

These solutions may be shown to be characteristic of the $y$-component of the orbit center by writing the appropriate eigenvalue equation. The operator corresponding to $y_0$ in the rectangular coordinate representation is

\[
y_0 = y + \frac{\varepsilon_b}{\varepsilon_b} \kappa_\alpha \quad \longrightarrow \quad y - i \frac{\varepsilon_b}{\varepsilon_b} \frac{\partial}{\partial y}
\]

The eigenvalue equation is

\[
y_0 \psi = \left[ y - i \frac{\varepsilon_b}{\varepsilon_b} \frac{\partial}{\partial y} \right] \psi_{y_{0}, y_{0}, \kappa_\alpha} (x, y, z) = \left[ y - i \frac{\varepsilon_b}{\varepsilon_b} (-i \frac{\partial}{\partial y}) (y - y_0) \right] \psi = y_0 \psi.
\]

The second solution is obviously characteristic of
\( \psi = \psi + \psi < \delta \) because of the delta function. The third solution may be shown to be characteristic of \( \psi \) by using the operator replacement

\[ \psi = \psi + \frac{\delta}{\delta \psi} \psi_0 = \psi_0 + \frac{\delta}{\delta \psi} \psi \cdot \]

The fourth solution uses

\[ \psi = \psi + \frac{\delta}{\delta \psi} \psi_0 = \psi_0 - \frac{\delta}{\delta \psi} \psi \cdot \]

The question of how to get from solutions characteristic of \( \psi \) to those characteristic of \( \chi \) may be answered by integrating (or summing) the wave function over the range of the characteristic quantity with the proper multiplying factor. For example, the third solution above may be transformed

\[ \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dy \, e^{i\psi \xi} \psi_0, \psi_1, \psi_2 \left( \psi, \gamma, \xi, \xi \right) = \psi_0, \psi_1, \psi_2 \left( \psi, \gamma, \xi, \xi \right) \]

since we know that

\[ \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dy_0 \, e^{i\psi_0 \xi} \psi_0, \psi_2 \left( \psi_0, \gamma, \xi, \xi \right) = \delta(\psi_0 - \psi) \cdot \]

The other solutions may be transformed similarly.

Another set of sixteen solutions in rectangular coordinates could be obtained by choosing the vector potential as

\[ \mathbf{A} = (-y \mathbf{B}, 0, 0) \]

which also gives a uniform magnetic field in the \( z \)-direction.
I.B Solutions in Cylindrical Coordinates

To further explore the range of possible wave functions describing a free electron in a magnetic field, solutions are found in the cylindrical coordinate and wave-vector representations. The Fourier transformation shows the identical form of the two representations.

I.B.1 Coordinate Representation

Solutions in cylindrical coordinates\(^{14}\) arise when one chooses a vector potential

\[
\vec{A} = \frac{i}{2} \vec{a} \times \vec{r} = (-\hat{y} \zeta, \hat{x} \zeta, 0)
\]

which gives the required uniform magnetic field in the z-direction. The Hamiltonian is

\[
\hat{H} = \frac{1}{2m}(\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2) + \frac{eB}{2mc}(\hat{x} p_y - \hat{y} p_x) + \frac{eB^2}{8mc^2}(x^2 + y^2).
\]

The quantum mechanical energy eigenvalue equation is obtained by substituting the usual equivalent operators: \(p_x \rightarrow -i\hbar \frac{\partial}{\partial x}, x \rightarrow x\), etc. The time independent Schroedinger equation is

\[
\hat{H}\psi = \frac{-i\hbar}{\partial t}(\frac{\partial \psi}{\partial x} + \frac{\partial \psi}{\partial y} + \frac{\partial \psi}{\partial z}) - i \frac{eB}{2mc}(x \frac{\partial \psi}{\partial y} - y \frac{\partial \psi}{\partial x}) + \frac{eB^2}{8mc^2}(x^2 + y^2) \psi = E \psi
\]

The transformation to cylindrical coordinates is made by using the following relations.

\[
\frac{\partial \psi}{\partial x} + \frac{\partial \psi}{\partial y} = \frac{\partial \psi}{\partial r} + \frac{1}{r} \frac{\partial \psi}{\partial \phi} - \frac{1}{r} \frac{\partial \psi}{\partial \phi} - \frac{1}{r} \frac{\partial \psi}{\partial \phi}
\]

\[
x \frac{\partial \psi}{\partial y} - y \frac{\partial \psi}{\partial x} = \frac{\partial \psi}{\partial \phi}
\]
Thus we obtain the equation in cylindrical coordinates.
\[
\mathcal{H}_\psi = -\frac{\epsilon}{2}\left( \frac{1}{\rho^2} \frac{\partial^2 \psi}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial \psi}{\partial \rho} + \frac{1}{\rho^2 \sin \theta} \frac{\partial^2 \psi}{\partial \theta^2} + \frac{1}{\rho^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right) - \frac{\epsilon \alpha}{2 \mu} \frac{\partial \psi}{\partial \rho} + \frac{\epsilon \beta^2}{\omega c^2} \tau \psi = E \psi
\]

Since neither \( \phi \) nor \( z \) appear explicitly, let us try solutions
\[
\psi_{\mu, \kappa_0}(\rho, \theta, \tau) = \frac{1}{2\pi} e^{i\mu \rho} e^{i\kappa_0 \theta} R(\theta).
\]
Thus the radial equation is
\[
-\frac{d}{d\rho} \left( \frac{dR}{d\rho} + \frac{1}{\rho} \frac{dR}{d\rho} - \frac{\mu^2}{\rho^2} R - \kappa_0^2 R \right) + \frac{\epsilon \alpha^2}{2 \mu c^2} R + \frac{\epsilon \beta^2}{\omega c^2} \tau^2 R = ER
\]
or rewritten
\[
\frac{d}{d\tau} \frac{dR}{d\tau} + \frac{1}{\tau} \frac{dR}{d\tau} + \left[ \frac{\epsilon \alpha^2}{2 \mu c^2} - \kappa_0^2 - \frac{\epsilon \beta^2}{\omega c^2} \mu - \frac{\mu^2}{\rho^2} - \frac{\mu}{\tau} \right] R(\tau) = 0
\]
This equation is solved easily in terms of \( \zeta = \tau^2 e^{i\mu / a c} \).

Using the new variable, the equation becomes
\[
\zeta \frac{d^2 R}{d\zeta^2} + \frac{dR}{d\zeta} + \left[ \frac{\epsilon \alpha^2}{2 \mu c^2} - \kappa_0^2 - \mu - \frac{\mu}{\zeta} - \frac{\mu}{\tau} \right] R(\zeta) = 0.
\]
This equation has singularities at infinity and at zero.

As \( \zeta \) goes to infinity, we have the limit equation: \( \zeta^2 \frac{d^2 R}{d\zeta^2} = 0 \), which has solutions: \( R = e^{\pm \zeta} \).

Since we want finite solutions at infinity, we choose the negative sign. As \( \zeta \) goes to zero, we have the limit equation: \( \zeta^2 \frac{d^2 R}{d\zeta^2} + \frac{dR}{d\zeta} + \left[ \frac{\epsilon \alpha^2}{2 \mu c^2} - \kappa_0^2 - \mu - \frac{\mu}{\zeta} - \frac{\mu}{\tau} \right] R(\zeta) = 0 \), with solutions: \( R = \zeta^{\pm \frac{\mu}{\omega c}} \).

Since we want finite solutions at the origin, we choose the positive sign. Thus we must look for solutions of the form
\[
R(\zeta) = e^{-\frac{1}{2} \zeta} \zeta^{\pm \frac{\mu}{2}} f(\zeta)
\]
The equation for \( f(\zeta) \) is
\[
\zeta \frac{d^2 f}{d\zeta^2} + \left( 1 + \frac{\mu}{2} - \frac{1}{\zeta} \right) \frac{df}{d\zeta} - \frac{1}{2} \left( 1 + \frac{2}{\zeta} - \frac{\epsilon \alpha^2}{2 \mu c^2} \right) f(\zeta) = 0.
\]
The confluent hypergeometric function of the first kind\( ^nF_m \).
\[ M(a,b,z) = 1 + \frac{a}{b} z + \frac{a(a+1)}{b(b+1)} z^2 + \ldots \]

satisfies the following differential equation\(^{16}\)
\[ z \frac{d^M}{dz^a} + (b-z) \frac{dM}{dz} - a M = 0 \]

which has a regular singularity at zero and an irregular singularity at infinity. Since we require that the wavefunction be finite at \(z = \infty\), the function \(f(z)\) must be a polynomial. This occurs if the parameter \(a = -s\) is a negative integer. We also require that the parameter \(b = 1 + 1/\mu\) be a positive number greater than zero, which is the reason for using the absolute value of \(|\mu|\).

The energy eigenvalues may be obtained from the equation for \(f(z)\), since \(a = -s = \frac{1}{2}(1+\mu+1/\mu - \frac{\lambda}{\alpha} \epsilon + \frac{\lambda}{\alpha} \epsilon z)\) then
\[ E_{s,\mu} = (2s + \mu + 1/\mu + 1) e^{\beta / 2\mu c} + \epsilon^2 \mu^2 / \lambda c, \quad s = 0, 1, 2, \ldots \]

Since we know that \(s\) is a positive integer, we may write the confluent hypergeometric function in terms of the associated Laguerre polynomials,
\[ M(-s, 1+1/\mu, \epsilon) = \frac{s! \mu!}{(s+1)!} L^{(1/\mu)}_{s}(\epsilon) \]

which are defined as follows.
\[ L^{(1/\mu)}_{s}(\epsilon) = \frac{1}{\mu!} \int e^{-\epsilon} \epsilon^{-s} \frac{d^s}{dz^s} [e^{-\epsilon} \epsilon^{\frac{1}{\mu}}] \]
\[ \int_{0}^{\infty} e^{-\epsilon} \epsilon^{s} L^{(1/\mu)}_{s}(\epsilon) L^{(1/\mu)}_{s}(\epsilon) d\epsilon = \delta_{s\mu} \Gamma(n+1)/n! \]

Thus the complete wave function may be written
\[ \psi_{s,\mu, \kappa}(\eta, \theta, z) = \left( \frac{\epsilon^{\frac{k}{c}}}{2\pi} \right)^{-\frac{1}{4}} e^{i \omega \eta} e^{-i k z} e^{\frac{i \epsilon}{2 k c} \left( \frac{\epsilon \mu}{\alpha c} \right) \frac{1}{1/\mu} - \frac{1}{2} \left( \frac{\epsilon \mu}{\alpha c} \right) L^{(1/\mu)}_{s}(\epsilon) \frac{1}{2 k c} \left( \frac{\epsilon \mu}{\alpha c} \right) \frac{1}{1/\mu} } \]

with eigenvalues
\[ E_{s,\mu} = (2s + \mu + 1/\mu + 1) e^{\beta / 2\mu c} + \epsilon^2 \mu^2 / \lambda c \]

If we now put on the condition that the
angular variation of the wave function must be periodic, with period $\pi r$, then the parameter $\mu = m$ must be an integer. In this case, it becomes simpler to define the energy quantum number, $\eta = s + \frac{1}{2}(m + |m|) = 0, 1, 2, \ldots, \infty$.

Thus we have

$$s = n - m = 0, 1, 2, \ldots, n \quad \text{for} \quad m = |m| = 0, 1, 2, \ldots, n$$

$$s = n \quad = 0, 1, 2, \ldots, \infty \quad \text{for} \quad -m = |m| = 0, 1, 2, \ldots, \infty.$$

The wave function must now be written in two parts, one for positive angular momentum, $m = 0, 1, \ldots, n$

$$\psi_{n,m,k_x}(r, \theta, z) = \left[ \frac{n!}{\pi r} \right]^{-\frac{1}{2}} e^{i k_x z} e^{i m \theta} e^{-\frac{a r^2}{r}} \left[ \frac{a r^2}{r} \right]^\frac{1}{2} L_n(m)(\frac{a r^2}{r})$$

and one for negative angular momentum, $m = 1, 2, \ldots, \infty$

$$\psi_{n,-m,k_x}(r, \theta, z) = \left[ \frac{n!}{\pi r} \right]^{-\frac{1}{2}} e^{i k_x z} e^{-i m \theta} e^{-\frac{a r^2}{r}} \left[ \frac{a r^2}{r} \right]^\frac{1}{2} L_n(m)(\frac{a r^2}{r}).$$

The energy eigenvalues are

$$E_{n,k_x} = (2n + 1) \frac{\hbar^2 k^2}{2 m \rho} + \frac{n k_x^2}{2 m}.$$

The wave function is shown to be an eigenfunction of angular momentum by applying the angular momentum operator.

$$L_z \psi_{n,m,k_x}(r, \theta, z) = -i \hbar \frac{\partial}{\partial \theta} \psi_{n,m,k_x}(r, \theta, z) = \frac{m \hbar}{\rho} \psi_{n,m,k_x}(r, \theta, z).$$

Classically the angular momentum is

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} = \mathbf{r} \times (m \mathbf{\omega} - \frac{\mathbf{\omega}}{c} \mathbf{r}) = \mathbf{r} \times (m \mathbf{v} - \frac{\mathbf{\omega}}{c} \mathbf{r}).$$

The component of angular momentum along the z-axis, for which m is the eigenvalue, is

$$L_z = m (x v_y - y v_x) - \frac{\hbar}{\rho} B (x^2 + y^2) = m v_y r - \frac{\hbar}{\rho} r^2.$$

If we note that the velocity may be written as

$$v_x = \omega (y_0 - y), \quad v_y = \omega (x - x_0)$$
where \( x, y \) are the coordinates of the classical center of the electron orbit and \( \omega = eB/mc \) is the Larmor frequency, (see section I.D.2). Then the z-component of the angular momentum may be written

\[
x_z = m \left[ (x_0 + \nu_0 / \omega) \nu_y - (y_0 - \nu_0 / \omega) \nu_x \right] - \frac{eB}{\omega} \left[ (x_0 + \nu_0 / \omega)^2 + (y_0 - \nu_0 / \omega)^2 \right]
\]

\[
= \frac{1}{2} \omega \left( \nu_2^1 + \nu_2^2 \right) / \omega - \frac{1}{2} \omega \left( x_2^1 + y_2^1 \right).
\]

Thus for a given energy the electron may have an arbitrary negative angular momentum about the origin simply by having the center of the electron orbit sufficiently far from the origin because the angular momentum of the electromagnetic field is included in the derivation through the vector potential term. The electron may have a positive angular momentum up to a maximum value set by putting the orbit center at the origin of coordinates, which is the classically expected value,

\[
x_z (\text{max}) = \frac{1}{2} m \left( \nu_2^1 + \nu_2^2 \right) / \omega = E_k / \omega \approx h \nu
\]

as found above, from the wave function.

I.B.2 Wave-Vector Representation

Now let us explore the wave-vector representation of the electron wave function in cylindrical coordinates. Again we have the Hamiltonian

\[
\hat{\mathcal{H}} = \frac{\hbar}{\omega} \left( \hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2 \right) + \frac{eB}{2mc} \left( \hat{x} \hat{p}_x - \hat{y} \hat{p}_y \right) + \frac{eB}{2mc} \left( x^2 + y^2 \right).
\]

The energy eigenvalue equation is now obtained by making
the substitutions:

\[ p_x \rightarrow \xi_k x, \quad x \rightarrow i \frac{\partial}{\partial p_x} = i \frac{\partial}{\partial \xi_k}, \quad \text{and so forth.} \]

The time independent Schrödinger equation is

\[ i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \left( \xi_k^2 + \xi_y^2 + \xi_z^2 \right) \psi + i \frac{\hbar eB}{2mc} \left( \xi_k \frac{\partial \psi}{\partial \xi_k} - \xi_y \frac{\partial \psi}{\partial \xi_y} \right) - \frac{e^2 B^2}{8mc^2} \frac{\partial^2 \psi}{\partial \xi_k^2} = \xi \psi. \]

The transformation to cylindrical coordinates requires that we define

\[ \xi^2 = \xi_k^2 + \xi_y^2, \quad \tan \phi = -\xi_x/\xi_y. \]

The definition of the angle \( \phi \) can be justified as follows.

In the classical motion of the electron in a magnetic field\(^{17} \) we write \( \mathbf{mv} = -\frac{e}{c} \mathbf{v} \times \mathbf{B} \), which may be integrated for the free electron to give \( \mathbf{mv} = -\frac{e}{c} \mathbf{v} \times \mathbf{B} \). If we identify the classical momentum, \( \mathbf{mv} = \imath \mathbf{k} - \frac{e}{c} \mathbf{v} \times \mathbf{B} \), then we may write

\[ \imath \mathbf{k} = -\frac{e}{c} \mathbf{v} \times \mathbf{B}. \]

This shows that as the electron describes an orbit in coordinate space, it simultaneously describes a similar orbit in \( k \)-space, reduced by a factor of \( 2\pi c/e \)

and rotated through an angle of \( \pi/2 \). We must also use

\[ \frac{\partial^2 \psi}{\partial k_x^2} + \frac{\partial^2 \psi}{\partial k_y^2} = \frac{\partial^2 \psi}{\partial k^2} + \frac{1}{k} \frac{\partial \psi}{\partial k} + \frac{i}{\hbar} \frac{\partial \psi}{\partial \phi} \]

\[ k_x \frac{\partial \psi}{\partial k_y} - k_y \frac{\partial \psi}{\partial k_x} = \frac{\partial \psi}{\partial \phi}. \]

Thus we obtain

\[ i\hbar \frac{\partial \psi}{\partial t} = \frac{\hbar^2}{2m} \left( \xi_k^2 + \xi_y^2 + \xi_z^2 \right) \psi + i \frac{\hbar eB}{2mc} \left( \xi_k \frac{\partial \psi}{\partial \xi_k} - \xi_y \frac{\partial \psi}{\partial \xi_y} \right) - \frac{e^2 B^2}{8mc^2} \frac{\partial^2 \psi}{\partial \xi_k^2} \]

Let us try solutions of the form

\[ \psi_k (k, \phi) = \frac{1}{\sqrt{2\pi}} e^{i\phi} \xi (k) \]

Thus

\[ \frac{d^2 \xi}{dk^2} + \frac{i}{k} \frac{d \xi}{dk} + \left[ \frac{2\imath m e^2}{\hbar^2 c^2} \xi - \xi^2 - \frac{e^2 B^2}{2mc^2} \right] \xi (k) = 0. \]
If we define the new variable

$$f = \kappa^2 (x_1 \kappa / c_3)$$

we have

$$\frac{d^2 f}{dt^2} + \frac{d^2 f}{dx^2} + \left[ \frac{m c}{x_1 \kappa} \left( \frac{\kappa}{c_3} \right)^2 - \mu - \frac{1}{\kappa^2} \right] f = 0$$

which is identical to the equation for $R(x)$, so that we can write down the solutions for $\kappa(t)$ directly,

$$\psi_{n,m} \kappa_x (k_x, \Phi, \kappa_x) = \left[ \frac{m c}{x_1 \kappa} \left( \frac{\kappa}{c_3} \right)^2 - \mu - \frac{1}{\kappa^2} \right]^{-1/2} e^{-i k_x x} \left[ \frac{z c_3}{x_1 \kappa} \right] \delta (k_x - \kappa_x), \quad m = 0, 1, \ldots, n$$

$$\psi_{n,-m} \kappa_x (k_x, \Phi, \kappa_x) = \left[ \frac{m c}{x_1 \kappa} \left( \frac{\kappa}{c_3} \right)^2 - \mu - \frac{1}{\kappa^2} \right]^{-1/2} e^{ik_x x} \left[ \frac{z c_3}{x_1 \kappa} \right] \delta (k_x - \kappa_x), \quad m = 1, 2, \ldots, n$$

with the same energy eigenvalues as before.

I.B.3 Fourier Transformation

The Fourier transformation between representations requires the cylindrical coordinate equivalent of the Fourier Transform. In rectangular coordinates we have

$$\psi_{n,m} \kappa_z (k_x, k_y, k_z) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \quad e^{-i(k_x x + k_y y)} \psi_{n,m} \kappa_z (x, y, z).$$

To transform to cylindrical coordinates, we must use

$$x = r \cos \theta, \quad y = r \sin \theta, \quad k_x = -k \sin \theta, \quad k_y = k \cos \theta$$

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy = \int_{0}^{\infty} r dr \int_{0}^{2\pi} d\theta$$

$$k_x x + k_y y = -k r \sin \theta \cos \phi + k r \sin \theta \sin \phi = k r \sin \theta (\theta - \phi).$$

Thus the Fourier Transform in the cylindrical system is

$$\psi_{n,m} \kappa_z (k_x, k_y, k_z) = \int_{-\infty}^{\infty} d\phi \int_{0}^{\infty} r dr \int_{-\infty}^{\infty} dz \quad e^{-i(k_x x + k_y y + k_z z)} \psi_{n,m} \kappa_z (r, \theta, \phi).$$

The integral over $z$ yields a delta function as before

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik_z z} dz = \delta(k_z).$$
The transformation goes as follows.

\[ \psi_{n,m,k^*}(k_x,k_y,k_z) = \left[ \frac{2\pi}{\sinh(z_0)} \right]^{1/2} \frac{1}{2\pi} \int_0^{\pi} d\theta' \int_0^{\pi/2} d\phi' \ e^{-ik_x \sin(\theta')} e^{ik_y \cos(\theta')} e^{ik_z \cos(\theta')} L_n^{(m)}(\frac{2\pi k^*}{\sinh(z_0)}) \delta(k_x-k_y) \]

The integral over the angle \( \theta \) may be written

\[ \frac{1}{2\pi} \int_0^{\pi} d\theta' e^{-ik_x \sin(\theta')} = \frac{1}{2\pi} e^{i\phi'} \int_0^{\pi/2} d\theta' \ e^{i\omega \theta'} e^{-ik_x \sin(\theta')} \]

The definition of the Bessel function of integral order is\(^{18}\)

\[ J_m(z) = \frac{1}{2\pi} \int_0^{\pi} d\theta' \ e^{-iz \sin \theta'} \]

Thus we have

\[ \psi_{n,m,k^*}(k_x,k_y,k_z) = \left[ \frac{2\pi}{\sinh(z_0)} \right]^{1/2} \frac{1}{2\pi} \int_0^{\pi} d\theta' \int_0^{\pi/2} d\phi' \ e^{i\phi'} \ e^{i\omega \theta'} \ e^{-ik_x \sin(\theta')} \ L_n^{(m)}(\frac{2\pi k^*}{\sinh(z_0)}) J_m(kr) \]

But this is just a form of the following Hankel transform\(^{19}\).

\[ \int_0^{\infty} e^{-i\chi \xi} L_n^{(m)}(\chi) J_m(\sqrt{\xi^2 + \gamma^2}) d\chi = (-i)^{m+1} \pi e^{-i\gamma \xi} L_n^{(m)}(\xi) \]

If we identify

\[ \chi = \frac{2\pi k^*}{\sinh(z_0)} \quad \xi = \frac{2\pi k^*}{\sinh(z_0)} \]

we have

\[ \psi_{n,m,k^*}(k_x,k_y,k_z) = (-i)^{m+1} \frac{2\pi}{\sinh(z_0)} \left[ \frac{2\pi}{\sinh(z_0)} \right]^{1/2} \delta(k_x-k_y) e^{i\phi'} e^{-ik_x \sin(\theta')} \ L_n^{(m)}(\frac{2\pi k^*}{\sinh(z_0)}) J_m(kr) \]

which is correct to within a factor of \((-i)^{m+1}\).

The transformation for negative angular momentum states follows in the same manner. In fact, both can be handled at the same time by using the \(s\)-notation of section I.B.1.

Since the wave functions in \( m \) are nearly identical to those in terms of \( k \), the inverse transformation follows the same pattern as above.
I.C. Transformation Between Rectangular and Cylindrical Coordinates

Since we have complete sets of wave functions, we may represent an arbitrary wave function written in cylindrical coordinates in terms of a complete set of wave functions written in rectangular coordinates and vice versa. Only those wave functions that are characteristic of a given energy eigenvalue \( n \) may be used since the energy cannot depend on which coordinate system the wave function is written in. For example, we may write

\[
\psi_{n, m, k_x}(r, \theta, z) = \int_0^\infty d\mu_y A_m(k_y) \psi_{n, k_y, k_z}(x, y, z)
\]

\[
\psi_{n, k_y, k_z}(x, y, z) = \Sigma_{m=-\infty}^{\infty} A_m(k_y) \psi_{n, m, k_z}(r, \theta, z).
\]

This type of transformation may be accomplished by using the integral transformation proved in Appendix I.

\[
\int_0^\infty dx e^{i k_x x} e^{-\frac{1}{2} x^2} H_n(x) e^{-\frac{1}{2} (x+y)^2} H_n(x+y) = \]

\[
= \sqrt{\pi} n! (i k_x - x)^m e^{-\frac{1}{2} (x^2 + x y + y^2)} L_n^{(m-n)} \left( \frac{2 x y}{\sqrt{\pi}} \right)
\]

If we make the following replacements

\[
x \rightarrow x \sqrt{e^2/c^2}, \quad y \rightarrow y \sqrt{e^2/c^2}, \quad x \rightarrow \frac{k_x}{\sqrt{e^2/c^2}}, \quad m \rightarrow m + n, \quad n \rightarrow n
\]

then we have

\[
\int_0^\infty d\mu_y \sqrt{\frac{e^2}{c^2}} e^{i k_y y} e^{-\frac{2 \pi e^2}{c^2} k_y^2} H_m^{(n)} \left( \frac{k_y}{\sqrt{e^2/c^2}} \right) e^{-\frac{1}{2} (x^2 + y^2)} H_n(x) \left( \frac{k_y}{\sqrt{e^2/c^2}} \right) =
\]

\[
= \sqrt{\pi} \pi^n (i k_y - x)^m e^{-\frac{e^2}{2c^2} (k_y^2 + 2 i x y + y^2)} L_n^{(m-n)} \left( \frac{2 i x y}{e^2/c^2} \right) =
\]

\[
= \sqrt{\pi} \pi^n e^{-i \theta} \left( \frac{e^2}{2c^2} \right)^m \alpha^m e^{-\frac{e^2}{2c^2} (x^2 + 2 i x y)} L_n^{(m)} \left( \frac{2 i x y}{e^2/c^2} \right).
\]

When we put in the normalization factors to obtain the
correct wave functions, we find that

\[ A_m(k_z) = \frac{1}{\sqrt{2\pi\kappa_0}} e^{-\frac{i\kappa_2^2\kappa_0}{2\kappa_0}} e^{-\frac{i\kappa_2^2\kappa_0}{2\kappa_0}} H_{m+n}(\kappa_0 \frac{\kappa_0}{\kappa_0}). \]

But we already know that the \( A_m(k_z) \) are orthonormalized,

\[ \int_0^\infty A_m^*(k_z) A_n(k_z) \, dk_z = \delta_{mn} \]

Thus the inverse transformation through summation over \( m \) follows directly as written above.

It is interesting to note that the \( A_m(k_z) \) are directly related to the wavefunctions in the rectangular wave-vector representation that are characteristic of \( \kappa_z \), thus being related to the vector potential \( \vec{A} = (-y, 0, 0) \).

\[ \psi_{n, k_x, k_z} (x, y, z) = A_{m-n}(k_z) e^{\frac{ik_z}{\kappa_0}(k_x-k_y)} e^{\frac{ik_z}{\kappa_0}(k_z-k_y)} \delta(k_x-k_y) \delta(k_z-k_y). \]

Although this is not the only such transformation, it was felt that at least one example of transformation between rectangular and cylindrical coordinate representations should be given.

I.D Solutions in terms of Velocity Variables

Now, the question arises whether solutions in terms of other variables might be more appropriate to the problem of introducing a periodic crystal lattice potential in the Hamiltonian. One such set of variables which will prove useful is the velocity and orbit-center variables to be treated in the present section. We will first treat the problem of the free electron and later generalize to a
Hamiltonian with an arbitrary potential.

I.D.1 Free Electron Solutions

The Hamiltonian for a free electron in a magnetic field may be written most simply as
\[ H = \frac{1}{2m} \mathbf{p}^2 = \frac{1}{2m} (v_x^2 + v_y^2 + v_z^2) \]
where we have made the identification
\[ m \mathbf{v} = \mathbf{p} + e \mathbf{A} \]
(Note that \( \varepsilon = \pm \varepsilon_0 \), the sign is included explicitly.) The velocity variables may be shown to be the time derivative of the corresponding coordinates by taking the quantum mechanical time derivative.

\[ \dot{x} = \frac{i}{\hbar} [H, x] = \frac{i \hbar}{m} [v_x, x] = \frac{i \hbar}{m} v_x [v_x, x] = \frac{i \hbar}{m} v_x \left( \frac{\partial}{\partial x} (p_x + eA_y) \right), x = \frac{i \hbar}{m} v_x [p_x, x] = \frac{i \hbar}{m} v_x (-\nabla) = v_x \]
The remaining two time derivatives go in a similar manner,

\[ \dot{y} = v_y, \quad \dot{z} = v_z. \]

But the components of the velocity are not independent. This may be shown by obtaining the commutation relations among them.

\[ [v_x, v_y] = v_x v_y - v_y v_x = \frac{i \hbar}{m} \left( (p_x + eA_y) (p_y + eA_x) - (p_y + eA_x) (p_x + eA_y) \right) = \frac{i \hbar}{m} \nabla \times \mathbf{A} \]

Like wise, the other two commutators are found to be

\[ [v_y, v_z] = -i \frac{eB_z}{m} B_x, \quad [v_z, v_x] = -i \frac{eB_y}{m} B_x. \]

The quantum mechanical Schroedinger equation
is formulated in terms of independent pairs of conjugate variables. To obtain these, we may choose one axis of our coordinate system to be parallel to the magnetic field, say the z-axis. Thus we have two independent pairs of conjugate variables whose commutation relations are 
\[ [\nu_x, \nu_y] = -i \frac{eB}{\hbar c}, \quad [\nu_x, \nu_z] = -i \frac{\hbar}{m} \]
\[ [\nu_y, \nu_z] = [\nu_x, \nu_z] = [\nu_x, \nu_y] = 0. \]

By analogy with the usual method of replacing variables with their quantum mechanical equivalents,
\[ p_x = -i \hbar \frac{\partial}{\partial \nu_x} = [\nu_x, x] \frac{\partial}{\partial \nu_x} \]
we have
\[ \nu_x \rightarrow [\nu_x, \nu_y] \frac{\partial}{\partial \nu_y} = -i \frac{eB}{\hbar c} \frac{\partial}{\partial \nu_y}, \quad \nu_x \rightarrow [\nu_x, \nu_z] \frac{\partial}{\partial \nu_z} = -i \frac{\hbar}{m} \frac{\partial}{\partial \nu_z}. \]

Thus Schroedinger's equation may be written
\[ \hbar \psi = \lambda \left[ -\frac{eB}{\hbar c} \frac{\partial^2 \psi}{\partial \nu_y^2} + \nu_y^2 \psi - \frac{\hbar}{m} \frac{\partial^2 \psi}{\partial \nu_z^2} \right] = E \psi. \]

Since the variable z does not appear in the equation, we may assume plane wave solutions in that direction,
\[ \psi_{\nu z}(\nu_y, z) = [2\pi]^{-\nu_y} e^{i\nu_y z} u(\nu_y) \]
The equation for the function \( u(\nu_y) \) may be written as
\[ \frac{d^2 u}{d\nu_y^2} + \left[ \lambda \left( \frac{eB}{\hbar c} \right)^2 - \nu_y^2 \left( \frac{eB}{\hbar c} \right)^2 - \left( \frac{eB}{\hbar c} \right)^2 \nu_y^2 \right] u(\nu_y) = 0 \]
which is just the harmonic oscillator equation in terms of the variable \( \nu_y \sqrt{eB/m} \), whose normalized solutions are
\[ u_n(\nu_y) = \left[ 2\pi \right]^{-\nu_y/2} e^{-\nu_y^2/2} \frac{\nu_y^n}{n!} H_n(\nu_y \sqrt{eB/m}) \]
Thus the wave function is
\[ \psi_{n, \nu z}(\nu_y, z) = [2\pi]^{-\nu_y/2} e^{i\nu_y z} e^{-\nu_y^2/2} \frac{\nu_y^n}{n!} H_n(\nu_y \sqrt{eB/m}). \]
This wave function is not yet complete because we need to specify one other characteristic value. We could specify either the $x$- or the $y$-component of the orbit center by multiplying the wave function by a delta function. An example of a complete solution characteristic of the $x$-component of the orbit center would be

$$\Psi_{n, y, x, \kappa_z}(v_y, x, z) = \Psi_{n, x, \kappa_z}(v_y, z) \delta(x - x)$$.

Note that this wave function is gauge independent, in the sense that we have made no assumptions about the vector potential $\vec{A}$, except that it is a function only of the coordinates. If we assume a specific form for the vector potential, we obtain solutions that are equivalent to those obtained previously. For example, if we take $\vec{A} = (0, 0, 0)$, then $v_y = \frac{\hbar}{m} k_y + \frac{e}{mc} x$ and

$$\Psi_{n, y, x}(v_y, z) = [z^n! \sqrt{\frac{\pi e^2}{\hbar mc^2}}]^{-1} e^{i u_y z} e^{-\frac{1}{2} (\frac{v_y}{\hbar c} + x \frac{e}{mc})^2} \psi_n(u_x \frac{e}{mc} + x \frac{e}{mc})$$

or we could take $\vec{A} = (-y, 0, 0)$, then $v_y = \frac{\hbar}{m} k_y$ and

$$\Psi_{n, y, x}(v_y, z) = [z^n! \sqrt{\frac{\pi e^2}{\hbar mc^2}}]^{-1} e^{i u_y z} e^{-\frac{1}{2} (\frac{v_y}{\hbar c})^2} \psi_n(u_x \frac{e}{mc})$$

Thus we see the intimate relation of the two functions used in the transformation from rectangular to cylindrical coordinates in section I.C.
I.D.2 Orbit Center Variables

There is one very important point that has so far been overlooked. We have used two pairs of conjugate variables to write the Hamiltonian, which is all that is needed in the free electron case. But three pairs of conjugate variables are necessary to write an arbitrary Hamiltonian. Since the missing variables do not appear in the free electron Hamiltonian, they must be constants of the motion. Let us look among the constants of the motion for the new variables. The z-component of the velocity is already a constant of the motion since the Hamiltonian is independent of z.

\[ \dot{v}_z = \frac{i}{\hbar} [\mathcal{H}, v_z] = 0 \]

The time derivatives of the x-component of velocity is

\[ \dot{v}_x = \frac{i}{\hbar} [\mathcal{H}, v_x] = \frac{i}{\hbar} [\mathcal{H}, v_x] = \frac{i}{\hbar} v_y [v_x, v_x] = \frac{i}{\hbar} v_y (i \frac{eB}{mc}) = -\frac{eB}{mc} v_y \]

But we know already that \( v_y = y \), so that we may integrate both sides of the equation to obtain

\[ v_x = -\frac{eB}{mc} y + \frac{eB}{mc} y_0 \]

where we have taken the constant of integration to be

\[ y_0 = y + \frac{me}{eB} v_x \]

which we will call the y-component of the center of the electron orbit. This is certainly a constant of the motion, as can be seen by taking its time derivative

\[ \dot{y}_0 = \frac{i}{\hbar} [\mathcal{H}, y_0] = \frac{i}{\hbar} [\mathcal{H}, y_0] + \frac{i}{\hbar} \frac{me}{eB} [\mathcal{H}, v_z] = v_z + \frac{i}{\hbar} \frac{me}{eB} (i \frac{eB}{mc} v_y) = 0 . \]
The same process may be used to define the remaining constant of the motion by taking the time derivative of the \( y \)-component of velocity.

\[
\dot{v}_y = \frac{i}{\hbar} [\mathcal{H}, v_y] = \frac{i}{\hbar} \left( \mathcal{P}_y v_x \right) - i \frac{\mathcal{P}_y}{\hbar} v_x = \frac{i}{\hbar} \mathcal{P}_y \left( - \frac{\mathcal{I}_y}{\mathcal{E}_0} \right) = \frac{i}{\hbar} \mathcal{P}_y v_x
\]

Integrating both sides and rearranging we obtain

\[
x^* = x - \frac{\mathcal{P}_y}{\mathcal{E}_0} v_y
\]

the \( x \)-component of the electron orbit center, which also can be shown to be a constant of the motion of the free electron in a magnetic field.

The orbit center variables are independent of the velocity variables, which may be shown as follows

\[
[x, v_x] = [x, v_y] = \frac{\mathcal{P}_x}{\mathcal{E}_0} [v_x, v_y] = \frac{i}{\hbar} [x, \mathcal{P}_y] = \frac{\mathcal{P}_x}{\mathcal{E}_0} \left( + i \frac{\mathcal{I}_y}{\mathcal{E}_0} \right) = 0
\]

and likewise we find that

\[
[x, v_x] = [x, v_y] = [x^*, v_x] = [x^*, v_y] = [x^*, v_z] = [y^*, x] = 0
\]

The orbit center variables are not independent of each other, the commutation relation between them being

\[
[x^*, y^*] = [x - \frac{\mathcal{P}_x}{\mathcal{E}_0} v_x, y + \frac{\mathcal{P}_y}{\mathcal{E}_0} v_y] = \frac{\mathcal{P}_x}{\mathcal{E}_0} \left( [x, v_x] - [v_x, y] - \frac{\mathcal{P}_y}{\mathcal{E}_0} [v_y, v_x] \right) = \frac{\mathcal{P}_x}{\mathcal{E}_0} \left[ \frac{i}{\hbar} \left( - \frac{\mathcal{I}_y}{\mathcal{E}_0} \right) - \frac{\mathcal{P}_y}{\mathcal{E}_0} \left( i \frac{\mathcal{I}_y}{\mathcal{E}_0} \right) \right] = \frac{i}{\hbar}
\]

Thus we have the required three independent pairs of conjugate variables.

Let us study the orbit center variables a bit more before going on. The classical radius of the electron orbit is

\[
\gamma = \frac{mc^2 \nu}{\epsilon_0} = \frac{\mathcal{P}_x}{\mathcal{E}_0} \sqrt{2 \mu \mathcal{E}_0}
\]
If we use the quantum mechanical value for the transverse component of the energy \( E_1 = (2n+1)\frac{e^2B}{2mc} \), then we have
\[
\gamma_n = \sqrt{(2n+1)\frac{e^2}{2B}}.
\]

The two components of the orbit center do not commute, so they cannot be determined simultaneously except to within a factor equal to or greater than the product of root-mean-square uncertainties
\[
\Delta x \cdot \Delta y \geq \frac{\hbar}{2} \cdot \frac{\hbar}{2} = \frac{\hbar^2}{4}
\]
which is proportional to the area of the smallest allowed electron orbit.

The energy eigenvalues are degenerate because of the existence of mutually noncommuting constants of the motion. This corresponds to the classical situation where the energy of the electron is independent of the position of the center of its orbit. Thus each value of the energy corresponds to an infinite set of pairs of values of \( x \) and \( y \). But to determine the wave function uniquely, either \( y \), \( x \), or some combination of the two must be specified precisely.

To find the spectrum of pairs of values of \( x \) and \( y \), let us introduce the operator:
\[
\rho^2 = x^2 + y^2,
\]
which is the quantum mechanical analogue of the square of the cylindrical radius vector of the center of the circular electron orbit. Since both \( x \) and \( y \) are constants of the
motion, it follows that $\hat{H}^2$ must also be a constant of the motion whose eigenvalues may be found as follows. The equivalent Schroedinger equation may be written as

$$\hat{H}^2 \psi = x^2 \psi - \left( \frac{\hbar}{2m} \right)^2 \frac{\partial^2 \psi}{\partial x^2} = \langle \hat{\xi}^2 \rangle \psi$$

where we have used the quantum mechanical replacement

$$y_0 \rightarrow [y_0, x_0] = -i \frac{\hbar}{\epsilon_0} \frac{\partial}{\partial \xi} .$$

But the equation is that of a quantum harmonic oscillator, whose eigenvalues we know to be

$$\langle \hat{\xi}^2 \rangle = (2s + 1) \frac{\hbar^2}{\epsilon_0} , \ s = 0, 1, 2, \ldots$$

Thus the geometric locations of the possible centers of the electron orbits lie on a discrete set of concentric circles whose center is at the origin of coordinates and whose radii are equal to

$$\sqrt{\langle \hat{\xi}^2 \rangle} = \sqrt{(2s + 1) \hbar^2 / \epsilon_0} .$$

This suggests that we look for the spectrum of eigenvalues for the actual radius of the electron orbit regardless of its position. Let us therefore introduce the radius-squared operator

$$\hat{r}^2 = (x-x_0)^2 + (y-y_0)^2$$

which is the quantum mechanical analogue of the square of the radius of the Larmor orbit. But this operator may be written as

$$\hat{r}^2 = \left( \frac{\hbar}{\epsilon_0} \right)^2 \left( \hat{\xi}^2 + \hat{\eta}^2 \right) = \left( \frac{\hbar}{\epsilon_0} \right)^2 \left( \hat{\xi}^2 - \hat{\eta}^2 \right).$$

Consequently, its eigenvalues are proportional to those of
the transverse component of the energy, or

\[ \langle \mathcal{H}^2 \rangle = \left( \frac{\hbar^2}{2m} \right)^2 \left( 2n + 1 \right) \frac{\hbar^2}{2m} = \left( 2n + 1 \right) \frac{\hbar^2}{2m} \]

and, like the energy, it is a constant of the motion.

For completeness, let us also find the eigenvalues of the angular momentum about an axis parallel to the magnetic field. The angular momentum operator about the z-axis has the form

\[ L_z = x p_y - y p_x = x \left( mv_y - \frac{eB}{c} x \right) - y \left( mv_x + \frac{eB}{c} y \right) \]

where we have assumed a vector potential

\[ A = \frac{e}{c} \mathbf{v} \times \mathbf{r} = (-i\mathbf{A}, \mathbf{v} \times \mathbf{A}, 0). \]

Now substituting for

\[ x = x_0 + \frac{eB}{c} v_y, \quad y = y_0 - \frac{eB}{c} v_x \]

and rearranging, we find that

\[ L_z = (x_0 + \frac{eB}{c} v_y) (\frac{eB}{c} v_x - \frac{eB}{c} x_0) - (y_0 - \frac{eB}{c} v_x) (\frac{eB}{c} v_y + \frac{eB}{c} y_0) = \]

\[ = \frac{m e^2}{2 \hbar} (v_x^2 + v_y^2) - \frac{eB}{c} (x_0 + y_0) = \frac{eB}{c} (\mathbf{r} \times \mathbf{p}) \]

Thus the angular momentum is a constant of the motion and is related to the eigenvalues of the orbit center and of the orbit radius as follows.

\[ \langle L_z \rangle = \hbar (n - s) \]

If we define the angular momentum quantum number \( m = \langle L_z \rangle / \hbar \)

then the relation between the three quantum number is

\[ m = n - s = n, n-1, \ldots, 1, 0, -1, \ldots, -\infty \]

which is the same as we found in section I.B.1, thus providing us with a new interpretation of the quantum
number s found in that section.

I.D.3 Orbit Center in Wave-vector Representation

So far we have been concerned with the coordinate representation in the above discussion. To clarify some popularly held concepts concerning the motion of a quasi-free electron in a uniform magnetic field, let us define the wave-vector representation of the orbit center variables. We again look for constants of the motion in terms of wave-vector components. Now we must choose a definite vector potential to obtain a unique solution, we will choose

\[ A = \frac{i}{\hbar} \mathbf{x} \times \mathbf{F} = (-i4\mathbf{B}, \frac{i}{4}\mathbf{B}, 0). \]

The time derivative of the x-component of the wave vector is

\[ \dot{k}_x = \frac{i}{\hbar} \dot{\mathbf{p}}_x = \frac{i}{\hbar} \left[ H, \mathbf{p}_x \right] = \frac{i}{\hbar} \mathbf{v}_x \mathbf{p}_x = \frac{i}{\hbar} \mathbf{v}_x \left[ \mathbf{c}_0 + \mathbf{e}_x \times \mathbf{p}_x, \mathbf{p}_x \right] = \]

\[ = \frac{\hbar}{\mathcal{A}} \mathbf{v}_x \mathbf{c}_0. \]

But we know from previous work that \( \mathbf{v}_x = -\frac{\hbar}{\mathcal{A}} \mathbf{c}_0 \) thus we have

\[ \dot{k}_x = \frac{\hbar}{\mathcal{A}} \mathbf{c}_0. \]

Integrating and rearranging, we may define the constant of the motion

\[ k_x^* = k_x - \frac{\hbar}{\mathcal{A}} \mathbf{x}_0 \]

as the x-component of the center of the orbit in \( k \)-space.

Likewise we may define the y-component as

\[ k_y^* = k_y - \frac{\hbar}{\mathcal{A}} \mathbf{y}_0 \]
Both can be shown to be constants of the motion and also independent of the velocity variables and of the z-component variables. The commutation relation is given by

$$[\kappa_x^*, \kappa_z^*] = i \hbar / 4 \pi c.$$  

Note that the k-space orbit center variables are directly proportional to the coordinate-space components of the orbit center.

$$\kappa_x^* = \frac{e}{\hbar} v_x + \frac{e}{\hbar} v_y = \frac{e}{\hbar} v_x,$$

$$\kappa_z^* = \frac{e}{\hbar} v_y - \frac{e}{\hbar} v_x = - \frac{e}{\hbar} v_x.$$  

Thus the operator corresponding to the square of the cylindrical radius vector in k-space of the center of the circular orbit is

$$\kappa^2 = (\kappa_x^*)^2 + (\kappa_z^*)^2 = \left( \frac{e}{\hbar} v_x \right)^2 + \left( - \frac{e}{\hbar} v_x \right)^2 = \left( \frac{e}{\hbar} v_x \right)^2.$$  

and thus has quantized values given by

$$\langle \kappa^2 \rangle = (2s+1) \hbar^2 / 4 \pi c.$$  

The root-mean-square uncertainty in the location of the center of the orbit in k-space is

$$\Delta \kappa_x \cdot \Delta \kappa_z = \frac{\hbar}{\hbar c} = \frac{1}{\sqrt{2}}$$

which is proportional to the area of the lowest energy orbit in reciprocal space. The square of the radius of the orbit in k-space is

$$\kappa^2 = (\kappa_x - \kappa_x^*)^2 + (\kappa_z - \kappa_z^*)^2 = \left( \frac{e}{\hbar} v_x \right)^2 (v_x + v_y^2)$$

and thus has quantized values of
\[ \langle k \rangle = (2n+1) eB/4\pi c \]

which is the justification for the concept of cylindrical surfaces in \( k \)-space whose intersections with the constant energy sphere give the allowed states of the electron in a uniform magnetic field.

I.D.4 Hamiltonian with an Arbitrary Potential

The Hamiltonian for an electron in a uniform magnetic field in an arbitrary potential may be written as:

\[ H = \frac{1}{2m} (\mathbf{p}^2 + \mathbf{v}_0^2 + \mathbf{v}_z^2) + V(x, y, z). \]

But to express the Hamiltonian in terms of independent pairs of conjugate variables, we must express \( x \) and \( y \) in terms of the \( v_x, v_y \) and \( x_0, y_0 \). We need not assume a specific vector potential to do this, so that our results will be gauge invariant. Thus we have

\[ x = x_0 + \frac{v_y}{\omega} \quad y = y_0 - \frac{v_x}{\omega} \]

where we have defined the Larmor frequency \( \omega = \frac{eB}{mc} \). Thus the Hamiltonian is written as

\[ H = \frac{1}{2m} (v_x^2 + v_y^2 + v_z^2) + V(\frac{x_0 + v_y}{\omega}, \frac{y_0 - v_x}{\omega}, x). \]

Now the so-called orbit center variables are no longer necessarily constants of the motion, as may be seen as follows,

\[ x_0 = \frac{i}{\hbar}[H, x_0] = \frac{i}{\hbar} [V, x_0] = \frac{i}{\hbar} [y_0, x_0] \frac{\partial V}{\partial y_0} = \frac{i}{\hbar \omega} (\frac{\partial V}{\partial y_0}) \]

since \( x_0 \) is independent of all variables except \( y_0 \), and
\[ \dot{\psi} = \frac{i}{\hbar} [H, \psi] = \frac{i}{\hbar} [V, \psi] = \frac{i}{\hbar} [x, \psi] \frac{\partial V}{\partial x} = -\frac{1}{m}\frac{\partial^2 \psi}{\partial x^2}. \]

This means that the energy will now depend explicitly on the position of the center of the electron orbit. This is the spirit with which we will approach the next problem of putting on a periodic potential.

II First Order Lattice Potential Energy Correction

We would like now to treat the periodic lattice potential as a perturbation on the energy of a free electron in a magnetic field. This would be physically reasonable only for magnetic fields greater than about one-hundred megagauss, but the calculation gives some insight into the physical problem and suggests a new approach to problem of the crystal electron in a magnetic field.

II.A. A Cosine Lattice Potential

We will first do the problem of a simple cosine lattice which will define most of the important concepts of the problem. Then we will generalize to an arbitrary periodic lattice potential.

II.A.1 Definition of Variables

In working out the perturbation problem, we
would like to use the more familiar variables, $P_i$ and $Q_i$, which satisfy the usual commutation relations.

$$ [P_i, Q_j] = -i \hbar \delta_{ij}, \quad [P_i, P_j] = [Q_i, Q_j] = 0. $$

Only the velocity variables appear in the free electron Hamiltonian, so that we will define $P_i, Q_i, P_z$ as follows.

$$ P_i = m v_i \sqrt{eB/c}, \quad Q_i = m v_i \sqrt{eB/c}, \quad P_z = m v_z \sqrt{eB/c}. $$

The orbit center variables then appear in terms of $P_i, Q_i$.

$$ P_x = -x_0 \sqrt{eB/c}, \quad Q_x = y_0 \sqrt{eB/c} $$

If we choose the magnetic field $B$, to lie parallel to the $z$-axis, then the remaining variable is defined as $Q_z = z \sqrt{eB/c}$. The $P_i, Q_i$ so defined, satisfy the above commutation relations. The sign of the electron charge $e = |e|$, has been included explicitly in the above definitions because a slightly different set of variables must be used to treat a positively charged particle.

In summary, the definitions of the new variables are

$$ P_i = \sqrt{eB/c} (P_z + \frac{e}{m} A_z), \quad Q_i = \sqrt{eB/c} (P_i + \frac{e}{m} A_i), \quad P_z = \sqrt{eB/c} P_z $$

$$ x = \sqrt{eB/c} (Q_z - P_z), \quad y = \sqrt{eB/c} (Q_y - P_y), \quad z = \sqrt{eB/c} Q_z $$

Defined in this form, the new variables are independent of the choice of the vector potential $\mathbf{A}$. And, since an arbitrary constant could have been included in the definition of the orbit center variables without altering any of our succeeding conclusions, the new variables are
also independent of our choice of the origin of coordinates.

The Hamiltonian of an electron in a magnetic field with an arbitrary potential in terms of the usual variables is

\[ H = \frac{\hbar}{2m} \left( (p_x + \xi A_x)^2 + (p_y + \xi A_y)^2 + p_z^2 \right) + V(x,y,z). \]

In terms of the new variables, it is

\[ H = \frac{\hbar^2}{2mc} \left( p_x^2 + p_y^2 + p_z^2 \right) + V(\sqrt{\xi}(q_x - P_x), \sqrt{\xi}(q_y - P_y), \sqrt{\xi}q_z) \]

Now that one pair of conjugate variables \( p_x, q_x \), is missing from the first term of the Hamiltonian, a perturbation treatment of the lattice potential is much easier to handle.

We will first treat the relatively simple cosine potential,

\[ V(x,y,z) = -\varepsilon \left[ \cos(2\pi x/a) + \cos(2\pi y/b) + \cos(2\pi z/d) \right] \]

which will bring out most of the gross features of the problem. The Hamiltonian will then be

\[ H^0 + H^i = \frac{\hbar^2}{2mc} \left( p_x^2 + p_y^2 + p_z^2 \right) + \varepsilon \left[ \cos(\alpha q_x - P_x) + \cos(\beta q_y - P_y) + \cos(\gamma q_z) \right] \]

where we have defined the parameters:

\[ \alpha = \frac{2\pi}{a}, \quad \beta = \frac{2\pi}{b}, \quad \gamma = \frac{2\pi}{d}. \]

The energy eigenvalue equation is obtained by making the usual substitution of operators for variables.

\[ q_i \rightarrow q_i, \quad p_i \rightarrow -i\hbar \frac{\partial}{\partial q_i} \]

The Schrödinger equation is then written as

\[ (H^0 + H^i)\psi = \frac{\hbar^2}{2mc} \left[ -\frac{\partial^2}{\partial q_i^2} + q_i^2 \psi - \varepsilon \frac{\partial}{\partial q_i} \right] \psi - \varepsilon \left[ \cos(q_i + \frac{\partial}{\partial q_i}) + \cos\beta(q_i + i\frac{\partial}{\partial q_i}) + \cos\gamma q_z \right] \psi = (E^0 + E^i)\psi. \]
The cosine of an operator is to be interpreted as the equivalent expansion of that operator in an infinite series. This may be illustrated by considering the exponential or shifting operator.

\[ e^{i\omega P} \rightarrow \exp \left( i\omega \frac{\partial}{\partial Q} \right) = 1 + i\omega \frac{\partial}{\partial Q} + \frac{(i\omega)^2}{2!} \frac{\partial^2}{\partial Q^2} + \ldots \]

When the shifting operator is allowed to operate on an analytic function, we have

\[ \exp \left( i\omega \frac{\partial}{\partial Q} \right) \psi(q) = \psi(q) + i\omega \frac{\partial \psi}{\partial Q} + \frac{(i\omega)^2}{2!} \frac{\partial^2 \psi}{\partial Q^2} + \ldots = \psi(q + i\omega t). \]

Thus the cosine operator is to be interpreted as follows.

\[ \cos \left( \omega t \frac{\partial}{\partial Q} \right) \psi(q, Q_1, Q_2) = \frac{1}{2} \left[ e^{i\omega Q_2} \exp \left( i\omega \frac{\partial}{\partial Q_1} \right) + e^{-i\omega Q_2} \exp \left( -i\omega \frac{\partial}{\partial Q_1} \right) \right] \psi(q, Q_1, Q_2) \]

\[ = \frac{1}{2} \left[ e^{i\omega Q_2} \psi(q, Q_1, Q_2 - i\omega t, Q_2) + e^{-i\omega Q_2} \psi(q, Q_1, Q_2 + i\omega t, Q_2) \right] \]

The \( Q_3 \) or \( z \)-component of the Schroedinger equation separates to give

\[ \frac{\hbar}{2m} \left( -\frac{\partial^2}{\partial Q_3^2} \right) \psi(q, Q_1, Q_2) + (E \cos \gamma Q_3 + E_z) \psi(q, Q_1, Q_2) = 0 \]

which reduces to the problem of a particle in a one-dimensional, periodic cosine potential which is treated in detail elsewhere.

### II.A.2 Zero Order Solutions

The zero order problem in the transverse plane is then

\[ \mathcal{H}_0 \psi^0 = \frac{\hbar}{2m} \left[ -i^* \frac{\partial^2}{\partial Q_2^2} \right] \psi^0 = E^0 \psi^0 (q, Q_1). \]

In terms of \( Q_1 \), this is just the simple harmonic oscillator problem whose solutions we have found in section I.A.1.
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Since the zero order Hamiltonian does not contain $\alpha$, let us assume free particle solutions in that direction, so that the zero order solutions and energies are

$$\psi_{n, k'}(Q, Q_4) = \left[\frac{\alpha}{\pi L_4 \sqrt{E^2 + \alpha^2}}\right]^{-\frac{1}{4}} e^{i\frac{Q}{\alpha}k_4} \psi_n(Q, k_4) e^{iQ \cdot k / \alpha}, \quad E_{n} = (2n + 1) \frac{\hbar \omega}{2\pi c}.$$

In normalizing, we have assumed that the classical center of the electron orbit remains inside the boundary of the crystal or $-\frac{1}{2}L_x \leq x_0 = \psi_0 e^{iQ \cdot k / \alpha} \leq \frac{1}{2}L_x$. Landau, in his classic work, makes this same assumption which, in terms of the present variables, seems much more reasonable than it did at that time. Much work has been done to clarify the effect of the boundary on the energy states. It now seems generally accepted that the boundary effect is small and that the above assumption is a reasonable one. The quantity $P'_x$ is to be interpreted as an eigenvalue of quasi-momentum in the $Q_x$-direction. If periodic boundary conditions are imposed, such that

$$\psi_{n, k'}(Q, Q_4) = \psi_{n, k'}(Q, Q_4 + L_4 \sqrt{E^2 + \alpha^2})$$

then the eigenvalues of $P'_x$ are determined by

$$\exp(iQ \cdot P'_x / \hbar) = \exp(i(Q_4 + L_4 \sqrt{E^2 + \alpha^2}) P'_x / \hbar).$$

Thus, we have that

$$P'_x = \frac{\pi \hbar}{L_4} \sqrt{E^2 + \alpha^2} n_4 + \sqrt{\hbar^2 c^2} \frac{P'_x}{\hbar} = \pi n_4,$$

where $n_4$ is an integer. The range of $n_4$ is determined by the range of the quasi-momentum $P'_x$, that is

$$-\frac{1}{2}L_x \leq x_0 = -P'_x e^{iQ \cdot k / \alpha} \leq \frac{1}{2}L_x,$$

the classical center of the electron.
orbit must also remain inside the crystal in the x-direction. Thus the range of \( n_3 \) is given by

\[
\begin{align*}
\text{range} &= L x L y e^{B/2 \pi t c} \quad \text{from} \quad P_t' (\text{range}) = \frac{\pi L y}{L x} \frac{\sqrt{e B}}{L y} \quad n_3 (\text{range}) = \frac{L y}{L x} = \frac{L y}{L x}.
\end{align*}
\]

This is the total number of states in each magnetic energy level, except for a factor of two due to the spin states of the electron which we will not consider explicitly in this work.

II.A.3 Energy Corrections

To get a first correction to the energy, we must find the average value of the periodic potential perturbation over the zero order wave functions as follows.

\[
\begin{align*}
E_1' &= \int_{-L_y/2}^{L_y/2} dQ_y \int_{-L_y/2}^{L_y/2} dQ_y \left( \psi_{n,P_x'}(Q_y,Q_y) \right)^* V(Q_y-P_x,Q_y-P_x) \psi_{n,P_x'}(Q_y,Q_y).
\end{align*}
\]

The operators \( P_x, P_y \) operate on the zero order wave function to give

\[
\begin{align*}
&\frac{-i \hbar}{2} \left[ e^{iQ_y \cdot P_y'}(Q_y,Q_y) + e^{-iQ_y \cdot P_y'}(Q_y,Q_y) \right] \\
&\frac{-i \hbar}{2} [e^{iQ_y \cdot P_y'}(Q_y,Q_y) + e^{-iQ_y \cdot P_y'}(Q_y,Q_y) + e^{iQ_y \cdot P_y'}(Q_y-P_x,Q_y) + e^{-iQ_y \cdot P_y'}(Q_y,P_x,Q_y)].
\end{align*}
\]

We may treat the two types of integrals over \( Q_y \) first.

\[
\begin{align*}
\int_{-L_y/2}^{L_y/2} dQ_y e^{-iQ_y \cdot P_y'/k} e^{i(Q_y \cdot \sigma P_x)R'/k} &= L_y \sqrt{2 \pi} e^{i \pi R_y} \\
\int_{-L_y/2}^{L_y/2} dQ_y e^{-iQ_y \cdot P_y'/k} e^{-iQ_y \cdot \sigma P_x} e^{iQ_y \cdot \sigma P_x} &= \frac{2 \pi}{\hbar} \sin(\pi L_y/k) = \frac{2 \pi}{\hbar} \sqrt{2 \pi} \sin(\pi L_y/k).
\end{align*}
\]

The two types of integrals over \( Q_y \) may be seen to be

\[
\begin{align*}
\int_{-L_y/2}^{L_y/2} dQ_y e^{-iQ_y \cdot P_y'/k} H_y(Q_y \cdot P_y) &= 2^{1/2} \pi \sqrt{2 \pi} e^{-i \pi /k} L_y(k^\prime) \\
\int_{-L_y/2}^{L_y/2} dQ_y e^{-iQ_y \cdot P_y'/k} H_y(Q_y \cdot P_y) &= 2^{1/2} \pi \sqrt{2 \pi} e^{-i \pi /k} L_y(k^\prime).
\end{align*}
\]
Combining these results with the normalization factors, we obtain

\[ E_1' = -\varepsilon \left\{ \cos \phi \ R_i \ e^{-\frac{i}{\lambda} \ \phi} \ L_n \left( \frac{1}{2} \ a^* \ t \right) + \ \frac{\kappa}{\pi \lambda} \ \sin \left( \frac{\pi \ t}{\lambda} \right) \ e^{-\frac{i}{\lambda} \ \phi} \ L_n \left( \frac{1}{2} \ a^* \ t \right) \right\} \]

\[ = -\varepsilon \left\{ \cos \left( \frac{\pi \ t}{\lambda} \right) \ e^{-\frac{i}{\lambda} \ \phi} \ L_n \left( \frac{\pi \ t}{\lambda} \right) + \ \frac{\kappa}{\pi \lambda} \ \sin \left( \frac{\pi \ t}{\lambda} \right) \ e^{-\frac{i}{\lambda} \ \phi} \ L_n \left( \frac{\pi \ t}{\lambda} \right) \right\} . \]

The second factor in the brackets has the form \( \sin x \) which is zero if there are an integral number of unit cells in the periodically extended crystal, \( L_y = n \), and which is small if \( L_y \) is large, in any case. Thus we will neglect it. Note also that \( \alpha \ R_i = \frac{\pi \ t}{\lambda} / a \), so that the energy with the correction is

\[ E_1'' + E_1' = (2 n + 1) e k B / 2 m = -\varepsilon \cos \left( \frac{\pi \ t}{\lambda} \right) \ \exp \left( -\frac{\pi \ t}{\lambda} \ \phi \right) \ L_n \left( \frac{\pi \ t}{\lambda} \right) . \]

Thus the energy now depends on the position of the center of the electron orbit. It is periodic in the position of the orbit center \( x_0 = \frac{\pi \ t}{\lambda} \ \frac{\kappa}{\pi \lambda} \ n \), which may now only take on discrete values, the range being \( x_0 (\gamma \ \alpha \ \phi) = L_y \). Thus each magnetic level is now spread out into a band of energies, the width of which is proportional to the lattice potential energy and is also a function of the magnetic field.

To get some quantitative feeling for what this correction means, let us take a metal with a Fermi energy \( \eta = 2.12 \text{ ev} \) and a lattice constant of \( a = 5.33 \times 10^{-8} \text{ cm} \). In the spirit of the nearly free electron approximation, we may assume that the lattice potential energy \( \varepsilon \), is equal to
the energy gap at the first Brillouin zone or \( \gamma = 0.27 \approx 0.42 \text{ eV} \). The magnetic energy must be greater than the lattice potential energy for the above correction to have any quantitative significance. This means we must have magnetic fields like

\[
B \geq \left( 0.42 \text{ eV} \times 5.79 \times 10^{-1} \text{ eV/gauss} \right) = 7.32 \times 10^7 \text{ gauss}
\]

Note that at this magnetic field, only the three lowest magnetic levels are completely filled by all the electrons in the solid. The classical radius of the electron orbit at the Fermi energy is then \( r = \frac{\hbar c}{eB} = 3.02 \times 10^{-6} \text{ cm} \), or about the same size as a lattice cell. Since the zeroth order Laguerre polynomial is unity, we have a correction factor

\[
\exp \left( -\pi r^2 \alpha^2 \right) = \exp (-3.18) = 0.041.
\]

The qualitative validity of the above approximation may extent to lower fields because as the field decreases, so does the exponential in the correction term, but the higher order Laguerre polynomials will also contribute, so that the field cannot be lowered too much. Note that the Laguerre polynomials will make the correction go to zero at certain values of the field, at least in this first approximation. This suggests the possibility of interesting experimental effects at high magnetic fields.
II.B. Arbitrary Periodic Potential

To demonstrate the requirements of a more general approach to the determination of the energy correction, an arbitrary periodic potential is specified by its Fourier series expansion in terms of reciprocal lattice vectors and the energy correction is calculated.

II.B.1 Definition of Variables

To obtain the set of three independent pairs of conjugate variables, we choose the magnetic field to lie along the z-axis and define the following variables by assuming a vector potential $\mathbf{A} = (-\frac{i}{\hbar} \mathbf{B}, \frac{j}{\hbar} \times \mathbf{B}, 0)$.

\[
P_i = \sqrt{\hbar} (P_x - \frac{e}{m} B_y), \quad P_k = \sqrt{\hbar} (P_y + \frac{e}{m} B_x), \quad P_3 = \sqrt{\hbar} P_z
\]

\[
Q_i = \sqrt{\hbar} (P_y + \frac{e}{m} B_x), \quad Q_k = \sqrt{\hbar} (P_x - \frac{e}{m} B_y), \quad Q_3 = \sqrt{\hbar} z
\]

The commutation relations are easily verified to be the following.

\[
[P_i, Q_j] = -i\hbar \delta_{ij}, \quad [P_i, P_j] = [Q_i, Q_j] = 0
\]

The factor of $\sqrt{\hbar/e}$ appears in the definitions so that the commutation relations will have this form. The sign of the electron charge has been included explicitly, so that $e = -ie$.

The transformation to and from the $x, y, z$-coordinates may be accomplished by using the following generating function.

\[
S(x, y, z, P_x, P_y, P_z) = P_x P_z + \sqrt{\hbar/e} (x P_z + y P_x + z P_y) + (eB/2c)x^2 y
\]

The inverse relations are as follows.
\[ P_x = \frac{1}{2} \sqrt{E_x} (P_1 + Q_2), \quad P_y = \frac{1}{2} \sqrt{E_y} (P_1 + Q_1), \quad P_z = \sqrt{E_z} P_3 \]
\[ X = \sqrt{E_x} (Q_2 - P_1), \quad Y = \sqrt{E_y} (Q_1 - P_1), \quad Z = \sqrt{E_z} Q_2 \]

The Hamiltonian in terms of the old variables is
\[ H = \frac{1}{2m} \left[ (P_x - \frac{\partial}{\partial X})^2 + (P_y - \frac{\partial}{\partial Y})^2 + (P_z - \frac{\partial}{\partial Z})^2 \right] + V(x, y, z). \]

In terms of the new variables, it is
\[ H = \frac{\hbar}{2\sqrt{mc}} \left[ \hat{P}_1^2 + \hat{Q}_1^2 + \hat{P}_3^2 \right] \cdot V(\sqrt{E_x}(Q_2 - P_1), \sqrt{E_y}(Q_1 - P_1), \sqrt{E_z} Q_2). \]

Now, only \( P_1, Q_1, P_3 \) appear in the first term, making a perturbation treatment of the lattice potential much easier to work with.

An arbitrary periodic lattice potential may be written
\[ V(\vec{r}) = \sum_{k} c(k^*) \exp(i \vec{k} \cdot \vec{r}) \]
\[ c(k^*) = \frac{1}{(2\pi)^3} \int_{\text{unit cell}} V(\vec{r}) \exp(-i\vec{k} \cdot \vec{r}) d\vec{r} = C(-k^*) \]

The reciprocal lattice vector is
\[ \vec{k}^* = n_x \vec{a}_1 + n_y \vec{a}_2 + n_z \vec{a}_3. \]

The periodicity of the lattice potential may be demonstrated by adding an arbitrary lattice vector
\[ \vec{R} = m_1 \vec{a}_1 + m_2 \vec{a}_2 + m_3 \vec{a}_3 \]

to the position vector \( \vec{r} \).
\[ V(\vec{r}) = V(\vec{r} + \vec{R}) \]
\[ \vec{k}^* \cdot \vec{R} = m_1 n_1 + m_2 n_2 + m_3 n_3 = \sigma, \quad e^{i\vec{k} \cdot \vec{R}} = 1. \]

Since the unit vectors of the crystal need have no specific relation to the system of coordinates chosen,
we may choose the $z$-axis to be always parallel to the magnetic field. Thus the Hamiltonian may be written, in terms of the new variables, as follows.

$$
H' = \frac{eB}{2\pi c} \left[ R^2 + Q^2 + R_x^2 \right] + \frac{\hbar}{2m} \sum \chi \exp \left[ \frac{2\pi i}{L_z} \left( R_x^2 (Q_x - R_x) + R_y^2 (Q_y - R_y) + R_z^2 (Q_z - R_z) \right) \right]
$$

where $R_x, R_y, R_z$ are the components of the reciprocal lattice vector resolved along the three respective coordinate axes.

II.B.2 Zero Order Eigenfunctions

The zero order eigenfunctions and eigenvalues may be found from the zero order Schroedinger equation.

$$
H' \psi' = \frac{eB}{2\pi c} \left[ -\nabla^2 \psi' + Q^2 \psi' - 4^4 \psi' \right] = E' \psi'
$$

The normalized solutions and eigenvalues are

$$
\psi_{n_1, n_2} (Q, Q_z) = \left[ \frac{x^n}{\pi x^n! \sqrt{\pi e^4 \hbar^4 L_z}} \right]^{-\frac{1}{2}} e^{iQ_x R_x^2} e^{-Q_y^2/2L_z^2} \chi_n(Q, k^z)
$$

$$
E_{n_1, n_2} = \frac{eB}{2\pi c} \left[ (2n+1) \frac{k^2}{2} + R^2 \right]
$$

where $H_n(Q, k^z)$ are the Hermite polynomials of order $n$.

In normalizing the wave-function in the $Q_z$-direction, we have assumed periodic boundary conditions,

$$
\psi_{n_1, n_2} (Q, Q_z) = \psi_{n_1, n_2} (Q, Q_z + L_z \sqrt{e^4 \hbar^4})
$$

where $L_z = N_{a_1} a_1 + N_{a_2} a_2 + N_{a_3} a_3$. $N_{a_1}, N_{a_2}, N_{a_3}$ are integers defining the number of unit cells in the crystal in the three directions parallel to the unit cell vectors. $a_1, a_2, a_3$ are the unit cell vectors resolved along the axis parallel to the magnetic field. The quasi-momentum eigenvalues $P_z$, are discrete under finite boundary conditions. The actual
values may be obtained from the periodicity conditions.

\[ P'_y = \frac{2\pi \hbar k_y \sqrt{\varepsilon/\varepsilon_B}}{L_y} \text{ from } \frac{1}{2} P'_y L_y \sqrt{\varepsilon/\varepsilon_B} = 2\pi \hbar k_y \]

The maximum value that \( P'_y \) may have for a given energy is

\[ P'_y (\text{max}) = \frac{\sqrt{2\pi m_c/\varepsilon_B} E - (2\pi n_k)^2}{L_y} \]

Since the variables \( r, q_a \) do not appear in the zeroth order Hamiltonian, we may choose an arbitrary function subject only to the periodic boundary conditions. Let us then choose an expansion in plane wave states.

\[ V(Q_a) = \left[ L_y \sqrt{\varepsilon/\varepsilon_B} \right]^{-1/2} \sum_{r'} A(r') \exp \left( iq_a Q_a \right) \]

The boundary condition is

\[ V(Q_a) = V(Q_a + L_y \sqrt{\varepsilon/\varepsilon_B}) \]

where \( L_y = N_x a_y + N_y a_y + N_z a_y \)

which yields values of the quasi-momentum in the \( Q_a \)-direction.

\[ P'_y = \frac{2\pi \hbar k_y \sqrt{\varepsilon/\varepsilon_B}}{L_y} \]

This corresponds to moving the center of the electron orbit in the \( y \)-direction from some point in the crystal to an equivalent point in the next part of the periodically extended crystal. The range of the eigenvalues of \( P'_y \) may be found by requiring that the \( x \)-component of the orbit center remain inside the crystal. Thus we have

\[ P'_y (\text{range}) = \frac{L_x \sqrt{\varepsilon/\varepsilon_B}}{2} \text{ or } P'_x (\text{range}) = \frac{L_x \sqrt{\varepsilon/\varepsilon_B}}{2\pi \hbar} \]

Note that the total magnetic flux penetrating the crystal is \( \Phi = L_y B \). If the spin of the electron is included, then the total number of states in the plane perpendicular to the magnetic field is
\[ z n_s(y_{avg}) = \Phi(z e/kc) \]

which is equal to the total number of superconducting flux quanta penetrating the crystal. In the case of the free electron in a magnetic field, this represents the degeneracy of each magnetic level. This means that as the magnetic field changes, the number of electrons that can be accommodated in each magnetic level changes by discrete steps corresponding to a change of one superconducting magnetic flux quantum. Thus we should write that the range of \( n_s \) is the integer which is just less than or equal to the number of flux quanta penetrating the sample.

II.B.3 Energy Correction

In the spirit of the nearly free electron approximation, let us assume a trial wave function of the following form.

\[ \psi^{P_x}_{n_s}(Q_x, Q_y, Q_z) = [2^n n! \pi^{n-1} \pi L_x L_y L_z e^B/e]^{-\frac{1}{2}} e^{-Q_x^2/2} H_n(Q_x, i/\kappa) \sum_{P_x} A(P_x) e^{iQ_x P_x^x} e^{iQ_y P_y^y} e^{iQ_z P_z^z} \]

To evaluate the parameters \( A(P_x) \), and to find the energy eigenvalues, we find the matrix elements as follows.

\[ \langle P_x', P_y', P_z' | H^0 + H' | P_x, P_y, P_z \rangle = [2^n n! \pi^{n-1} \pi L_x L_y L_z e^B/e]^{-\frac{1}{2}} \int_{-\frac{1}{2} L_x a \kappa c}^{\frac{1}{2} L_x a \kappa c} dz_0 \int_{-\frac{1}{2} L_y a \kappa c}^{\frac{1}{2} L_y a \kappa c} dz_0 \int_{-\frac{1}{2} L_z a \kappa c}^{\frac{1}{2} L_z a \kappa c} dz_0 \cdot e^{-Q_x^2/2} H_n(Q_x, i/\kappa) e^{-iQ_x P_x^x} e^{-iQ_y P_y^y} (H^0 \cdot H') \psi^{P_x}_{n_s}(Q_x, Q_y, Q_z). \]

The integral over \( H^0 \) gives simply

\[ \frac{e^B}{2mc} [(2n+1) \pi + P_z^2] A(P_x^0). \]
If we let
\[ H' = \sum_{\mathbf{R}} C(\mathbf{R}) \exp\left\{ i\mathbf{a} \cdot (\mathbf{Q} - \mathbf{R}) + \mathbf{p} \cdot (\mathbf{Q} - \mathbf{R}) + i\mathbf{Q} \cdot \mathbf{b}\right\}, \quad \mathbf{a} = 2\pi R_x \mathbf{e}_x, \quad \mathbf{p} = 2\pi R_y \mathbf{e}_y, \quad \mathbf{b} = 2\pi R_z \mathbf{e}_z, \]
then its operation on \( \psi^0 \) gives
\[ H' \psi^0_{\mathbf{Q}_2}(\mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3) = \sum_{\mathbf{R}_1} C(\mathbf{R}_1) e^{i\mathbf{Q}_1 \cdot \mathbf{R}_1 + i\mathbf{Q}_2 \cdot \mathbf{R}_1} \left\{ \begin{array}{c}
\sum_{\mathbf{R}_2} \mathcal{A}(\mathbf{R}_2^0) e^{i\mathbf{Q}_2 \cdot \mathbf{R}_2^0} e^{i(\mathbf{Q}_2 \cdot \mathbf{R}_2 + \mathbf{Q}_3 \cdot \mathbf{R}_2^0)} \\
\mathcal{H}(\mathbf{Q}_2 \cdot \mathbf{R}_2 + \mathbf{Q}_3 \cdot \mathbf{R}_2^0)
\end{array} \right\} \psi^0_{\mathbf{Q}_2}. \]

Integrating over \( \mathbf{Q}_2 \), we have
\[ \left[ \frac{1}{L_x L_y L_z} \right] \int_{-\frac{1}{2}L_x}^{\frac{1}{2}L_x} d\mathbf{Q}_2 e^{-i\mathbf{Q}_2 \cdot \mathbf{R}_2} e^{i\mathbf{Q}_2 \cdot \mathbf{R}_2} = \delta(\mathbf{Q}_2 + \mathbf{Q}_1 - \mathbf{Q}_3). \]
The actual solution is
\[ \left[ L_x L_y L_z \mathcal{S}\left(\mathbf{P}_2^0 - \mathbf{P}_2^0\right) \right] \mathcal{S}\left(\mathbf{P}_2^0 + \mathbf{P}_2^0\right) \to \mathcal{S}(2\pi R_z) \mathcal{S}(P_2^0 + P_2^0) \]
which approaches a delta function in the limit as the crystal becomes infinite. For this reason, we will assume that all terms are negligible except when
\[ P_2^0 + 2\pi R_z = P_2^0. \]
The integral over \( \mathbf{Q}_2 \) is
\[ \left[ \frac{1}{L_x L_y L_z} \right] \int_{-\frac{1}{2}L_x}^{\frac{1}{2}L_x} d\mathbf{Q}_2 e^{-i\mathbf{Q}_2 \cdot \mathbf{R}_2} e^{i\mathbf{Q}_2 \cdot \mathbf{R}_2} = e^{-\pi R_z} \mathcal{S}(P_2^0 + \mathbf{P}_2^0). \]
The reasoning behind the delta function is the same as above. We will assume the crystal to be large enough so that all terms are negligible except when
\[ P_2^0 + 2\pi R_z = P_2^0. \]

The integral over \( \mathbf{Q}_1 \) is
\[ \left[ \frac{1}{L_x L_y L_z} \right] \int_0^{\infty} d\mathbf{Q}_1 e^{-\mathbf{Q}_1^2/2} h_{\mathbf{Q}_1} \mathcal{H}(\mathbf{Q}_1, \mathbf{P}_2, \mathbf{P}_3) = \exp \left\{ -\frac{1}{2}(x + iZ_{10} + P_3) \right\} \mathcal{L}_n \left( \frac{1}{2}(x + iZ_{10}) \right). \]
The integrals over \( H' \) give
\[ \sum_{\mathbf{R}} C(\mathbf{R}) \mathcal{A}(\mathbf{R}_2^0 + \mathbf{P}_2^0) e^{-\frac{1}{2}(x + iZ_{10} + P_3)} \mathcal{L}_n \left( \frac{1}{2}(x + iZ_{10}) \right) e^{-i\mathbf{Q}_2 \cdot \mathbf{R}_2}. \]
Since the matrix element may also be written
\[ \langle R''_x, R''_y | H | R'_x, R'_y \rangle = E_k A(R'_x) \]
we may write the infinite set of simultaneous equations as
\[
\begin{align*}
\{ E - \frac{g_e}{2} \left[ (2 \mu \hbar \omega) + P_y'^2 \right] \} A(R'_x) &= \\
&= \frac{g_e}{2} C(R'_x) A(R'_x - 2n \hbar R_y^0 \sqrt{\hbar}) e^{-\frac{P_x'^2}{2\hbar}} \left( R_y'^2 - 2i \mu \hbar \omega R_y^0 R_y'^0 + \hbar \omega^2 \right) \sum_{n \neq 0} e^{i \mu \hbar \omega R_y^0 (R_y'^0 + R_y^0)} C(R_y'^0) \\
&= \frac{g_e}{2} C(R'_x) A(R'_x - 2n \hbar R_y^0 \sqrt{\hbar}) e^{-\frac{P_x'^2}{2\hbar}} \left( R_y'^2 - 2i \mu \hbar \omega R_y^0 R_y'^0 + \hbar \omega^2 \right) \sum_{n \neq 0} e^{i \mu \hbar \omega R_y^0 (R_y'^0 + R_y^0)} C(R_y'^0).
\end{align*}
\]
This set of simultaneous equations would lead to an exact solution to the eigenvalue problem, it it could be solved. To obtain an approximate solution, we assume that the off-diagonal elements are small enough to be neglected in the evaluation of the determinant for the energy values. The determinant will then vanish if one of the diagonal elements vanishes, which leads to
\[
E_{n}\beta, R_y^0 = \frac{g_e}{2} \left[ (2 \mu \hbar \omega) + P_y'^2 \right] + \frac{g_e}{2} C(R'_x, 0, 0) e^{-\frac{P_x'^2}{2\hbar}} \sum_{n \neq 0} e^{i \mu \hbar \omega R_y^0 (R_y'^0 + R_y^0)} C(R_y'^0) e^{-\frac{P_x'^2}{2\hbar}}.
\]
The first term is the expression of the magnetic energy levels. The second term is the usual parabolic dependence on the z-component of the wave-vector near the center of the Brillouin zone. In the third term, the sum is over
\[ R_x^0 = n \alpha + n \beta + \alpha \beta \] only, since the diagonal terms are given by setting \( R_y^0 = R_y^0 = 0 \). The result reduces to that of section II.A.3 when the following assumptions are made:
\[ C(R_x^0) = 0 \] except for \( C(\alpha \beta) = C(-\alpha \beta) = -\frac{1}{2} \varepsilon \), \( \alpha \beta = \frac{1}{a} \).

This result now provides a powerful tool for determining the actual Fourier coefficients in the expansion of the periodic lattice potential in reciprocal
lattice space. At sufficiently high fields, one-hundred megagauss and greater, only the lowest magnetic levels will be filled. The magnetic susceptibility may then be calculated numerically with accuracy for various magnetic fields and for an arbitrary direction in a crystal lattice with assumed values of the Fourier coefficients which may then be compared directly with experiment.

Note that the matrix elements for transitions between magnetic levels may be calculated with ease using the integral transform of Appendix I.

III. Extension of the Sommerfeld Quantization Technique

In an effort to clarify the Onsager semiclassical quantization scheme, as it is usually applied to the theory of metallic electrons in a magnetic field, the Sommerfeld quantization technique is studied in terms of the principle of the argument in the theory of the complex variable.

III.A Contour Integration

The argument principle is usually stated as follows.

Theorem: Let \( f(z) \) be analytic in a domain D. Let C be a simple closed path in D within which \( f(z) \) is analytic except for a finite number of poles and zeros
and on which \( f(z) \) is non-zero. Then

\[
\oint_C \frac{f'(z)}{f(z)} \, dz = N_\ast - N_p
\]

where \( N_\ast \) is the total number of zeros of \( f(z) \) inside \( C \) and \( N_p \) is the total number of poles of \( f(z) \) inside \( C \), zeros and poles being counted according to their respective multiplicities.

Proof: The logarithmic derivative \( \frac{d}{dz} \log f(z) = \frac{f'(z)}{f(z)} \) has isolated singularities at the zeros and poles of \( f(z) \). At a zero, \( z_\ast \), of order \( N_\ast \), the function \( f(z) \), may be written as a product

\[
f(z) = (z - z_\ast)^N q(z)
\]

where \( q(z) \) is not zero at \( z = z_\ast \). The logarithmic derivative is then

\[
\frac{d}{dz} \log f(z) = \frac{d}{dz} \left[ N \log (z - z_\ast) + \log q(z) \right] = \frac{N}{z - z_\ast} + \frac{f'(z)}{f(z)} .
\]

Hence the logarithmic derivative has a pole of first order, with a residue \( N \) equal to the multiplicity of the zero provided the curve \( C \) encloses \( z = z_\ast \). The same argument holds when considering the poles of \( f(z) \) with \( N \) replaced by \(-N\). The theorem then follows from the consideration of the Cauchy residue theorem given in standard texts\(^{22}\).

III.B Phase Integral

This theorem may now be applied to the elucidation of the Sommerfeld quantization technique in the following
manner. The Hamiltonian of a particle in one dimension is
\[ H = \frac{p^2}{2m} + V(x). \]
The time independent energy eigenvalue equation is obtained by replacing the variables by quantum mechanical operators:
\[ x \rightarrow x, \quad p \rightarrow [p, x] = i\hbar \frac{\partial}{\partial x}. \]
Thus we obtain
\[ \frac{\partial^2 \psi}{\partial x^2} + \frac{\hbar^2}{m} [E - V(x)] \psi = 0. \]
Note that this equation may also be written
\[ \frac{\partial^2 \psi}{\partial x^2} + \frac{\hbar^2}{m} \psi = 0 \quad \text{since} \quad p^2 = \frac{\hbar^2}{m} [E - V(x)] \]
in the classical sense.

Let us now expand the logarithm of the wave function in an asymptotic series in powers of Planck's constant \( \hbar \).
\[ \log \Psi(x) = \frac{1}{\hbar} [S_0(x) + \frac{\hbar}{i} S_1(x) + \left( \frac{\hbar^2}{8} \right) S_2(x) + \ldots]. \]
This expansion does not converge in its present form but this will not concern us since we will replace the variable \( x \) by its complex form \( z \) and integrate the logarithmic derivative about a closed contour \( C \) in the complex \( z \)-plane which just encloses all the zeros of the wave function, \( \Psi(x) \). This can be done because the wave function, \( \Psi(x) \), is finite everywhere inside the range of interest, and all the zeros of the wave function lie on the real axis between the turning points of the potential, that is, for
\[ \frac{1}{2m} p^2 = E - V(x) > 0. \]
Thus we may write
\[ 2\pi i N_0 = \Phi_c \int \frac{\psi'(z)}{\psi(z)} dz = \frac{1}{\lambda} \Phi_c \sum_{n=0}^{\infty} \frac{\lambda^2}{n^2} \delta_{c} \sum_{n=0}^{\infty} \frac{\lambda^2}{n^2} \delta_{c} + \cdots \]
where \( N_0 \) is the number of zeros contained inside the contour \( C \).

Now the Schroedinger equation can give the form of the \( S' \) functions as follows.
\[ \psi'' \psi = (\psi \psi')' + (\psi \psi')^2 = \frac{1}{\lambda} \sum_{n=0}^{\infty} \frac{\lambda^2}{n^2} \delta_{c} \sum_{n=0}^{\infty} \frac{\lambda^2}{n^2} \delta_{c} + \cdots = -\hbar^2 \frac{\lambda^2}{\lambda^2} \]
The equation must be satisfied for an arbitrary value of \( \hbar \), so the coefficient of each power of \( \hbar \) may be set independently equal to zero. Thus we get
\[
\begin{align*}
(\psi')' &= -\frac{\lambda^2}{\lambda^2} \\
\psi'' + 2\psi' \psi &= 0 \\
\psi'' + (\psi')^2 + 2\psi' \psi &= 0
\end{align*}
\]
Now the Bohr-Sommerfeld phase integral is
\[ \Phi_c \sum_{n=0}^{\infty} \frac{\lambda^2}{n^2} \delta_{c} dz = \Phi_c \int_{C} \frac{\lambda^2}{\lambda^2} dz \]
where the \( \pm \) signs have been incorporated into the contour integration. Note that the second term may be written as
\[ \Phi_c \sum_{n=0}^{\infty} \frac{\lambda^2}{n^2} \delta_{c} dz = -\int_{C} \Phi_c \frac{[E-\nu(z)]'}{[E-\nu(z)]} dz = -\frac{1}{\lambda^2} \pi (\lambda i \nu) \]
where \( \nu \) is the number of zeros of the function \( E-\nu(z) = 0 \) inside the contour \( C \). Therefore the Bohr-Sommerfeld phase integral may be written as
\[ \Phi_c \int_{C} \frac{\lambda^2}{\lambda^2} dz = 2\pi \pi \left( \nu_0 + \frac{1}{2} \nu \right) + O(\lambda^2) \]
To obtain the energy eigenvalues from this relation, the contour integration
\( \zeta_c \rho dx = \sqrt{2m} \zeta_c \sqrt{E-V(x)} \, dz \)

is performed over the area of interest in the complex z-plane with the energy \( E \), as a parameter.

### III.C Harmonic Oscillator Potential

In the case of the harmonic oscillator potential 
\( V(x) = ax^2 \)

there is a cut in the complex plane joining the two points 
\( x = \pm \sqrt{E/\alpha} \)

across which the contour must not pass if it is to stay on the same Riemann surface. Thus we will take the contour to surround the cut completely in one sense or another. All the zeros of the oscillator wave function lie on the real axis between the above two points. Thus the contour will enclose all these zeros and the number of the zeros will be equal to \( n_\nu \). The momentum function 
\( p^2 = 2m(E-V(x)) = 2m(E-ax^2) \)

is zero at only the above two points, so that \( n_\nu = 2 \). Thus
\[ \sqrt{2m} \zeta_c \sqrt{E-ax^2} \, dz = 2\pi \hbar (n_\nu + \nu_\nu) + O(t^3). \]

The only pole of the above function is at infinity. One way to evaluate the integral is to make the replacement

\( z = -iv \) , \( dz = dt/t^2 \)

where the negative sign preserves the positive sense of the contour integral.
\[ \int \sqrt{E - \alpha x^2} \, dx = \int \sqrt{E t^2 - a} \, dt / t^3. \]

Now the contour need only surround the pole at \( t = \infty \), which may be found from the residue theorem.

\[ i \sqrt{E} \int \frac{dt}{t^3} \sqrt{E t^2 - \alpha} \int = i \sqrt{E} \int \frac{dt}{t^3} \left[ \sqrt{E} - \frac{1}{2} \frac{\sqrt{E}}{t} + O(t^{-1}) \right] = i \sqrt{E} \pi i \left( -\frac{1}{2} \frac{\sqrt{E}}{t} \right) = \frac{\pi E}{\sqrt{\alpha}}. \]

Thus the contour integral has the value \( \pi E / \sqrt{\alpha} \), and the energy is

\[ E = \frac{\pi E}{\sqrt{\alpha}} \frac{\hbar^2}{2m} + O(t^{-1}). \]

In the case of the harmonic oscillator potential, it turns out that the higher order terms in \( \hbar \) can be shown to have zero residues since no one of them has a term like \( \frac{1}{t^2} \) or its equivalent in their Laurent series expansions. This, of course, may not be the case in other types of potentials.

III.D Onsager Quantization

The Hamiltonian for a free electron in a magnetic field may be written in terms of the velocities.

\[ \mathcal{H} = \frac{1}{2m} \left( v_x^2 + v_y^2 + v_z^2 \right) \]

Let us restrict our attention to the plane perpendicular to the magnetic field which we will take to be in the \( z \)-direction. The commutation relation between the two components of velocity was found in section I.D.1 to be

\[ [v_x, v_y] = -ie\hbar B / m^2 c. \]

Thus if we consider \( v_x \) to be a momentum like variable and \( v_y \) to be coordinate like, then the operator replacement is
\[ V_x \rightarrow [v_x, v_y] \frac{\partial}{\partial v_x} = -i \left( \frac{e k B}{m c} \right) \left( \frac{\partial}{\partial v_x} \right) \]

and Schrödinger's equation may be written as

\[ \frac{\hbar}{i} \left[ -\left( \frac{e k B}{m c} \right) \frac{\partial^2}{\partial v_x^2} + v_y \psi \right] = E \psi . \]

This is just a form of the harmonic oscillator equation, for which we may write the phase integral directly as follows.

\[ \frac{1}{2 \pi i} \oint_c V_x dV_y = [v_x, v_y] (n + v_y) = -i \left( \frac{e k B}{m c} \right) (n + v_y) \]

But since the energy may be written as

\[ v_x = \frac{\hbar}{m} E - V_x \]

then the contour integration yields

\[ \oint_c V_x dV_y = \oint_c \sqrt{E - V_x^2} dV_y = \frac{\hbar}{m} E \cdot \pi = 2 \pi \left( \frac{e k B}{m c} \right) (n + V_x) \]

and we obtain the energy eigenvalues

\[ E = (\lambda n + 1) \frac{e k B}{mc} . \]

Thus, the variables \( \bar{v} \), which Onsager defines, are equivalent to the velocity variables as defined above (see appendix IV).

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Integration over Hermite Functions

Prove the following integration.

\[ I_{m,n}(x,y) = \int_{-\infty}^{\infty} e^{-\frac{1}{2}z^2} H_n(z) e^{-\frac{1}{2}(x+z)^2} H_n(x+z) e^{iyz} \, dz = \]
\[ = \sqrt{\pi} 2^m n! (i\pi - x)^m n e^{-\frac{1}{2}(x^2 + 2ixy + y^2)} L_n^{(m-n)}(x^2 + y^2) \]

To prove this integration, use the generating function for the Hermite polynomials.

\[ e^{zt - t^2} = \sum_{n=0}^{\infty} H_n(z) t^n / n! \] \[ \therefore H_n(x) = \lim_{t \to \infty} \frac{d^n}{dt^n} (e^{zt - t^2}) \]

then

\[ I(x,y) = \int_{-\infty}^{\infty} e^{-\frac{1}{2}z^2} e^{zt - t^2} e^{-\frac{1}{2}(x+z)^2} e^{z(x+z)u - u^2} e^{iyz} \, dz \]

where

\[ I_{m,n}(x,y) = \lim_{t \to \infty} \frac{d^m}{dt^m} \left( \lim_{u \to \infty} \frac{d^n}{du^n} I(x,y) \right). \]

Thus

\[ I(x,y) = e^{-t^2 - \frac{1}{2}x^2 + 2xy - u^2} \int_{-\infty}^{\infty} e^{-z^2 + z(2t-x+2u+iy)} \, dz \]

Let \( z = x + t - \frac{1}{2}xu + \frac{1}{2}iy \), then \( \int_{-\infty}^{\infty} e^{-2t^2} dz = \sqrt{\pi} \) and

\[ I(x,y) = \sqrt{\pi} e^{-\frac{1}{2}t^2 - \frac{1}{2}x^2 + xu - u^2 + (t-\frac{1}{2}xu + ty)^2} \]
\[ = \sqrt{\pi} e^{-\frac{1}{2}t^2 - \frac{1}{2}(x^2 + 2xy - ta + xy - thy - ty)} \]
\[ = \sqrt{\pi} e^{-\frac{1}{2}(x^2 + 2(x+y)u)} e^{t(\pi-x)} e^{u(x+2u+y)}. \]

Expand the last exponential in an infinite series.

\[ I(x,y) = \sqrt{\pi} e^{-\frac{1}{2}(x^2 + 2(x+y)u)} e^{t(\pi-x)} \sum_{n=0}^{\infty} \frac{(2t+x+y)^n}{n!} u^n / n! \]

The limit of the n-th derivative is

\[ I_n(x,y) = \lim_{t \to \infty} \frac{d^n}{dt^n} I(x,y) = \sqrt{\pi} e^{-\frac{1}{2}(x^2 + 2(x+y)u)} e^{t(\pi-x)} (2t+x+y)^n. \]

Expand the exponential and the polynomial in powers of t

\[ I_n(x,y) = \sqrt{\pi} e^{-\frac{1}{2}(x+y)^2} \sum_{k=0}^{n} \frac{(x+y)^k}{k!} \sum_{m=0}^{k} \frac{n! (x+y)^m (2t)^{n-m}}{m! (n-k)!}. \]
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The limit of the m-th derivative is
\[
I_{m,n}(x,y) = \lim_{t \to 0^+} \frac{d^m}{dt^m} I_m(x,y) = \sqrt{\pi} \frac{(-1)^m}{(m+n)!} \left( \frac{k}{n} \right)^m \left( \frac{\alpha}{k} \right)^n \frac{\Gamma(n)}{\Gamma(n+m)} \frac{1}{(n-m-k)!} \frac{1}{(n-k)!} \frac{1}{(n-k)!} \frac{1}{(m+n+k)!} \left( \frac{x^2 + 2\alpha y + y^2}{k^2} \right)^n. \]

The generalized Laguerre polynomials are defined as
\[
L_n^{(\alpha)}(x) = \sum_{k=0}^{n} \frac{(-1)^k}{k!} \frac{(x+\alpha)!}{(n-k)!} \frac{(\alpha+k)!}{(n-k)!} x^k. \]

If we identify \( \alpha = m-n \) and \( z = \frac{1}{2}(x^2 + y^2) \), we see that
\[
L_n^{(m-n)}(\frac{x^2 + y^2}{k^2}) = \sum_{k=0}^{n} \frac{(-1)^k}{k!} \frac{m!}{(n-k)!} \frac{(m+n)!}{(n-k)!} x^k. \]

Thus we have the required result.
\[
I_{m,n}(x,y) = \sqrt{\pi} \frac{x^n}{n!} \left( \frac{\alpha}{k} \right)^n \frac{\Gamma(n)}{\Gamma(n+m)} \frac{1}{(n-m-k)!} \frac{1}{(n-k)!} \frac{1}{(n-k)!} \frac{1}{(m+n+k)!} \left( \frac{x^2 + 2\alpha y + y^2}{k^2} \right)^n. \]

Appendix II

High Field Correction to the de Haas–van Alphen Effect

The usual treatments of the de Haas–van Alphen effect make the approximation that the Fermi energy, \( \eta \), is much greater than the magnetic field energy, \( eB/2mc \). It seems reasonable to ask what corrections need to be made when this approximation no longer holds. A more precise calculation may be done as follows.

The energy eigenvalues of an electron in a uniform magnetic field are
\[
E = (2m+1) \frac{eB}{2mc} + \frac{ck^2}{2m} \]
there being, \( eB/2mc \), states for each energy level. If we regard \( \kappa_z \) as practically continuous, the number of states below \( E \) is
\[ Z(E) = \left( \frac{\sqrt{n!}}{4\pi n^{3/2}} \right) \mathcal{R} \left\{ \frac{e^{-n/2}}{\sqrt{2\pi n}} \right\} \]

where the sign \( \mathcal{R} \) indicates that only the real part of the complex sum is to be considered, and the Bohr magneton is \( \mu = e^2/hmc \).

The free energy is
\[ F = N\eta - 2 \int Z(E) \left( 1 + e^{(E-E_s)/kT} \right)^{-1} dE. \]

After an integration by parts, we find
\[ F = N\eta + A \int_0^\infty \phi(\epsilon) \frac{d}{d\epsilon} \left( 1 + e^{(E-E_s)/kT} \right)^{-1} d\epsilon \]
where we have defined the following.
\[ A = (2\pi)^{3/2} (\mu B)^{5/2} / \sqrt{2} \pi \Gamma^2, \quad \epsilon = E/\mu B, \quad E_s = \eta/\mu B, \quad \theta = kT/\mu B \]

To evaluate \( \phi \), we use Poisson's summation formula
\[ \phi(\epsilon) = \sum_{n=0}^{\infty} \frac{(-\epsilon)^n}{n!} \int_0^\infty \frac{e^{-x/\epsilon}}{(x+\epsilon)^{n+1}} dx. \]

The integral may be written in terms of Fresnel functions\(^{25}\)
\[ c(x) = \frac{1}{\sqrt{\pi}} \int_0^x t^{-1/2} \cos t dt \quad s(x) = \frac{1}{\sqrt{\pi}} \int_0^x t^{-1/2} \sin t dt \]
if we define \( t = \pi x / (E-x) \). Then we have
\[ \int_0^E (E-x)^{-1/2} \cos \pi x dx = (\pi x)^{-1/2} \int_0^{\pi x} t^{-1/2} \cos (2\pi x - t) dt \]
\[ = \pi^{-1/2} \left[ c(\pi x) \cos (\pi x) + s(\pi x) \sin (\pi x) \right]. \]

Thus the function is
\[ \phi(\epsilon) = \frac{3}{4} \epsilon^{3/4} + \frac{1}{4} \epsilon^{-1/4} - \frac{3}{4} \epsilon^{3/4} \frac{\pi}{4} \left[ c(\pi \epsilon) \cos (\pi \epsilon) + s(\pi \epsilon) \sin (\pi \epsilon) \right]. \]

Now to do the integral over \( \epsilon \), we change the variable to
\[ x = (E-E_s)/\pi \theta = (E-\eta)/\pi kT \]
and we have
\[ F = N \eta + A \int_{-\infty}^{\infty} \phi(\xi - \pi x) \frac{d}{dx} \left(1 + e^{\pi x}\right)^{-1} \, dx \]

Note that
\[ \frac{d}{dx} \left(1 + e^{\pi x}\right) = -\left(1 + e^{\pi x}\right)^{-1} \pi e^{\pi x} = -\pi \left(e^{\pi x} + e^{-\pi x}\right)^{-1} = -\frac{1}{2} \pi \operatorname{sech}^2(\pi x). \]

We may expand \( \phi \) in powers of \( x \) to obtain
\[ F = N \eta + A \left\{ \int_{-\infty}^{\infty} \phi(\xi) + \frac{1}{2} \xi \phi'(\xi) + \frac{1}{2} \xi^2 \phi''(\xi) + \cdots \right\} \operatorname{sech}^2(\pi x) \, dx \]
where the odd powers of \( x \) have been dropped since they integrate to zero anyway because of the symmetrical limits. The derivatives of \( \phi(\xi) \) are
\[ \phi(\xi) = \frac{1}{3} \xi^5 e^{\xi} - \frac{3}{5} \xi^3 e^{\xi} - \frac{1}{8} \xi e^{\xi} \cos(\xi) \left( \frac{c_1(x^2)}{c_2(x^2)} \cos(x^2) + s(x^2) \sin(x^2) \right) \]
\[ \phi''(\xi) = \frac{1}{3} \xi^5 e^{\xi} - \frac{2}{5} \xi^3 e^{\xi} + \frac{1}{5} \xi e^{\xi} \cos(\xi) \left( \frac{c_1(x^2)}{c_2(x^2)} \cos(x^2) + s(x^2) \sin(x^2) \right) \]
\[ \phi'''(\xi) = -\frac{3}{2} \pi \xi^5 e^{\xi} \sin(\xi) \cos^2(\xi) \left( \frac{c_1(x^2)}{c_2(x^2)} \cos(x^2) + s(x^2) \sin(x^2) \right) \]
and etc. may be obtained by differentiating \( \phi(\xi) \) either before or after the expansion in a Poisson sum. Note that the term in square brackets is the same in each case, the double differentiation merely multiplying by a factor \( -4\pi^2 \xi^2 \). Thus we may reverse the order of summation and integration, and using
\[ \frac{\pi}{4} \int_{-\infty}^{\infty} \left(1 + \frac{1}{2} \xi \phi'(\xi) + \frac{1}{4} \xi^2 \phi''(\xi) + \cdots \right) \operatorname{sech}^2(\pi x) \, dx = \frac{-1}{2} \frac{\pi^2 \eta}{\operatorname{sech}(\pi^2 \eta)} \]
we may write the final result as
\[ F = N \eta - A \left\{ \frac{3}{3} \xi^5 e^{\xi} - \frac{3}{5} \xi^3 e^{\xi} (1 - \pi x) - \frac{1}{8} \xi e^{\xi} \phi(x) - \cdots \right. \]
\[ -\frac{3}{2} \pi \xi^5 e^{\xi} \sin(\xi) \left( \frac{c_1(x^2)}{c_2(x^2)} \cos(x^2) + s(x^2) \sin(x^2) \right) \left/ \operatorname{sech}(\pi^2 \eta) \right. \]

The additional terms from the sixth and higher derivatives, written as \( O(\xi^m e^\xi) \) above, do not depend on the magnetic field and thus do not contribute to the magnetic
susceptibility. In fact the only terms that do contribute may be written as follows.

\[ F_1 + F_2 = A \left\{ \frac{1}{\beta} \varepsilon_{\beta}^{\infty} + \frac{3}{\pi^2} \theta \varepsilon_{\infty}^{\infty} \right\} (-i)^{\frac{1}{2}} \left[ C(x \pi L_e) \cos(x \pi L_e) + S(x \pi L_e) \sin(x \pi L_e) \right] / \sinh(x \pi L_e) \]

To show that this result agrees with that obtained previously and to show the actual form of the high magnetic field correction term, we can use the following asymptotic expansion.

\[ C(x \pi L_e) \cos(x \pi L_e) + S(x \pi L_e) \sin(x \pi L_e) = \frac{1}{x \pi L_e} \cos \left( \frac{z - \pi L_e}{x \pi L_e} \right) - \frac{1}{\sqrt{x \pi L_e}} \varepsilon_{\infty}^{\infty} \left( -1 \right)^{m} \pi^{(2m + 1)} / \pi \left( \frac{z}{x \pi L_e} \right)^{2m+1} \]

Thus we have

\[ F_2 = \frac{1}{x \pi L_e} \frac{1}{4} A \theta \varepsilon_{\infty}^{\infty} \left( -1 \right)^{m} \pi^{2m+1} \frac{1}{x \pi L_e} \cos \left( \frac{z - \pi L_e}{x \pi L_e} \right) - \frac{1}{\sqrt{x \pi L_e}} \varepsilon_{\infty}^{\infty} \left( -1 \right)^{m} \pi^{(2m + 1)} \left( \frac{z - \pi L_e}{x \pi L_e} \right)^{2m+1} \frac{1}{x \pi L_e} \cos \left( \frac{z - \pi L_e}{x \pi L_e} \right) - \frac{1}{\sqrt{x \pi L_e}} \varepsilon_{\infty}^{\infty} \left( -1 \right)^{m} \pi^{(2m + 1)} \left( \frac{z - \pi L_e}{x \pi L_e} \right)^{2m+1} \frac{1}{x \pi L_e} \cos \left( \frac{z - \pi L_e}{x \pi L_e} \right) \]

the same as found previously, now with a correction factor in powers of the ratio of the magnetic field energy to the Fermi energy. Note that to obtain the actual magnetic susceptibility, we must include the variation of the Fermi level with magnetic field which is obtained by setting \( \partial \phi / \partial \gamma = 0 \) which gives

\[ N = \frac{A}{x \pi L_e} \left\{ \frac{1}{\beta} \varepsilon_{\beta}^{\infty} + \frac{3}{4 \pi} \varepsilon_{\infty}^{\infty} \right\} (-i)^{\frac{1}{2}} \left[ C(x \pi L_e) \sin(x \pi L_e) - \frac{S(x \pi L_e) \cos(x \pi L_e)}{2 \pi} \right] \]

\[ \left( L_{1,2}, L_{3,4} / \pi \right) \frac{\pi \varepsilon_{\infty}^{\infty} \varepsilon_{\beta}^{\infty} \theta \varepsilon_{\infty}^{\infty} \left( -1 \right)^{m} \frac{1}{x \pi L_e} \cos \left( \frac{z - \pi L_e}{x \pi L_e} \right) \sin \left( \frac{y + 1}{x \pi L_e} \right) \right] / \sinh(x \pi L_e) \]

from which \( \eta \) must be obtained for each magnetic field, such that the total number of particles \( N \), remains constant.
Mean Radius of Cylindrical Wave Functions

To study further the cylindrical wave functions of an electron in a magnetic field, let us obtain the average value of the radius vector of the wave function, that is

\[ \langle r^{3}\rangle = \int_{0}^{\infty} r^{2} |\Psi_{j,\mu,\kappa}(r,\theta,z)|^{2} r^{2}dr \]

\[ = \frac{2^{1/2}}{(2\pi\mu)^{1/2}} \int_{0}^{\infty} e^{-2r} r^{\mu+i\kappa} L_{\mu}^{(i\kappa)}(r) L_{\mu}^{(i\kappa)}(r) d\xi \]

We will expand the second associated Laguerre polynomial

\[ L_{\mu}^{(i\kappa)}(r) = \sum_{k=0}^{\infty} \frac{(2+i\kappa)}{(2k-\mu-i\kappa)!} (-2)^{k} r^{k} / k! \]

and use a Mellin transform

\[ \int_{0}^{\infty} \xi^{\mu-1} e^{-2\xi} L_{\mu}^{(i\kappa)}(\xi) d\xi = \frac{\Gamma(\mu) \Gamma(2+i\kappa-1)}{\Gamma(2+i\kappa-1) \Gamma(2-i\kappa)} \]

to operate on the integral

\[ G = \int_{0}^{\infty} e^{-2\xi} \xi^{\mu+i\kappa} L_{\mu}^{(i\kappa)}(\xi) \xi^{2} \xi^{\mu} \xi^{i\kappa} \xi^{(2-i\kappa)} \xi^{(2+i\kappa-1)} \xi^{(2+i\kappa)} \xi^{(2-i\kappa)} = \sum_{k=0}^{\infty} \frac{(2+i\kappa)}{(2k-\mu-i\kappa)!} (-2)^{k} r^{k} / k! \]

Thus we have

\[ \langle r^{3}\rangle = \frac{2^{1/2}}{(2\pi\mu)^{1/2}} \int_{0}^{\infty} e^{-2r} r^{\mu+i\kappa} L_{\mu}^{(i\kappa)}(r) L_{\mu}^{(i\kappa)}(r) d\xi \]

To check the formula, set \( \mu = 0 \). Then only the \( \kappa \)th term gives a non-zero contribution.

\[ \langle r^{0}\rangle = \sum_{k=0}^{\infty} \frac{(2+i\kappa)}{(2k-\mu-i\kappa)!} (-2)^{k} r^{k} / k! \]

as expected, since this is just the normalization factor.

If we set \( \mu = 1 \), then only the \( \kappa = 5, 5-1 \) terms contribute.

\[ \langle r^{5}\rangle = \frac{(2+i\kappa)}{(2k-\mu-i\kappa)!} (-2)^{k} r^{k} / k! \]

If \( \mu = 2 \) then three terms contribute to give
\langle \tau^2 \rangle = \left( \frac{2\alpha}{\hbar} \right)^2 \left[ 2s(s+1) + (2l+1)(2l+2) \right]

Thus the deviation of \( \tau^2 \) is

\[ \Delta(\tau^2) = \sqrt{\langle \tau^2 \rangle - \langle \tau^2 \rangle^2} = \frac{2\alpha}{\hbar} \sqrt{2s(s+1)(2l+1)(2l+2)} \]

This may now be compared with the turning points of the wave function, that is, the value of \( r \) for which the potential equals the kinetic energy. Writing the differential equation as

\[ \chi \frac{d^2 R}{dz^2} + \frac{dR}{dz} + \left[ s + \frac{1}{2} - \frac{\hbar^2}{4m^2} - \frac{1}{4} \right] R = 0 \]

we see that the turning points come at

\[ \chi = \frac{\hbar^2}{8mc^2} \gamma^2 = \left( 2s + 1 - 2m \right) \pm \sqrt{(2s + 1 - 2m)^2 - \frac{\hbar^2}{mc^2}} \]

Thus for \( m = 0 \) the turning points are

\[ \gamma_1^2 = 0 \quad \text{and} \quad \gamma_2^2 = \frac{\alpha^2}{\hbar^2} (4s + 2) = 2 \langle \tau^2 \rangle \]

Appendix IV Conjugate Variables

A general set of conjugate variables which could be used in treating the motion of an electron in a magnetic field are defined.

The kinetic momentum or quasi-momentum is defined as follows: \( \vec{\pi} = \vec{p} + e \vec{A} \) where \( \vec{p} \) is the momentum of the electron. \( \vec{A} \) is the vector potential such that the magnetic field is given by \( \vec{B} = \nabla \times \vec{A} \). \( e \) is the charge of the electron, the sign being explicitly included. \( c \) is the velocity of light since Gaussian units are used. Note that the classical velocity of the electron is given
by \( \tilde{\tau} = \frac{i}{\hbar} \Pi \) hence the quasi-momentum cognomen.

The quasi-momentum operators satisfy the following commutation relations:

\[
[\Pi_x, \Pi_y] = -i \hbar \frac{\partial}{\partial x} B_z, \quad [\Pi_y, \Pi_z] = -i \hbar \frac{\partial}{\partial y} B_x, \quad [\Pi_z, \Pi_x] = -i \hbar \frac{\partial}{\partial z} B_y.
\]

This may be shown, for example, as follows:

\[
[\Pi_x, \Pi_y] = \left[ P_x + \frac{\partial}{\partial x} A_x, P_y + \frac{\partial}{\partial y} A_y \right] = \frac{\partial}{\partial x} \left[ P_x A_y \right] + \frac{\partial}{\partial y} \left[ A_x P_y \right]
= \frac{\partial}{\partial x} \left( \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) = -i \hbar \frac{\partial}{\partial x} B_z.
\]

Now we need three more variables to form a complete set. Let us define the quasi-coordinate vector as follows:

\[
\vec{\tau} = \vec{p} + \frac{\hbar}{2} \vec{F}
\]

where we must choose the vector \( \vec{F} \) such that each component of the quasi-momentum is independent of each component of the quasi-coordinate vector. This will yield nine equations of the following form:

\[
[\Pi_x, \tau_i] = \left[ P_x + \frac{\partial}{\partial x} A_i, P_i + \frac{\partial}{\partial x} F_i \right] = \frac{\partial}{\partial x} \left[ P_i A_i \right] + \frac{\partial}{\partial x} \left[ A_i P_i \right]
= \frac{\partial}{\partial x} \left( \frac{\partial F_i}{\partial x} - \frac{\partial A_i}{\partial x} \right) = 0
\]

Thus, we have

\[
\frac{\partial F_i}{\partial x^i} = \frac{\partial A_i}{\partial x^i}, \quad i, j = x, y, z
\]

or

\[
\frac{\partial F_x}{\partial x} = \frac{\partial A_x}{\partial x} \quad \frac{\partial F_y}{\partial x} = \frac{\partial A_x}{\partial y} \quad \frac{\partial F_z}{\partial x} = \frac{\partial A_x}{\partial z}
\]

\[
\frac{\partial F_x}{\partial y} = \frac{\partial A_y}{\partial x} \quad \frac{\partial F_y}{\partial y} = \frac{\partial A_y}{\partial y} \quad \frac{\partial F_z}{\partial y} = \frac{\partial A_y}{\partial z}
\]

\[
\frac{\partial F_x}{\partial z} = \frac{\partial A_z}{\partial x} \quad \frac{\partial F_y}{\partial z} = \frac{\partial A_z}{\partial y} \quad \frac{\partial F_z}{\partial z} = \frac{\partial A_z}{\partial z}
\]
\[ \frac{\partial F_x}{\partial x} = \nabla A_x \quad \frac{\partial F_y}{\partial y} = \nabla A_y \quad \frac{\partial F_z}{\partial z} = \nabla A_z. \]

The commutation relations for the quasi-coordinates may be written directly once the independence equations are satisfied.

\[ [\gamma_x, \gamma_y] = -i k \frac{\partial}{\partial z} \left( \frac{\partial F_y}{\partial y} - \frac{\partial F_x}{\partial x} \right) \]
\[ = -i k \frac{\partial}{\partial z} \left( \frac{\partial A_x}{\partial y} - \frac{\partial A_y}{\partial x} \right) = i k \frac{\partial}{\partial z} B_z \]

where the partial differentials of \( F \) have been replaced by those for \( A \), which are known. Thus, we have the quasi-coordinate commutators

\[ [\gamma_x, \gamma_y] = i k \frac{\partial}{\partial z} B_z, \quad [\gamma_y, \gamma_z] = i k \frac{\partial}{\partial x} B_z, \quad [\gamma_z, \gamma_x] = i k \frac{\partial}{\partial y} B_z, \]

the negatives of the quasi-momentum commutators.

The above nine equations may be reduced to three vector equations:

\[ \frac{\partial F}{\partial x} = \nabla A_x \quad \frac{\partial F}{\partial y} = \nabla A_y \quad \frac{\partial F}{\partial z} = \nabla A_z \]

or

\[ \nabla F_x = \frac{\partial}{\partial x} A_x \quad \nabla F_y = \frac{\partial}{\partial y} A_y \quad \nabla F_z = \frac{\partial}{\partial z} A_z \]

The general solution for the unknown vector \( \vec{F} \) may be written symbolically as

\[ \vec{F} = \int (\nabla \vec{A}) \cdot d\vec{r} \]

where the order of the unit vectors must be maintained, as with dyadics.

Six pairs of the independence relations may be combined, in to the single vector equation

\[ \nabla \times \vec{F} = -\nabla \times \vec{A} \]
which may be solved to give
\[ \vec{F} = -\vec{A} + \nabla \phi \]
where the function \( \phi \) must be chosen so that the remaining independence relations are satisfied.

If we choose the symmetrical vector potential
\[ \vec{A} = \frac{1}{4} \hat{\mathbf{a}} \times \vec{F} \]
then we have
\[ \vec{F} = -\frac{i}{\hbar} \hat{\mathbf{a}} \times \vec{A} = -\vec{A} \]
which satisfies the independence relations identically.

Thus instead of the usual three independent pairs of conjugate variables, we have two independent triplets of conjugate variables.

10. The wave-vector representation \( k \), is used rather than the momentum representation \( p \), because the \( k \)'s have the dimensions of reciprocal length which makes the later equations more symmetrical between the coordinate and wave-vector representations.

11. We have implicitly assumed that the wave-vectors are continuous variables. This is true only in the case where the electron is not restricted in its motion in space. If finite boundary conditions are put on the motion of the electron, say be putting it in a box with infinite potential walls, then the wave-vectors are no longer continuous and the partial differential operators must be replaced by partial difference operators. This is only of minor concern in this problem since, for reasonable sized boxes (with a volume of more than one cubic centimeter) the wave-vectors may be assumed to be quasicontinuous without loss of generality.


13. If the discrete nature of the wave-vectors were considered, the integrals would become sums but the resulting delta functions would be the same.


16 The confluent hypergeometric function of the second kind

\[ U(a, b, z) = \frac{\Gamma(a)}{\Gamma(a-b)} - z^{1-b} \frac{M(\text{a}, \text{b}, z)}{\Gamma(\text{a}) \Gamma(\text{a-b})} \]

also satisfies the confluent hypergeometric differential equation. This solution converges for all values of b, even when b is a negative integer. But since it goes to infinity at \( z = 0 \),

\[ U(a, b, z) = z^{1-b} \frac{\Gamma(\text{b}-1)}{\Gamma(a)} + O(|z|^{\text{b}-1}) \quad \text{as} \quad |z| \to 0 \]

it is not in general integrable over any interval that includes the origin and thus cannot be a valid solution to the wave equation if the region of interest includes the origin.


19 Magnus, p. 183


