Quantenmechanik I
Lösungsblatt 4

Exercise 4.1 Charged particle in an external electromagnetic field

a) By direct computation,

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{x}_i} = m_i \dot{x}_i - \frac{q_i}{c} A(x_i).$$

b) Hence

$$\dot{x}_i = \frac{1}{m_i}\left(p_i + \frac{q_i}{c} A(x_i)\right)$$

and

$$\begin{aligned} H(x_i, p_i) &= \sum_i \dot{x}_i p_i - \mathcal{L}(x_i, \dot{x}_i) \\ &= \sum_i \frac{1}{m_i}\left(p_i + \frac{q_i}{c} A(x_i)\right) p_i - \sum_i \frac{1}{2m_i}\left(p_i + \frac{q_i}{c} A(x_i)\right)^2 \\ &\quad + \sum_i q_i \varphi_i(x_i) + \sum_i \frac{q_i}{c}\left(p_i + \frac{q_i}{c} A(x_i)\right) A(x_i) \\ &= \sum_i \frac{1}{2m_i}\left[p_i^2 + \frac{q_i}{c}\left(p_i A(x_i) + A(x_i) p_i\right) + \frac{q_i^2}{c^2} A(x_i)^2\right] + \sum_i q_i \varphi_i(x_i) \end{aligned}$$

Notice that since we promote the p_i to operators they do not commute in general with $A(x_i)$. We have finally

$$H(x_i, p_i) = \sum_i \frac{1}{2m_i}\left(p_i + \frac{q_i}{c} A(x_i)\right)^2 + \sum_i q_i \varphi_i(x_i).$$

c) For an electron the degrees of freedom are the spatial coordinates (x, y, z) and the charge is e. Therefore we have

$$\begin{aligned} H(\mathbf{x}, \mathbf{p}) &= \frac{1}{2m}\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)^2 + e\,\varphi \\ &\longrightarrow \frac{1}{2m}\left(-i\hbar\,\nabla + \frac{e}{c}\mathbf{A}\right)^2 + e\,\varphi, \end{aligned}$$

so that the Schrödinger equation $i\hbar\frac{\partial}{\partial t}\Psi = H\Psi$ corresponds exactly to what we want.

d) After a gauge transformation, the left-hand side of the Schrödinger equation becomes

$$i\hbar\left[\exp\left(-\frac{ie}{\hbar c}\chi\right)\frac{\partial}{\partial t}\Psi - \frac{ie}{\hbar c}\left(\frac{\partial}{\partial t}\chi\right)\exp\left(-\frac{ie}{\hbar c}\chi\right)\Psi\right] = \exp\left(-\frac{ie}{\hbar c}\chi\right)\left[i\hbar\frac{\partial}{\partial t}\Psi - \frac{e}{c}\left(\frac{\partial}{\partial t}\chi\right)\Psi\right]$$

Let's expand the right-hand side:

$$\left[\frac{1}{2m}\left(i\hbar\nabla - \frac{e}{c}\mathbf{A}\right)^2 + e\,\varphi\right]\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi - \frac{i\hbar e}{2mc}\left(\nabla\cdot\mathbf{A}\right)\Psi - \frac{i\hbar e}{mc}\mathbf{A}\cdot\nabla\Psi + \frac{e^2}{2mc^2}\mathbf{A}^2\Psi + e\varphi\Psi$$

The different pieces transform as

$$
\begin{aligned}
-\frac{\hbar^2}{2m}\nabla^2\Psi &\longrightarrow -\frac{\hbar^2}{2m}\nabla^2\left[\exp\left(-\frac{ie}{\hbar c}\chi\right)\Psi\right] \\
&= \exp\left(-\frac{ie}{\hbar c}\chi\right)\left[-\frac{\hbar^2}{2m}\nabla^2\Psi + \frac{i\hbar e}{mc}\nabla\chi\nabla\Psi + \frac{i\hbar e}{2mc}\left(\nabla^2\chi\right)\Psi + \frac{e^2}{2mc^2}\left(\nabla\chi\right)^2\Psi\right] \\
-\frac{i\hbar e}{2mc}\left(\nabla\cdot\mathbf{A}\right)\Psi &\longrightarrow -\frac{i\hbar e}{2mc}\exp\left(-\frac{ie}{\hbar c}\chi\right)\left(\nabla\cdot\mathbf{A}+\nabla^2\chi\right)\Psi \\
-\frac{i\hbar e}{mc}\mathbf{A}\cdot\nabla\Psi &\longrightarrow -\frac{i\hbar e}{mc}\exp\left(-\frac{ie}{\hbar c}\chi\right)\left(\mathbf{A}+\nabla\chi\right)\left[\nabla\Psi - \frac{ie}{\hbar c}\left(\nabla\chi\right)\Psi\right)\right] \\
&= \exp\left(-\frac{ie}{\hbar c}\chi\right)\left[-\frac{i\hbar e}{mc}\mathbf{A}\cdot\nabla\Psi - \frac{i\hbar e}{mc}\nabla\chi\nabla\Psi - \frac{e^2}{mc}\mathbf{A}\cdot\left(\nabla\chi\right)\Psi - \frac{e^2}{mc}\left(\nabla\chi\right)^2\Psi\right] \\
\frac{e^2}{2mc^2}\mathbf{A}^2\Psi &\longrightarrow \frac{e^2}{2mc^2}\exp\left(-\frac{ie}{\hbar c}\chi\right)\left[\mathbf{A}^2 + 2\mathbf{A}\cdot\left(\nabla\chi\right) + \left(\nabla\chi\right)^2\right]\Psi \\
e\varphi\Psi &\longrightarrow \exp\left(-\frac{ie}{\hbar c}\chi\right)\left[e\varphi - \frac{e}{c}\frac{\partial}{\partial t}\chi\right]\Psi
\end{aligned}
$$

so that the right-hand side of the Schrödinger equation becomes

$$
\exp\left(-\frac{ie}{\hbar c}\chi\right)\left[-\frac{\hbar^2}{2m}\nabla^2\Psi - \frac{i\hbar e}{2mc}\left(\nabla\cdot\mathbf{A}\right)\Psi - \frac{i\hbar e}{mc}\mathbf{A}\cdot\nabla\Psi + \frac{e^2}{2mc^2}\mathbf{A}^2\Psi + e\varphi\Psi - \frac{e}{c}\left(\frac{\partial}{\partial t}\chi\right)\Psi\right]
$$

$$
= \exp\left(-\frac{ie}{\hbar c}\chi\right)\left[\frac{1}{2m}\left(i\hbar\nabla - \frac{e}{c}\mathbf{A}\right)^2 + e\varphi - \frac{e}{c}\frac{\partial}{\partial t}\chi\right]\Psi
$$

Canceling the exponential factor and removing the term $-\frac{e}{c}\frac{\partial}{\partial t}\chi$ on both side, one recover the initial Schrödinger equation.

Exercise 4.2 Landau problem

a) Obviously, $\varphi = 0$ and $\mathbf{A}$ time-independent ensure that $\mathbf{E} = 0$, and

$$
\mathbf{B} = \nabla\times\mathbf{A} = \frac{1}{2}B\ \nabla\times\begin{pmatrix}-y\\ x\\ 0\end{pmatrix} = \begin{pmatrix}0\\ 0\\ B\end{pmatrix}
$$

We have therefore

$$
\begin{aligned}
H\Psi &= \frac{1}{2m}\left(i\hbar\nabla - \frac{e}{c}\mathbf{A}\right)^2\Psi \\
&= \frac{1}{2m}\left[-\hbar^2\nabla^2\Psi - i\hbar\frac{e}{c}\left(\nabla\cdot\mathbf{A}\right)\Psi - 2i\hbar\frac{e}{c}\mathbf{A}\cdot\nabla\Psi + \frac{e^2}{c^2}\mathbf{A}^2\right]
\end{aligned}
$$

One can check that $\nabla\cdot\mathbf{A} = 0$, $\mathbf{A}\cdot\nabla = \frac{1}{2}B\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$ and $\mathbf{A}^2 = \frac{1}{4}B^2\left(x^2+y^2\right)$. Moreover since the electron moves in the plane (x, y) the Laplacian reads $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$. Therefore

$$
H\Psi = \frac{1}{2m}\left[-\hbar^2\left(\frac{\partial^2}{\partial x^2}\Psi + \frac{\partial^2}{\partial y^2}\Psi\right) - i\hbar\frac{eB}{c}\left(x\frac{\partial}{\partial y}\Psi - y\frac{\partial}{\partial x}\Psi\right) + \frac{e^2B^2}{4c^2}\left(x^2+y^2\right)\Psi\right]
$$

or in terms of momenta $p_x \sim -i\hbar\frac{\partial}{\partial x}$ and $p_y \sim -i\hbar\frac{\partial}{\partial y}$

$$
H = \frac{1}{2m}\left[p_x^2 + p_y^2 + \frac{eB}{c}\left(xp_y - yp_x\right) + \frac{e^2B^2}{4c^2}\left(x^2+y^2\right)\right]
$$

b) We have

$$\begin{array}{rclcrcl} q &=& a\,x + b\,p_y & \qquad & p &=& e\,y + f\,p_x \\ Q &=& c\,y + d\,p_x & & P &=& g\,x + h\,p_y \end{array},$$

and the usual commutation relations $[x, p_x] = [y, p_y] = i\hbar$ and $[x, y] = [p_x, p_y] = [x, p_y] = [y, p_x] = 0$.

The commutators $[q, P]$ and $[Q, p]$ are automatically zero. For the others, we have

$$\begin{cases} [q, Q] = ad\,[x, p_x] + bc\,[p_y, y] = i\hbar\,(ad - bc) \\ [p, P] = eh\,[y, p_y] + gf\,[p_x, x] = i\hbar\,(eh - gf) \\ [q, p] = af\,[x, p_x] + be\,[p_y, y] = i\hbar\,(af - be) \\ [Q, P] = ch\,[y, p_y] + dg\,[p_x, x] = i\hbar\,(ch - dg) \end{cases} \implies \begin{cases} ad - bc = 0 \\ eh - gf = 0 \\ af - be = 1 \\ ch - dg = 1 \end{cases}$$

In order to compute the Hamiltonian, one has to invert the transformation above. We find

$$\begin{array}{rclcrcl} x &=& \frac{1}{ah-bg}\,(h\,q - b\,P) & \qquad & p_x &=& \frac{1}{de-cf}\,(e\,Q - c\,p) \\ y &=& \frac{1}{cf-de}\,(f\,Q - d\,p) & & p_y &=& \frac{1}{bg-ah}\,(g\,q - a\,P) \end{array},$$

and the Hamiltonian is then

$$\begin{aligned} H \;=\; \frac{1}{2m}\Bigg[& \frac{(eQ - cp)^2 + 2\beta(eQ - cp)(fQ - dp) + \beta^2(fQ - dp)^2}{(cf - de)^2} \\ & + \frac{(gq - aP)^2 + 2\beta(gq - aP)(hq - bP) + \beta^2(hq - bP)^2}{(ah - bg)^2}\Bigg] \end{aligned}$$

where we habe used the notation $\beta = eB/2c$. For the cross-terms in qP and Qp to vanish, one needs

$$\begin{array}{rcl} ce + \beta\,(cf + de) + \beta^2 df &=& 0 \\ ag - \beta\,(ah + bg) + \beta^2 bh &=& 0 \end{array}$$

Following the hint, we set $a = c = 1/\sqrt{2}$, and thus

$$\begin{array}{c} d = b \\ f = \sqrt{2}\,(1 + be) \\ h = \sqrt{2}\,(1 + bg) \end{array} \implies \begin{array}{c} cf - de = 1 \\ ah - bg = 1 \\ g = e \end{array}$$

$$\implies \quad \begin{array}{c} \frac{1}{\sqrt{2}}e + \beta(1 + 2be) + \beta^2 b(1 + be) = 0 \\ \frac{1}{\sqrt{2}}e - \beta(1 + 2be) + \beta^2 b(1 + be) = 0 \end{array}$$

$$\implies \quad e = -\frac{1}{2b} \quad \implies \quad -\frac{1}{2\sqrt{2}}\frac{1}{b} + \beta^2\frac{\sqrt{2}}{2}b = 0 \quad \implies \quad b = \pm\frac{1}{\sqrt{2}}\frac{1}{\beta}$$

We are free to choose the sign of b, so let's take $-$

$$a = c = f = h = \frac{1}{\sqrt{2}} \qquad b = d = -\frac{1}{\sqrt{2}}\frac{1}{\beta} \qquad e = g = \frac{1}{\sqrt{2}}\beta$$

so that we have finally

$$\begin{cases} q = \frac{1}{\sqrt{2}}\left(x - \frac{1}{\beta}p_y\right) \\ Q = \frac{1}{\sqrt{2}}\left(y - \frac{1}{\beta}p_x\right) \\ p = \frac{1}{\sqrt{2}}\,(\beta y + p_x) \\ P = \frac{1}{\sqrt{2}}\,(\beta x + p_y) \end{cases} \iff \begin{cases} x = \frac{1}{\sqrt{2}}\left(q + \frac{1}{\beta}P\right) \\ y = \frac{1}{\sqrt{2}}\left(Q + \frac{1}{\beta}p\right) \\ p_x = \frac{1}{\sqrt{2}}\,(\beta Q - p) \\ p_y = \frac{1}{\sqrt{2}}\,(\beta q - P) \end{cases}$$

And the Hamiltonian becomes then

$$H = \frac{1}{m}\left(P^2 + \beta^2 Q^2\right)$$

which corresponds to the Hamiltonian of an harmonic oscillator

$$H = \frac{1}{2m_0}P^2 + \frac{m_0\omega_0^2}{2}Q^2$$

with $m_0 = m/2$ and $\omega_0 = 2\beta/m = eB/mc$.

c) Since the Hamiltonian of the system is the one of an harmonic oscillator, the energy levels are

$$E_n = \hbar\omega_0\left(n + \frac{1}{2}\right) = \frac{\hbar eB}{mc}\left(n + \frac{1}{2}\right)$$

Exercise 4.3 Particle in a one-dimensional square potential

a) For a constant potential $V(x) = V_i$, the time-independent Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\psi''(x) + V_i\psi(x) = E\psi(x)$$

$$\Longleftrightarrow \quad \psi''(x) = \frac{2m}{\hbar^2}\left(V_i - E\right)$$

The solution will depend on the sign of the right-hand side:

$$\Longrightarrow \quad \psi(x) = \begin{cases} A\exp\left(\frac{k_i x}{\hbar}\right) + B\exp\left(-\frac{k_i x}{\hbar}\right), & k_i = \sqrt{2m\left(V_i - E\right)} \quad \text{if} \quad E < V_i \\ A\exp\left(i\frac{k_i x}{\hbar}\right) + B\exp\left(-i\frac{k_i x}{\hbar}\right), & k_i = \sqrt{2m\left(E - V_i\right)} \quad \text{if} \quad E > V_i \end{cases}$$

where A and B are arbitrary constants.

We have then to treat the following cases:

1) $\underline{V_1 < E < 0}$

Let's denote by ψ_1, ψ_2 and ψ_3 the wavefunction in the regions $(0, a)$, (a, b) and (b, ∞) respectively. We have

$$\begin{aligned} \psi_3(x) &= Ae^{k_3 x/\hbar} + Be^{-k_3 x/\hbar} & k_3 &= \sqrt{-2mE} \\ \psi_2(x) &= Ce^{k_2 x/\hbar} + De^{-k_2 x/\hbar} & k_2 &= \sqrt{2m\left(V_2 - E\right)} \\ \psi_1(x) &= Ee^{ik_1 x/\hbar} + Fe^{-ik_1 x/\hbar} & k_1 &= \sqrt{2m\left(E - V_1\right)} \end{aligned}$$

The infinite potential for $x < 0$ implies $\psi_1(0) = 0$ and thus $F = -E$ and

$$\psi_1(x) = 2iE\sin\left(\frac{k_1 x}{\hbar}\right)$$

By continuity we must have $\psi_1(a) = \psi_2(a)$ and $\psi_1'(a) = \psi_2'(a)$ and thus

$$\hbar\frac{\psi_1'(a)}{\psi_1(a)} = \frac{k_1}{\tan\left(k_1 a/\hbar\right)} = \hbar\frac{\psi_2'(a)}{\psi_2(a)} = k_2\frac{Ce^{k_2 a/\hbar} - De^{-k_2 a/\hbar}}{Ce^{k_2 a/\hbar} + De^{-k_2 a/\hbar}}$$

$$\Longrightarrow \quad \left(Ce^{k_2 a/\hbar} + De^{-k_2 a/\hbar}\right) = \frac{k_2}{k_1}\tan\left(k_1 a/\hbar\right)\left(Ce^{k_2 a/\hbar} - De^{-k_2 a/\hbar}\right)$$

$$\Longrightarrow \quad \frac{D}{C} = e^{2k_2 a/\hbar}\,\frac{1 - \frac{k_2}{k_1}\tan\left(k_1 a/\hbar\right)}{1 + \frac{k_2}{k_1}\tan\left(k_1 a/\hbar\right)}$$

The wavefunction must vanish at infinity, hence $A = 0$. By continuity in b, we have

$$\hbar\frac{\psi_2'(b)}{\psi_2(b)} = k_2\frac{Ce^{k_2 b/\hbar} - De^{-k_2 b/\hbar}}{Ce^{k_2 b/\hbar} + De^{-k_2 b/\hbar}} = \hbar\frac{\psi_3'(b)}{\psi_3(b)} = -k_3$$

$$\Longrightarrow \quad \frac{D}{C} = e^{2k_2 b/\hbar}\,\frac{k_2 + k_3}{k_2 - k_3}$$

2) $\underline{0 < E < V_2}$

3) $\underline{E > V_2}$

b)

c)

Exercise 4.4 Symplectic transformations

We have:

$$\begin{aligned} M\Omega M^T &= \begin{pmatrix} -B & A \\ -D & C \end{pmatrix} \begin{pmatrix} A^T & C^T \\ B^T & D^T \end{pmatrix} \\ &= \begin{pmatrix} AB^T - BA^T & AD^T - BC^T \\ CB^T - DA^T & CD^T - DC^T \end{pmatrix} = \Omega = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix} \end{aligned}$$

Therefore:

$$\begin{aligned} \sum_k (A_{ik}B_{jk} - B_{ik}A_{jk}) &= 0 \\ \sum_k (C_{ik}D_{jk} - D_{ik}C_{jk}) &= 0 \\ \sum_k (A_{ik}D_{jk} - B_{ik}C_{jk}) &= \delta_{ij} \end{aligned}$$

Then, using the relations above, the commutators become:

$$\begin{aligned} [Q_i, Q_j] &= \sum_k \sum_l [A_{ik}\ q_k + B_{ik}\ p_k, A_{jl}\ q_l + B_{jl}\ p_l] \\ &= \sum_k \sum_l (A_{ik}\ A_{jl}\ [q_k, q_l] + A_{ik}\ B_{jl}\ [q_k, p_l] + B_{ik}\ A_{jl}\ [p_k, q_l] + B_{ik}\ B_{jl}\ [p_k, p_l]) \\ &= \sum_k \sum_l [A_{ik}B_{jl}\,(i\hbar\ \delta_{kl}) + B_{ik}A_{jl}\,(-i\hbar\ \delta_{kl})] \\ &= i\hbar \sum_k (A_{ik}B_{jk} - B_{ik}A_{jk}) \\ &= 0 \\ [P_i, P_j] &= \sum_k \sum_l [C_{ik}\ q_k + D_{ik}\ p_k, C_{jl}\ q_l + D_{jl}\ p_l] \\ &= i\hbar \sum_k (C_{ik}D_{jk} - D_{ik}C_{jk}) \\ &= 0 \\ [Q_i, P_j] &= \sum_k \sum_l [A_{ik}\ q_k + B_{ik}\ p_k, C_{jl}\ q_l + D_{jl}\ p_l] \\ &= i\hbar \sum_k (A_{ik}D_{jk} - B_{ik}C_{jk}) \\ &= i\hbar\ \delta_{ij} \end{aligned}$$

And hence we see that the commutation relations are preserved.