PART IX

Charged particle in an uniform magnetic field. Landau levels.

$\vec{B} = (0, 0, B)$

Let us choose $\vec{A} = (-By, 0, 0)$

$\vec{B} = \vec{\nabla} \times \vec{A}$

$$\left.\begin{aligned} B_x &= \frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} = 0 \\ B_y &= \frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} = 0 \\ B_z &= \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} = B \end{aligned}\right\} \quad \text{OK}$$

Hamiltonian of a charged particle in the field.

$$\hat{H} = \frac{(\hat{\vec{p}} - q\vec{A})^2}{2m} = \frac{(\hat{p}_x + qBy)^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{\hat{p}_z^2}{2m}$$

Schroedinger eq.

$$\hat{H}\psi = \varepsilon\psi$$

(I) $$\left\{\frac{(\hat{p}_x + qBy)^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{\hat{p}_z^2}{2m}\right\}\psi = \varepsilon\psi$$

(II) $$\psi = e^{ik_x x + ik_z z}\,\chi(y)$$

k_x and k_z are arbitrary

Physical meaning: free propagation along x and z direction, confinement in y-direction.

Substitute (II) in (I)

$$\begin{cases} (\hat{p}_x + qBy)\psi = (-i\hbar\frac{\partial}{\partial x} + qBy)\psi = (\hbar k_x + qBy)\psi \\ (\hat{p}_x + qBy)^2\psi = (\hbar k_x + qBy)^2\psi = q^2B^2(y-y_0)^2\psi \\ \text{where } y_0 = -\frac{\hbar k_x}{qB} \end{cases}$$

$$\left\{ \hat{p}_z^2\psi = \hbar^2 k_z^2\psi \right.$$

Hence eq. (I) is transformed to

$$\left(\frac{q^2B^2}{2m}(y-y_0)^2+\frac{\hbar^2k_z^2}{2m}+\frac{\hat{p}_y^2}{2m}\right)\chi=\varepsilon\chi$$

introduce $\boxed{\omega_c=\frac{|q|B}{m}}$ - cyclotron frequency

$$\left(\frac{\hat{p}_y^2}{2m}+\frac{m\omega_c^2}{2}(y-y_0)^2\right)\chi=\underbrace{\left(\varepsilon-\frac{\hbar^2k_z^2}{2m}\right)}_{\varepsilon'}\chi$$

This is 1D harmonic oscillato problem.

Solution is known.

$$\varepsilon_n'=\hbar\omega_c(n+1/2)$$

For wave functions see pp 62-66.

Hence

$$\boxed{\varepsilon=\varepsilon(n,k_z)=\hbar\omega_c\left(n+\frac{1}{2}\right)+\frac{\hbar^2k_z^2}{2m}}$$

Landau levels.

The solution is impertant for number of effects in solid state physics.

Quantum Hall effect, Shubnikov-de Haas effect,

...

Time independent non-degenerate perturbation theory

Let $\hat{H}_0$ be a Hamiltonian and <u>all</u> eigenstates and eigenvalues of $\hat{H}_0$ are known:

(1) $$\boxed{\hat{H}_0 \psi_n^{(0)} = \varepsilon_n^{(0)} \psi_n^{(0)}}, \quad n = 1, 2, 3 \ldots$$

Perturbation theory is a method which allows to find solutions for Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ where $\hat{V}$ is a small perturbation.

(2) $$\boxed{(\hat{H}_0 + \hat{V})\psi = \varepsilon \psi}$$

Solutions for ψ and ε have form of series in powers of $\hat{V}$.

Represent ψ as

$$\psi = \sum_m C_m \psi_m^{(0)}$$

and substitute this in (2)

$$(\hat{H}_0+\hat{V})\sum_m c_m \psi_m^{(0)} = \sum_m c_m(\hat{H}_0+V)\psi_m^{(0)} =$$

$$= \sum_m c_m(\varepsilon_m^{(0)} + \hat{V})\psi_m^{(0)}$$

So $$\sum_m c_m(\varepsilon_m^{(0)}+\hat{V})\psi_m^{(0)} = \sum_m c_m \varepsilon \psi_m^{(0)}$$

multiply this eq by $\psi_k^{(0)*}$ and integrate over x.

$$\int (\psi_k^{(0)}(x))^* \psi_m^{(0)}(x)\,dx \equiv \langle k|n\rangle = \delta_{kn}$$

$$\int (\psi_k^{(0)}(x))^* V(x)\psi_m^{(0)}(x)\,dx \equiv \langle k|\hat{V}|m\rangle \equiv V_{km}$$

$$\Rightarrow c_k \varepsilon_k^{(0)} + \sum_m V_{km} = \varepsilon c_k \Longrightarrow$$

$$\Rightarrow (3) \quad \boxed{(\varepsilon - \varepsilon_k^{(0)})c_k = \sum_m V_{km} c_m}$$

Thus, we have reduced initial differential eq. (2) to the matrix eq. (3).

Look for solution as a series in powers of $\hat{V}$.

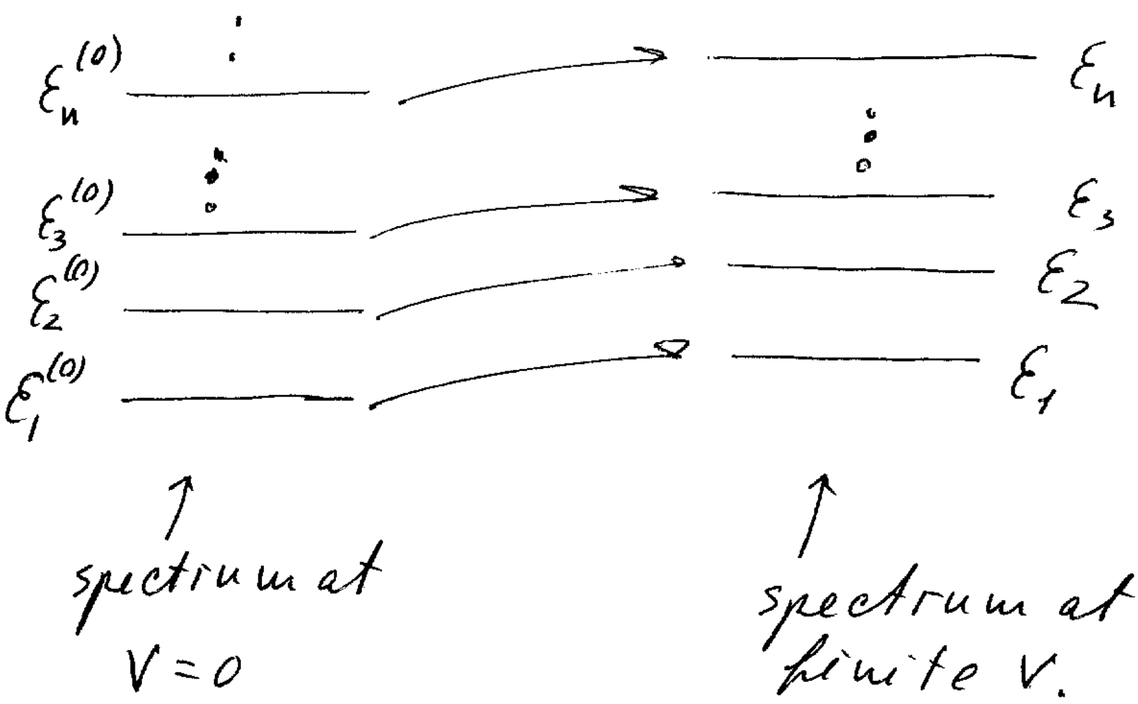
$$\mathcal{E} = \mathcal{E}^{(0)} + \mathcal{E}^{(1)} + \mathcal{E}^{(2)} + \dots$$

$$C_m = C_m^{(0)} + C_m^{(1)} + C_m^{(2)} + \dots$$

(0) – corresponds to zero order in V

(1) – corresponds to first order in V

...



Consider state ψ_n. In zero order $\psi_n = \psi_n^{(0)}$

Hence

$$C_n^{(0)} = 1, \quad C_m^{(0)} = 0, \quad m \neq n$$

Eq. (3) reads in this case

$$\left(\mathcal{E}_n - \mathcal{E}_K^{(0)}\right) C_K = \sum_m V_{Km} C_m , \quad K = 1, 2, 3 \ldots\ldots$$

consider the case $K = n$

$$(4) \quad \left(\cancel{\mathcal{E}_n^{(0)}} + \mathcal{E}_n^{(1)} + \mathcal{E}_n^{(2)} + \ldots - \cancel{\mathcal{E}_n^{(0)}}\right)\Big(\underbrace{C_n^{(0)}}_{=1} + C_n^{(1)} + \ldots\Big) = \sum_m V_{nm}\left(C_m^{(0)} + C_m^{(1)} + \ldots\right)$$

equating terms of the first order in V one finds

$$(5) \quad \boxed{\mathcal{E}_n^{(1)} = V_{nn} \equiv \langle n | V | n \rangle \equiv \int \psi_n^{(0)*}(x)\, V(x)\, \psi_n^{(0)}(x)\, dx}$$

first order correction to energy

now consider $K \neq n$

$$\left(\mathcal{E}_n^{(0)} + \mathcal{E}_n^{(1)} + \mathcal{E}_n^{(2)} + \ldots - \mathcal{E}_K^{(0)}\right)\Big(\underbrace{C_K^{(0)}}_{=0} + C_K^{(1)} + \ldots\Big) = \sum_m V_{Km}\left(C_m^{(0)} + C_m^{(1)} + \ldots\right)$$

equate 1st order terms in V

$$\left(\mathcal{E}_n^{(0)} - \mathcal{E}_K^{(0)}\right) C_K^{(1)} = V_{Kn}$$

Hence

(6) $$\boxed{C_k^{(1)} = \frac{V_{kn}}{\mathcal{E}_n^{(0)} - \mathcal{E}_k^{(0)}}, \quad k \neq n}$$

1st order correction to the wave function

Condition of validity of the pert. theory

$$|C_k^{(1)}| \ll 1 \Longrightarrow \boxed{|V_{kn}| \ll |\mathcal{E}_n^{(0)} - \mathcal{E}_k^{(0)}|} \quad (7)$$

The coefficient $C_n^{(1)}$ remains undetermined. To find it let us look at the normalization

$$1 = \langle \psi_n | \psi_n \rangle = \langle \sum C_m \psi_m^{(0)} | \sum_k C_k \psi_k^{(0)} \rangle =$$

$$= |C_n|^2 + \sum_{k \neq n} |C_k|^2 = |1 + C_n^{(1)} + C_n^{(2)} + \dots|^2 + \sum_{k \neq n} |C_k|^2 =$$

$$= 1 + 2C_n^{(1)} + (C_n^{(1)})^2 + C_n^{(2)} + \dots + \sum_{k \neq n} |C_k|^2$$

Equating the first order terms we find

(8) $$\boxed{C_n^{(1)} = 0}$$

The second order correction to energy.

Consider eq (4) (page 168) up to 2nd order in V

$$\left(\mathcal{E}_n^{(1)}+\mathcal{E}_n^{(2)}\right)\left(\underset{}{\overset{1}{\overset{\shortparallel}{C_n^{(0)}}}}+\overset{0}{\overset{\shortparallel}{C_n^{(1)}}}+\dots\right)=V_{nn}\left(\underset{1}{\underset{\shortparallel}{C_n^{(0)}}}+\underset{0}{\underset{\shortparallel}{C_n^{(1)}}}+\dots\right)+$$

$$+\sum_{k\neq n}V_{nk}\left(\underset{0}{\underset{\shortparallel}{C_k^{(0)}}}+C_k^{(1)}+\dots\right)$$

↑ given by eq (6) (page 169)

equatin 2nd order terms we find

$$(9)\quad \boxed{\mathcal{E}_n^{(2)}=\sum_{k\neq n}\frac{V_{nk}V_{kn}}{\mathcal{E}_n^{(0)}-\mathcal{E}_k^{(0)}}=\sum_{k\neq n}\frac{|V_{kn}|^2}{\mathcal{E}_n^{(0)}-\mathcal{E}_k^{(0)}}}$$

2nd order correction to energy

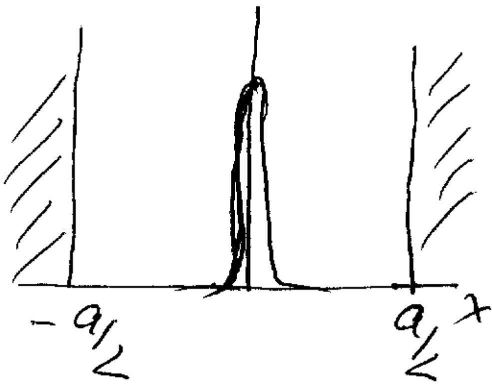
recall that $V_{nk}=V_{kn}^*$ since $\hat{V}$ is Hermitian.

Example 1

Problem from the 1st assignment:
δ-function perturbation inside infinite well.

$$V_0(x) = \begin{cases} \infty, & x < -a/2 \\ 0, & -a/2 < x < a/2 \\ \infty, & x > a/2 \end{cases}$$

perturbation $V = g\,\delta(x)$



Problem: Using pert. theory find 1st order correction to the energy of the ground state.

$$\psi_1^{(0)} = \sqrt{\frac{2}{a}} \cos kx = \sqrt{\frac{2}{a}} \cos \frac{\pi x}{a}, \quad k = \frac{\pi}{a}$$

$$\varepsilon_1^{(0)} = \frac{\hbar^2 k^2}{2m} = \frac{\pi^2 \hbar^2}{2ma^2}$$

$$\delta \mathcal{E} = \mathcal{E}^{(1)} = \langle \psi^{(0)} | V | \psi^{(0)} \rangle =$$ see eq ⑤ page 168

$$= \int \sqrt{\frac{2}{a}} \cos\frac{\pi x}{a} \, g\,\delta(x) \sqrt{\frac{2}{a}} \cos\frac{\pi x}{a} \, dx = \frac{2g}{a}$$

$$\mathcal{E}_1 = \mathcal{E}_1^{(0)} + \mathcal{E}_1^{(1)} = \frac{\pi \hbar^2}{2ma^2} + \frac{2g}{a}$$

Example 2

ground state of the hydrogen-like uranium ion (nuclear charge $Z=92$).
This is a pure Coulomb problem if one neglects finite size of the uranium nucleus.

(I) $$V_c(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r}$$

In this approximation the ground state energy is (see p 148 and account for rescaling $e^2 \to Ze^2$)

$$\mathcal{E}_{1s}^{(0)} = -\frac{Z^2 m_e e^4}{2\,(4\pi\varepsilon_0 \hbar)^2} = -Z^2 13.6\,eV = -115\,kV$$

The wave function is

$$\psi_{1s}^{(0)} = \frac{1}{\sqrt{\pi (a_B/Z)^3}}\, e^{-\frac{r}{(a_B/Z)}} = \frac{Z^{3/2}}{\sqrt{\pi a_B^3}}\, e^{-Zr/a_B}$$

$$a_B = \frac{4\pi \varepsilon_0 \hbar^2}{m_e e^2} = 0.529\, 10^{-10}\, m$$

See page 150 and account for rescaling $e^2 \to Z e^2$

The U nucleus has finite radius $R \approx 7\, 10^{-15}$ m. Let us consider the nucleus as a charged sphere (charge on the surface).

Uniformly charged sphere is a more realistic model, but for simplicity I consider .

Problem: <u>find the 1s energy shift due to the finite nuclear size</u>

Potential of the sphere is

$$\tilde{V} = \begin{cases} -\dfrac{Ze^2}{4\pi\varepsilon_0 r}, & r > R \\ -\dfrac{Ze^2}{4\pi\varepsilon_0 R}, & r < R \end{cases}$$

It can be represented as $\tilde{V} = V_0 + V$, where the perturbation V is

$$V = \begin{cases} 0, & r > R \\ \dfrac{Ze^2}{4\pi\varepsilon_0}\left(\dfrac{1}{r} - \dfrac{1}{R}\right), & r < R. \end{cases}$$

$$\delta\varepsilon = \varepsilon_{1s}^{(1)} = \langle \psi_{1s}^{(0)} | V | \psi_{1s}^{(0)} \rangle = \int |\psi_{1s}^{(0)}(r)|^2 V(r)\, d^3r =$$

$$= \frac{Z^3}{\pi a_B^3} \int_0^R e^{-\frac{2Zr}{a_B}} \frac{Ze^2}{4\pi\varepsilon_0}\left(\frac{1}{r} - \frac{1}{R}\right) 4\pi r^2 dr$$

$$\frac{2ZR}{a_B} = \frac{2\cdot 92\cdot 7\, 10^{-15}}{0.5\, 10^{-10}} \sim 3\, 10^{-2} \ll 1 \Longrightarrow e^{-\frac{2Zr}{a_B}} \simeq 1$$

Hence

$$\delta\varepsilon \simeq \frac{4Z^4}{a_B^3}\left(\frac{e^2}{4\pi\varepsilon_0}\right) \int_0^R \left(\frac{1}{r} - \frac{1}{R}\right) r^2 dr = \frac{2}{3} Z^4 \frac{R^2}{a_B^2}\left(\frac{e^2}{4\pi\varepsilon_0 a_B}\right) =$$

$$= \frac{2}{3}(92)^4 \left(\frac{7\cdot 10^{-15}}{0.5\, 10^{-10}}\right)^2 27.2\,\text{eV} \simeq 25\,\text{eV}.$$

Example 3

1D Harmonic oscillator.

$$H_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

with perturbation $V = \lambda x$.

Problem: find correction to the ground state energy up to the second order in λ.

1) Exact solution:

$$H_0 \Rightarrow \varepsilon = \varepsilon^{(0)} = \frac{1}{2}\hbar\omega$$

$$H = H_0 + \lambda x = \underbrace{\frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\left(x + \frac{\lambda}{m\omega^2}\right)^2}_{\text{harmonic oscillator}} - \frac{\lambda^2}{2m\omega^2}$$

Hence $\varepsilon = \frac{1}{2}\hbar\omega - \frac{\lambda^2}{2m\omega^2} \Rightarrow$

$$\Rightarrow \boxed{\delta\varepsilon = -\frac{\lambda^2}{2m\omega^2}}$$

Perturbation theory solution

$$\begin{cases} \psi_0^{(0)} = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\frac{\alpha x^2}{2}} \quad , \quad \mathcal{E}_0^{(0)} = \frac{1}{2}\hbar\omega \\ \psi_1^{(0)} = \sqrt{2\pi}\left(\frac{\alpha}{\pi}\right)^{3/4} x e^{-\frac{\alpha x^2}{2}} \quad , \quad \mathcal{E}_1^{(0)} = \frac{3}{2}\hbar\omega \\ \alpha = \frac{m\omega}{\hbar} \end{cases}$$

— see pages 62-66

first order correction (eq ⑤ page 168)

$$\mathcal{E}_0^{(1)} = \langle\psi_0^{(0)}|V|\psi_0^{(0)}\rangle = \left(\frac{\alpha}{\pi}\right)^{1/2}\int_{-\infty}^{+\infty} e^{-\alpha x^2}\lambda x\,dx = 0$$

Second order correction (eq ⑨ page 170)

$$\mathcal{E}_0^{(2)} = \sum_{k\neq 0}\frac{|\langle\psi_k^{(0)}|V|\psi_0^{(0)}\rangle|^2}{\mathcal{E}_0^{(0)} - \mathcal{E}_k^{(0)}}$$

$$\langle\psi_1^{(0)}|V|\psi_0^{(0)}\rangle = \sqrt{2\pi}\left(\frac{\alpha}{\pi}\right)\int_{-\infty}^{+\infty} x\, e^{-\alpha x^2}\lambda x\,dx = \frac{\lambda}{\sqrt{2\alpha}}$$

one can show that $\langle\psi_k^{(0)}|V|\psi_0^{(0)}\rangle = 0$ for $k \geq 2$.

Hence

$$\mathcal{E}_0^{(2)} = \frac{(\lambda/\sqrt{2\alpha})^2}{\frac{\hbar\omega}{2} - \frac{3\hbar\omega}{2}} = -\frac{\lambda^2}{2\alpha\hbar\omega} = -\frac{\lambda^2}{2m\omega^2}$$

agrees with exact answer on page 175.