The States of Metal-Electrons in a Magnetic Field

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The problem of metal-electrons in a magnetic field has been treated in detail. However, as far as known here, the periodicity of the lattice has not been taken into account so far. Because this is of importance for many applications, it seems derirable, to find expressions for the eigen-values and eigenfunctions of the metal electrons in the magnetic field. We confine however the computation to the first terms of the Fourier-expansion of the potential. We take as the direction of the magnetic field the Z-direction and write the vector-potential in the form $A_y=H\chi$, $A_x=A_2=0$ The lattic-potential we write as

$$V=V_0+2V_1(\cos\frac{2\pi\chi}{a}+\cos\frac{2\pi y}{a}+\cos\frac{2\pi z}{a})$$

The problem is then to solve the Schrödinger-equation

$$\triangle\psi+\frac{2ieH}{\hbar c}\times\frac{\partial\psi}{\partial y}+\frac{2m}{\hbar^2}(E-V-\frac{e^2H^2\chi^2}{2mc^2})\psi=0$$

The magnetic field shall be taken into account completely, while the potential is considered as a small perturbation.

We take as the boundary-conditions, that ψ is periodic in a cube with edges of length L. The satisfacion of this condition is not simple. As we will see however the functions satisfy the boundary-conditions, as long as one disregards the electrons in the vicinity of the surface.

According to our program we consider the variable part of the potential as a small perturbation and solve at first the equation

$$\triangle\psi_0+\frac{2ieH}{\hbar c}\chi\frac{\partial\psi}{\partial y}+\frac{2m}{\hbar^2}(E_0-V_0-\frac{e^2H^2X^2}{2mc^2})\psi=0$$

For this purpose we write

$$\psi_0=\frac{1}{L}\varphi_n(\chi-\frac{2\pi}{L}\frac{\hbar c}{eH}k_y)e^{\frac{2\pi i}{L}(k_z z-k_y y)}$$

and obtain for φ_n the equation

$$\frac{d^2\varphi_n}{dx^2}+\frac{2m}{\hbar^2}[E_0-\frac{4\pi^2\hbar^2}{2mL^2}k_z^2-\frac{e^2H^2}{2mc^2}(\chi-\frac{2\pi\hbar c}{eHL}k_y)^2-Vooo]\varphi_n=0$$

Introducing here the abbreviation

$$\varepsilon=E_0-\frac{4\pi^2\hbar^2}{2mL^2}k_2^2-Vooo$$

we write the equation as

$$\varphi_n''+[\frac{2m\varepsilon}{\hbar^2}-\frac{e^2H^2}{\hbar^2c^2}(\chi-\frac{2\pi}{L}\ \frac{\hbar c}{eH}k_y)^2]\varphi_n=0$$

with $\alpha=\frac{eH}{\hbar c}$, $\xi=\sqrt{\alpha}\chi$, $\chi_0=\frac{2\pi}{L}\ \frac{\hbar c}{eH}=\frac{2\pi}{L\alpha}$. $\xi_0=\sqrt{\alpha}\chi_0=\frac{2\pi}{L\sqrt{\alpha}}$

We can write the equation in the form

$$\frac{d^2\varphi_n}{d\xi^2}+[\frac{2m}{\hbar^2}\ \frac{\varepsilon}{\alpha}-(\xi-\xi_0 k_y)^2]\varphi_n=0$$

This is the known equation of the Hermite orthogonal functions. For the eigen-values one gets

$$\frac{2m}{\hbar^2}\ \frac{\varepsilon}{\alpha}=\frac{2mc}{e\hbar}\ \frac{\varepsilon}{H}=2n+1.$$

where n can be any positive integer including zero.

$$\varepsilon=E_0-\frac{4\pi^2\hbar^2}{2mL^2}k_2^2-Vooo=\frac{e\hbar H}{2mc}(2n+1)\quad n=0,\ 1,\ 2,\cdots\cdots$$

With the Bohr magneton $\mu=\frac{e\hbar}{2mc}$ we get then

$$\varepsilon=\mu H(2n+1)$$

The corresponding eigenfunctions can be written in the form

$$\varphi_n=e^{-\frac{1}{2}(\xi-\xi_0k_y)}H_n(\xi-\xi_0k_y)\sqrt{\frac{1}{2^n n!}\sqrt{\frac{\alpha}{\pi}}}$$

Here $H_n(\xi)$ is the n-th Hermite polynomial

$$H_n=(-)^n e^{\xi^2}\frac{d^n e^{-\xi^2}}{d\xi^n}$$

Thus we obtain as our zero-order eigen function

$$\psi_0(k_z,n,k_y)=[\frac{1}{2^n n!},\ \frac{\sqrt{\alpha}}{\pi}]^{1/2}\frac{1}{L}e^{\frac{2\pi i}{L}(k_z z-k_y y)}e^{-\frac{1}{2}(\xi-\xi_0k_y)^2}H_n(\xi-\xi_0k_y)$$

on account of the postulated periodicity of the eigenfunctions, k_y and k_z are integers.

For the computation of the perturbation we write

$$\psi=\psi_0+\psi_1, \quad E=E_0+E_1$$

and substitute this in the Schrödinger-equation. We consider ψ_1 as a small perturbation and consider it as small as compared with ψ_0, $\psi_1<<\psi_0$ and correspondingly we assume $E_1<<E_0$. When we neglect quantities of second order we obtain for ψ_1 the equation.

$$\triangle\psi_1+\frac{2ieH}{\hbar c}\chi\frac{\partial\psi_1}{\partial y}+\frac{2m}{\hbar^2}[E_0-V_0-\frac{e^2H^2}{2mc^2}\chi^2]\psi_1=[V-V_0-E_1]\psi_0$$

In order that this equation has a solution we have to satisfy the condition

$$E_1\int\psi_0^*\psi_0 d\tau=\int\psi_0^2(V-V_0)\psi_0 d\tau$$

Here we have to substitute for ψ_0 all possible solutions of the homogeneous undisturbed equation, which correspond to the same eigenvalue. We introduce the abbreviation

$$\varphi_n(\chi-\chi_0 k_y)=[\frac{1}{2^n n!}\sqrt{\frac{\alpha}{\pi}}]^{\frac{1}{2}} e^{-\frac{1}{2}(\xi-\xi_0 k_y)^2} H_n(\xi-\xi_0 k_y)$$

and we have, on account of the existing degeneration with respect to k_y, to assume a linear combination of all possible eigenfunctions with different k_y. However the electrons shall be inside the periodicity-cube of volume L^3, so that

$$k_y\chi_0=\frac{2\pi}{L\alpha}k_y$$

must take values between the two boundaries of the cube. These boundaries we take as $x=O$ and $x=L$. We have then for k_y the condition

$$0\leqq k_y\chi_0\leqq L \quad \text{or} \quad 0\leqq k_y\leqq\frac{L}{\chi_0}=\frac{L^2\alpha}{2\pi}$$

Therefore, when we write for ψ_0

$$\psi_0=\frac{1}{L}\sum C_{k_y}\varphi_n(\chi-\chi_0 k_y)e^{\frac{2\pi i}{L}(k_z z-k_y y)}$$

k_y in this sum takes all integer values between zero and $\frac{L^2\alpha}{2\pi}$ Now we take for ψ_0^* all solutions with different k_y and the same n and k_z. By substitution of ψ_0 and ψ_0^* in the equation for E_1 we obtain, observing that the eigenfunctions are normalized and orthogonal.

$$E_1 C_{k'_y} = \frac{1}{L^2} \sum C_{k_y} \int e^{-\frac{2\pi i}{L}(k_y y - k^1_y y)} \varphi_n(x - x_0 k_y)\varphi_n(x - x_0 k^1_y)(V - V_0) d\chi\, dy dz$$

Here is $V - V_0 = 2V_1(\cos\frac{2\pi\chi}{a} + \cos\frac{2\pi y}{a} + \cos\frac{2\pi z}{a})$ and the integration is to be taken over the cube L^3. Carrying out the integration over Z the term $\cos\frac{2\pi z}{a}$ gives a zero-contribution and in the other two terms we obtain the value L. We get thus,

$$\frac{2V_1}{L} \Sigma C_{k_y} \int e^{-\frac{2\pi i}{L}(k_y - k_y{}^1)y} \varphi_n(x - x_0 k_y)\varphi_n(\chi - x_0 k^1_y)(\cos\frac{2\pi x}{a} + \cos\frac{2\pi y}{a}) d\chi dy$$

Here now we write $L = Ga$, where G is the number of lattice-distances a which are contained in the length L. We consider at first the term $\cos\frac{2\pi x}{a}$ This gives a nonvanishing value only, when $k_y = k'_y$ and the integration yields the value L. In the integration over the term $\cos\frac{2\pi y}{a} = \frac{1}{2}(e^{\frac{2\pi iy}{a}} + e^{\frac{-2\pi iy}{a}})$ we get an exponential function $e^{\frac{-2\pi i}{L}(k_y - k'_y \pm G)y}$. so that we obtain here a nonvanishing contribution only when $k_y = k_y' \mp G$ and this value is again L. Thus we find in total,

$$C_{k'_y} 2V_1 \int \varphi_n^2(\chi - x_0 k_y')\cos\frac{2\pi\chi}{a} dx + C_{k_y' + G} V_1 \int \varphi_n(x - x_0 k_y')\varphi_n[x - x_0(k_y' - G)] d\chi$$
$$+ C_{k_y' - G} V_1 \int \varphi_n(x - x_0 k'_y)\varphi_n[\chi - x_0(k'_y + G)] d\chi = E_1 C_{k'_y}$$

The integral over χ should be taken from zero to L. However on account of the fact that the Hermite orthogonal functions vanish sufficiently in infinity, we can take it from $-\infty$ to ∞.

Here we introduce the abbreviations

$$J_1 = \int \varphi_n(x - x_0 k_y')\varphi_n[x - x_0\ (k_y' \pm G)] d\chi = \frac{1}{2^n n! \pi^{\frac{1}{2}}} \int e^{-\frac{1}{2}(\xi - \xi_0)^2 - \frac{1}{2}(\xi - \xi_0{}^1)^2}$$
$$H_n(\xi - \xi_0) H_n(\xi - \xi_0{}^1) d\xi$$

Here we have used the notation $\xi = \sqrt{\alpha}\,\chi$. $\xi_0 = \sqrt{\alpha} \times_0 k_y{}^1$, $\xi_0{}^1 = \sqrt{\alpha} x_0(k'_y \pm G)$

$$J_2 = \int \varphi_n{}^2(x - x_0 k'_y)\cos\frac{2\pi\chi}{a} d\chi = \frac{1}{2^n n! \pi^{1/2}} \int e^{-(\xi - \xi_0)^2} Hn^2(\xi - \xi_0)\cos\frac{2\pi\xi}{a\sqrt{\alpha}} d\xi$$

For the computation of these integrals we use the formulas.

$$H_n(x - x_0) = \sum_{\mu=0}^{n} (-)^{\mu} \binom{n}{\mu} (2x_0)^{\mu} H_{n-\mu}(\chi);\quad H_n(x + x_0) = \sum_{\mu=0}^{n} \binom{n}{\mu} (2\chi_0)^{\mu} H_{n-\mu}(\chi)$$

At first we consider the integrals J_1 we write.

$$\frac{1}{2}(\xi-\xi_0)^2+\frac{1}{2}(\xi-\xi_0{}^1)^2=\xi^2-\xi(\xi_0+\xi^1{}_0)+\frac{1}{2}(\xi_0{}^2+\xi_0{}^{12})$$

$$=[\xi-\frac{1}{2}(\xi_0+\xi_0{}^1)]^2+\frac{1}{4}(\xi_0-\xi_0{}^1)^2=y^2+\frac{1}{4}(\xi_0-\xi_0{}^1)^2$$

$$, \quad y=\xi-\frac{1}{2}(\xi_0+\xi_0{}^1)$$

we obtain then

$$J_1=\frac{1}{2^n n!\pi^{1/2}}e^{-\frac{1}{4}(\xi-\xi_0{}^1)^2}\int_{-\infty}^{\infty}e^{-y^2}H_n[y+\frac{1}{2}(\xi_0-\xi_0{}^1)]H_n(y-\frac{1}{2}(\xi_0-\xi_0{}^1))dy$$

$$=\frac{e^{-\frac{1}{4}(\xi_0-\xi_0{}^1)^2}}{2^n n!\pi^{1/2}}\sum_{\mu_1\nu=0}(-)^{\nu}\int_{-\infty}^{\infty}\binom{n}{\nu}\binom{n}{\mu}(\xi_0-\xi_0{}^1)^{\mu+\nu}e^{-y^2}H_{n-\mu}(y)H_{n-\nu}(y)dy$$

$$=\frac{e^{-\frac{1}{4}(\xi_0-\xi_0{}^1)^2}}{2^n n!\pi^{1/2}}\sum_{\nu=0}^{\infty}(-)^{\nu}\binom{n}{\nu}^2(\xi_0-\xi_0{}^1)^{2\nu}2^{n-\nu}(n-\nu)!\pi^{1/2}$$

$$J_1=e^{-\frac{1}{4}(\xi_0-\xi_0{}^1)^2}\sum_{\nu=0}^{n}(-)^{\nu}\binom{n}{\nu}\frac{1}{\nu!}\left[\frac{1}{2}(\xi_0-\xi_0')^2\right]^{\nu}=e^{-\frac{1}{4}(\xi_0-\xi_0{}^1)^2}\frac{1}{n!}L_n(\frac{1}{2}(\xi_0-\xi_0{}^1)^2)$$

Here $L_n(\times)$ is the n-th Lagnerre polynomial of order n and argument X.

For the computation of the integral

$$J_2=\frac{1}{2^n n!\pi^{1/2}}\int_{-\infty}^{\infty}e^{-(\xi-\xi_0)^2}H_n{}^2(\xi-\xi_0)\cos\frac{2\pi\xi}{a\sqrt{\alpha}}d\xi$$

we consider

$$J_2{}^1=\frac{1}{2^n n!\pi^{1/2}}\int_{-\infty}^{\infty}e^{\frac{2\pi im}{a\sqrt{\alpha}}\xi}e^{-(\xi-\xi_0)^2}H_n{}^2(\xi-\xi_0)d\xi \quad \text{With} \quad m=\pm1$$

we write

$$\xi^2-2\xi_0\xi-\frac{2\pi im}{a\sqrt{\alpha}}\xi+\xi_0{}^2=(\xi-\xi_0-\frac{\pi im}{a\sqrt{\alpha}})^2-\frac{2\pi im}{a\sqrt{\alpha}}\xi_0+\frac{\pi^2m^2}{a^2\alpha}$$

$$=y^2-\frac{2\pi im}{a\sqrt{\alpha}}\xi_0+\frac{\pi^2m^2}{a^2\alpha} \quad \text{With} \quad y=\xi-\xi_0-\frac{\pi im}{a\sqrt{\alpha}}$$

we obtain then

$$J_2{}^1=\frac{1}{2^n n!\pi^{1/2}}e^{(\frac{2\pi im}{a\sqrt{a}}\xi_0-\frac{\pi^2m^2}{a^2\alpha})}\int_{-\infty}^{\infty}e^{-y^2}Hn(y+\frac{\pi im}{a\sqrt{\alpha}})dy$$

$$=\frac{1}{2^n n!\pi^{1/2}}e^{\frac{2\pi im}{a\sqrt{\alpha}}\xi_0\frac{-\pi^2m^2}{a^2\alpha}}\sum_{\mu_1\nu=0}^{n}\binom{n}{\nu}\binom{n}{\mu}(\frac{2\pi im}{a\sqrt{\alpha}})^{\nu+\mu}\int_{-\infty}^{\infty}e^{-y^2}H_{n-\nu}(y)H_{n-\mu}(y)dy$$

$$=\frac{1}{2^n n!\pi^{1/2}} e^{\frac{2\pi i m}{a\sqrt{a}}\xi_0-\frac{\pi^2m^2}{a^2\alpha}} \sum_{\nu=0}^{n} (-)^{\nu} \binom{n}{\nu}^2 \left(\frac{2\pi m}{a\sqrt{\alpha}}\right)^{2\nu} 2^{n-\nu} (n-\nu)!\pi^{1/2}$$

$$=\frac{1}{2^n n!\pi^{1/2}} e^{\frac{2\pi i m}{a\sqrt{\alpha}}\xi_0-\frac{\pi^2m^2}{a^2\alpha}} \sum_{\nu=0}^{n} (-)^{\nu} \binom{n}{\nu}\frac{n!(n-\nu)!}{\nu!(n-\nu)!}\left(\frac{2\pi^2m^2}{a^2\alpha}\right)^{\nu} \pi^{1/2}2^n$$

we obtain therefore finally

$$J_2'=e^{\frac{2\pi i m}{a\sqrt{\alpha}}\xi_0-\frac{\pi^2m^2}{a^2\alpha}} \sum_{\nu=0}^{n} \frac{(-)^{\nu}}{\nu!}\binom{n}{\nu}\left(\frac{2\pi^2m^2}{a^2\alpha}\right)^{\nu}$$

$$=e^{\frac{2\pi i m}{a\sqrt{a}}\xi_0-\frac{\pi^2m^2}{a^2\alpha}} \frac{1}{n!}L_n\left(\frac{2\pi^2m^2}{a^2\alpha}\right)$$

Therefore we have obtained the result for J_2

$$J_2=\frac{1}{2^n n!\pi^{1/2}}\int_{-\infty}^{\infty} e^{-(\xi-\xi_0)^2}Hn^2(\xi-\xi_0)\cos\frac{2\pi\xi}{a\sqrt{\alpha}}d\xi$$

$$=\frac{1}{n!}\cos\left(\frac{4\pi^2}{\alpha La}k_y'\right)e^{-\frac{\pi^2}{a^2\alpha}} L_n\left(\frac{2\pi^2}{a^2\alpha}\right)$$

$$J_2=\frac{1}{2^n n!\pi^{1/2}}\int_{-\infty}^{\infty} e^{-(\xi-\xi_0)^2}H_n^2(\xi-\xi)_0)\cos\frac{2\pi\xi}{a\sqrt{\alpha}}d\xi$$

$$=\frac{1}{n!}\cos\left(\frac{4\pi^2}{\alpha La}k_y'\right)e^{-\frac{\pi^2}{a^2\alpha}} L_n\left(\frac{2\pi^2}{a^2\alpha}\right)$$

With this, our equation takes then the form

$$C_{k_y'+G}\frac{e^{-\frac{\pi^2}{a^2\alpha}}L_n\left(\frac{2\pi^2}{a^2\alpha}\right)}{n!}+C_{k_y'}\left[2\cos\frac{4\pi^2 k_y'}{\alpha La}\frac{e^{-\frac{\pi^2}{a^2\alpha}}L_n\left(\frac{2\pi^2}{a^2\alpha}\right)}{n!}-\frac{E_1}{V_1}\right]$$

$$+C_{k_y'-G}\frac{e^{\frac{-\pi^2}{a^2\alpha}}L_n\left(\frac{2\pi^2}{a^2\alpha}\right)}{n!}=0$$

or $$C_{k_y'+G}+C_{k_y'}\left[2\cos\frac{4\pi^2 k_y'}{\alpha La}-\frac{E_1 e^{\frac{\pi^2}{a^2\alpha}}n!}{V_1 L_n\left(\frac{2\pi^2}{a^2\alpha}\right)}\right]+C_{k_y'-G}=0$$

When we call this equation the equation for C_{k_y}, we see that the coefficient $C_{k_y'+G}$ appears in the equation for $C_{k_y'+G}$ and the same is true for $C_{k_y'-G}$ and also for $C_{k_y'\pm\nu G}$. In this way we obtain a system of equations for the Coefficients $C_{k_y'\pm\nu G}$ with $\nu=0, \pm1, \pm2, \pm3,\ldots\ldots$

Considering now a fixed value of k_y and introducing the abbreviation

$$\varepsilon_1(\nu)=2\cos\frac{4\pi^2(k_y+\nu G)}{\alpha La}-E_1\frac{e^{\frac{\pi^2}{a^2\alpha}}n!}{V_1\,L_n\left(\frac{2\pi^2}{a^2\alpha}\right)}$$

We write this system in the form

$$C_{k_y+(\nu-1)G}+\varepsilon_1(\nu)C_{k_y+\nu G}+C_{k_y+(\nu+1)G}=0$$

and here the ν is confined to a region defined by the inequality

$$-\frac{k_y}{G}\leq\nu\leq\frac{Ga^2\alpha}{2\pi}-\frac{k_y}{G}$$

and k_y is confined to the region defined by

$$0\leq k_y\leq\frac{L}{x_0}=\frac{G^2a^2\alpha}{2\pi}$$

In order that this system of equations has a solution, the determinant of the coefficients must vanish.

Here for simplicity of the computation, we allow only values of the magnetic field such that $\frac{4\pi^2}{\alpha La}G$ is an integer multiple of 2π. We take therefore

$$\frac{4\pi^2}{\alpha La}G=2N\pi$$

where N can be any integer.

Then the $\varepsilon_1(\nu)$ in all our equations take the same value and the determinant of this system of coefficients takes the form

$$\begin{vmatrix} \varepsilon_1 & 1 & 0 & 0 & 0\cdots\cdots\cdots \\ 1 & \varepsilon_1 & 1 & 0 & 0\cdots\cdots\cdots \\ 0 & 1 & \varepsilon_1 & 1 & 0\cdots\cdots\cdots \\ 0 & 0 & 1 & \varepsilon_1 & 1\cdots\cdots\cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{vmatrix}=D_{G/N}(\varepsilon_1)$$

It has on account of the inequality for ν which takes now the form

$$-\frac{k_y}{G}\leq\nu\leq\frac{G}{N}-\frac{k_y}{G}$$

G/N rows and columns.

To solve this equation we write

$$\varepsilon_1 = 2\cos\zeta$$

and find then easyly that

$$D_n = \frac{\sin(n+1)\zeta}{\sin\zeta}$$

Now this determinant shall vanish and thus we get as the solution

$$\zeta_\nu = \nu\frac{\pi}{n+1} \qquad \nu = 1, 2, \cdots\cdots n$$

In this way we obtain as the eigenvalues in our approximation

$$E_0 = V_0 + \frac{4\pi^2\hbar^2}{2mL^2}k_z^2 + 2\mu H(n+\frac{1}{2}) + \frac{2V_1}{n!}e^{-\frac{\pi N}{2}}L_n(N\pi)[\cos\frac{2\pi N}{G}k_y - \cos\frac{\nu\pi N}{G+N}]$$

Here ν takes all values between 1 and G/N $\nu = 1, 2, 3 \cdots G/N$ and N is given by

$$N = \frac{2\pi}{\alpha a^2} = \frac{2\pi\hbar C}{eHa^2}$$

磁場中金屬電子之狀態

竟 流

本文係計算金屬結晶中的電子在均勻磁場作用下的能量固有值（The energy-eigen value）。其方法爲視電子的位能爲很小的擾動（Perturbation）用 Fourier 級數將其展開而僅考慮其第一項，但磁場的作用是以嚴密的方法加以考慮的爲簡單計，本文在磁場大小爲某一定值的整數倍的假設下計算擾動的大小，如是擾動行列（Perturbation Matrix）可寫成 Tchebycheff 多項式而最後結果亦可以 Laguerre 多項式表示之。