Exercise 8: Change of variables in short-time action

$q = f(x)$ remember $\Delta q^2 = O(\varepsilon)$, $\Delta x^2 = O(\varepsilon)$ ⇝ kin. energy up to $O(\Delta x^4)$

$$\Delta q_j = f(x_j) - f(x_{j-1}) = f(x_j) - f(x_j - \Delta x_j) = \qquad (f_j := f(x_j))$$

$$= f_j - \left(f_j - f_j' \Delta x_j + \tfrac{1}{2} f_j'' \Delta x_j^2 - \tfrac{1}{6} f_j''' \Delta x_j^3 \right)$$

$$= f_j' \Delta x_j - \tfrac{1}{2} f_j'' \Delta x_j^2 + \tfrac{1}{6} f_j''' \Delta x_j^3$$

$$\Delta q_j = f(x_{j-1} + \Delta x_j) - f(x_{j-1}) = f_{j-1}' \Delta x_j + \tfrac{1}{2} f_{j-1}'' \Delta x_j^2 + \tfrac{1}{6} f_{j-1}''' \Delta x_j^3$$

$$\Delta q_j^2 = f_j' f_{j-1}' \Delta x_j^2 + \tfrac{1}{2} \Delta x_j^3 \left(f_j' f_{j-1}'' - f_{j-1}' f_j'' \right) + \Delta x_j^4 \left(-\tfrac{1}{4} f_j'' f_{j-1}'' + \tfrac{1}{6} f_j''' f_{j-1}' + \tfrac{1}{6} f_{j-1}''' f_j' \right)$$

NR: $f_j' f_{j-1}'' - f_{j-1}'' f_j'' = f'(x_j) f_{j-1}'' - f''(x_j) f_{j-1}' = \left(f_{j-1}' + \Delta x_j f_{j-1}'' \right) f_{j-1}'' - \left(f_{j-1}'' + \Delta x_j f_j''' \right) f_{j-1}'$

$$= \Delta x_j \left(f_{j-1}''^{\,2} - f_{j-1}' f_{j-1}''' \right)$$

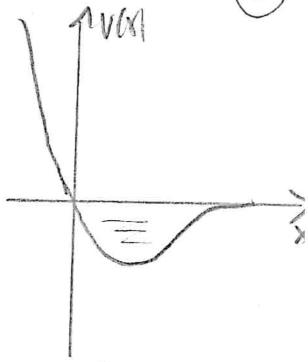
$$\Delta q_j^2 = f_j' f_{j-1}' \Delta x_j^2 + \Delta x_j^4 \left(\tfrac{1}{2} f''^2 - \tfrac{1}{2} f' f''' - \tfrac{1}{4} f'' f'' + \tfrac{1}{3} f''' f' \right)$$

↑ j or j-1 are irrelevant as this is $O(\Delta x^4)$ term

$$= f_j' f_{j-1}' \Delta x^2 + \Delta x_j^4 \left(\tfrac{1}{4} f''^2 - \tfrac{1}{6} f' f''' \right)$$

#

Exercise 9: The Morse oscillator



$$V(x) = \frac{\hbar^2\lambda^2}{2m}\left(e^{-2x} - 2e^{-x}\right)$$

interaction between molecules

Let $e^{-x} = r \leadsto f(r) = -\ln r \leadsto f'(r) = -\frac{1}{r}$, $f''(r) = \frac{1}{r^2}$, $f'''(r) = -\frac{2}{r^3}$

$$\leadsto (Sf)(r) = \frac{2}{r^2} - \frac{3}{2}\frac{1}{r^2} = \frac{1}{2}\frac{1}{r^2}$$

$$\tilde{V}(r) = \left(-\frac{1}{r}\right)^2\left[\frac{\hbar^2\lambda^2}{2m}\left(r^2 - 2r + \varepsilon\right)\right] + \tilde{V}_0 - \frac{\hbar^2}{8m}\frac{1}{r^2}$$

$$E := -\frac{\hbar^2\lambda^2}{2m}\varepsilon$$

$$= \frac{\hbar^2\lambda^2}{2m} + \tilde{V}_0 + \frac{\hbar^2(\lambda^2\varepsilon - \frac{1}{4})}{2mr^2} - \frac{\hbar^2\lambda^2}{m}\frac{1}{r}$$

$$= \frac{\hbar^2 L(L+1)}{2mr^2} - \frac{\alpha}{r}$$

where $\tilde{V}_0 = -\frac{\hbar^2\lambda^2}{2m} = \tilde{E}$

$\alpha = \frac{\hbar^2\lambda^2}{m}$

and $L(L+1) = \varepsilon\lambda^2 - \frac{1}{4} \leadsto \varepsilon = \left(L + \frac{1}{2}\right)^2\frac{1}{\lambda^2}$

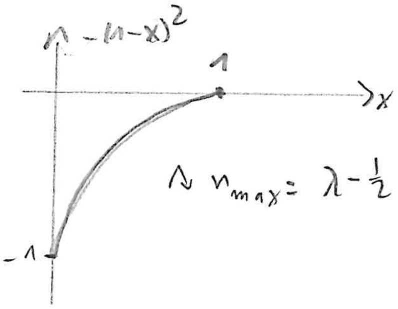
Coulomb spectrum:

$$\tilde{E}_n = -\frac{m\alpha^2}{2\hbar^2}\frac{1}{(n+L+1)^2} = -\frac{m\hbar^4\lambda^4}{2\hbar^2 m^2}\frac{1}{(n+L+1)^2} \overset{!}{=} \tilde{V}_0 = -\frac{\hbar^2\lambda^2}{2m}$$

$\leadsto \lambda^2 = (n+L+1)^2 \leadsto \lambda = n+L+1 \equiv N$ and $L + \frac{1}{2} = \lambda - n - \frac{1}{2}$

$$\leadsto \varepsilon = \left(\lambda - n - \tfrac{1}{2}\right)^2\frac{1}{\lambda^2}$$

$$\leadsto E_n = -\frac{\hbar^2\lambda^2}{2m}\left(1 - \frac{n+\frac{1}{2}}{\lambda}\right)^2$$



$\leadsto n_{max} = \lambda - \frac{1}{2}$

or $n = 0, 1, 2, \ldots < \lambda - \frac{1}{2}$

Eigenfunctions:

$$\psi(r) = N \left(\frac{r}{Na_B}\right)^{L+1} e^{-r/Na_B} L_n^{2L+1}\left(\frac{2r}{Na_B}\right) \qquad z := \frac{e^{-x}}{Na_B} = \frac{r}{Na_B}$$

$$Na_B = \lambda \frac{\hbar^2}{m\alpha} = \lambda \frac{\hbar^2 m}{m \hbar^2 \lambda^2} = \frac{1}{\lambda} \quad \rightsquigarrow \quad z = \lambda r$$

$$\phi(x) = N' (z)^{L+1} e^{-z} L_n^{2L+1}(2z)$$

$$= N' z^{\lambda-n} e^{-z} L_n^{2(\lambda-n)-1}(2z)$$

$$= N' \left(\lambda e^{-x}\right)^{\lambda-n} \exp\{-\lambda e^{-x}\} L_n^{2(\lambda-n)-1}(2\lambda e^{-x})$$

Exercise 10: Particle on ring - Non-trivial UIR

Lecture $K(\varphi'',\varphi';t) = \sum_{n\in\mathbb{Z}} e^{-in\delta} K_n(\varphi'',\varphi',t)$, $0\leq\delta\leq 2\pi$

$$= \sum_n \sqrt{\frac{mR^2}{2\pi i\hbar t}}\, e^{-in\delta} \exp\left\{\frac{i}{\hbar}\frac{mR^2}{2t}(\varphi''-\varphi'-2\pi n)^2\right\}$$

$$= \sqrt{\frac{mR^2}{2\pi i\hbar t}}\, e^{\frac{i}{\hbar}\frac{mR^2}{2t}(\varphi''-\varphi')^2} \sum_n \exp\left\{-\frac{i}{\hbar}\frac{mR^2}{2t}4\pi n(\varphi''-\varphi') - in\delta + \frac{i}{\hbar}\frac{mR^2}{2t}4\pi^2 n^2\right\}$$

$$\tau := -\frac{\hbar t}{2mR^2\pi}, \quad z := \frac{\varphi''-\varphi'}{2\pi}$$

$$= \sqrt{\frac{mR^2}{2\pi i\hbar t}}\, e^{-i\frac{\pi z^2}{\tau}} \sum_n \exp\left\{2\pi i n\left(\frac{z}{\tau}-\frac{\delta}{2\pi}\right) - i\frac{\pi n^2}{\tau}\right\}$$

$$= \frac{1}{2\pi}\sqrt{\frac{i}{\tau}}\, e^{-i\frac{\pi z^2}{\tau}}\, \Theta\left(\frac{z}{\tau}-\frac{\delta}{2\pi}\,\middle|\, -\frac{1}{\tau}\right)$$

let $\tilde{z} := z - \frac{\delta\tau}{2\pi}$

$$= \frac{1}{2\pi} e^{-i\frac{\pi z^2}{\tau}} \underbrace{\sqrt{\frac{i}{\tau}}\, \Theta\left(\frac{\tilde{z}}{\tau}\,\middle|\,-\frac{1}{\tau}\right)}_{=\Theta(\tilde{z}|\tau)\, e^{i\pi\tilde{z}^2/\tau}} = \frac{1}{2\pi}\exp\left\{\frac{i\pi}{\tau}(\tilde{z}^2-z^2)\right\}\Theta(\tilde{z}|\tau)$$

with $\frac{\pi}{\tau}(\tilde{z}^2-z^2) = \frac{\pi}{\tau}\left(-2z\frac{\delta\tau}{2\pi}+\frac{\delta^2\tau^2}{4\pi^2}\right) = -\delta z + \frac{\delta^2\tau}{4\pi}$

$$= \frac{1}{2\pi}\exp\left\{-iz\delta + i\frac{\delta^2}{4\pi}\tau\right\} \sum_{l\in\mathbb{Z}} \exp\left\{i\pi l^2\tau + 2\pi i l\left(z-\frac{\delta}{2\pi}\tau\right)\right\}$$

$$K(\varphi'', \varphi', t) = \frac{1}{2\pi} \sum_{\ell} \exp\left\{ i\pi\tau \left(\ell^2 - \frac{\ell\delta}{\pi} + \left(\frac{\delta}{2\pi}\right)^2 \right) \right\} \exp\left\{ 2\pi i z \left(\ell - \frac{\delta}{2\pi} \right) \right\}$$

$$= \frac{1}{2\pi} \sum_{\ell} \exp\left\{ i\pi\tau \left(\ell - \frac{\delta}{2\pi} \right)^2 \right\} \exp\left\{ i 2\pi z \left(\ell - \frac{\delta}{2\pi} \right) \right\}$$

$$= \frac{1}{2\pi} \sum_{\ell} \exp\left\{ -\frac{i}{\hbar} \frac{\hbar^2 t}{2mR^2} \left(\ell - \frac{\delta}{2\pi} \right)^2 \right\} \exp\left\{ i(\varphi'' - \varphi') \left(\ell - \frac{\delta}{2\pi} \right) \right\}$$

Spectral repr.

$$\leadsto \quad E_\ell = \frac{\hbar^2}{2mR^2} \left(\ell - \frac{\delta}{2\pi} \right)^2 , \quad \psi_\ell(\varphi) = \frac{1}{\sqrt{2\pi}} \exp\left\{ i \left(\ell - \frac{\delta}{2\pi} \right) \varphi \right\}$$

Note:

$$-\frac{\hbar^2}{2mR^2} \frac{\partial^2}{\partial \varphi^2} \psi_\ell(\varphi) = E_\ell \, \psi_\ell(\varphi) \quad \#$$

"Free particle on a ring" !

Exercise 11: The Aharonov-Bohm effect

Electromagn. field $\vec{E}, \vec{B}$ characterised by potentials ϕ and $\vec{A}$

$$\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} - \vec{\nabla}\phi \,, \quad \vec{B} = \vec{\nabla} \times \vec{A}$$

Physics is invariant under gauge transformations Λ (gauge field)

$$\vec{A} \to \vec{A}' := \vec{A} + \vec{\nabla}\Lambda \,, \quad \phi \to \phi' := \phi - \frac{1}{c}\frac{\partial \Lambda}{\partial t}$$

• Classical description:

$$L(\dot{\vec{r}}, \vec{r}) = \frac{m}{2}\dot{\vec{r}}^2 + \frac{e}{c}\dot{\vec{r}}\cdot\vec{A} - e\phi$$

$$\leadsto L'(\dot{\vec{r}}, \vec{r}) = \frac{m}{2}\dot{\vec{r}}^2 + \frac{e}{c}\dot{\vec{r}}\cdot(\vec{A} + \vec{\nabla}\Lambda) - e\phi + \frac{e}{c}\frac{\partial \Lambda}{\partial t}$$

$$= L(\dot{\vec{r}}, \vec{r}) + \frac{e}{c}\frac{d}{dt}\Lambda(\vec{r}, t)$$

cl. dynamics ruled by Lorentz force $\vec{F}(\vec{r},t) = e\vec{E}(\vec{r},t) + \frac{e}{c}\dot{\vec{r}} \times \vec{B}(\vec{r},t)$

• Quantum description:

$$H = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2 + e\phi$$

$$\leadsto H' = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A}'\right)^2 + e\phi' \quad \text{and } \psi' = e^{\frac{ie}{\hbar c}\Lambda}\psi$$

$$\leadsto H'\psi' = \frac{1}{2m}\left(\vec{p} - \frac{e}{c}\vec{A} - \frac{e}{c}\vec{\nabla}\Lambda\right)^2\psi' + e\phi\psi' - \frac{e}{c}\dot{\Lambda}\psi'$$

with $\vec{p}\psi' = \frac{\hbar}{i}\vec{\nabla}\left(e^{\frac{ie}{\hbar c}\Lambda}\psi\right) = e^{\frac{ie}{\hbar c}\Lambda}\left(\frac{e}{c}\vec{\nabla}\Lambda + \vec{p}\right)\psi$

$$H'\psi' = e^{\frac{ie}{\hbar c}\Lambda}\left[\frac{1}{2m}\left(\vec{p}-\frac{e}{c}\vec{A}\right)^2 + e\phi - \frac{e}{c}\dot{\Lambda}\right]\psi$$

$$i\hbar\partial_t\psi' = e^{\frac{ie}{\hbar c}\Lambda}\left[i\hbar\,\frac{ie}{\hbar c}\dot{\Lambda} + i\hbar\partial_t\right]\psi = e^{\frac{ie}{\hbar c}\Lambda}\left(-\frac{e}{c}\dot{\Lambda} + i\hbar\partial_t\right)\psi$$

Hence $H\psi = i\hbar\partial_t\psi \iff H'\psi' = i\hbar\partial_t\psi'$

Now let $\vec{B}=\vec{0} \rightsquigarrow \vec{\nabla}\times\vec{A}=\vec{0} \rightsquigarrow \vec{A}=\vec{\nabla}\Lambda$ pure gauge field
no time dependence except

$$\rightsquigarrow \quad \Lambda(\vec{r}) = \int_{\vec{r}_0}^{\vec{r}} d\vec{x}\cdot\vec{A}(\vec{x})$$

$\vec{r}_0$ ~ arbitrary

scalar potential to keep particle out of any area with $\vec{B}\neq\vec{0}$

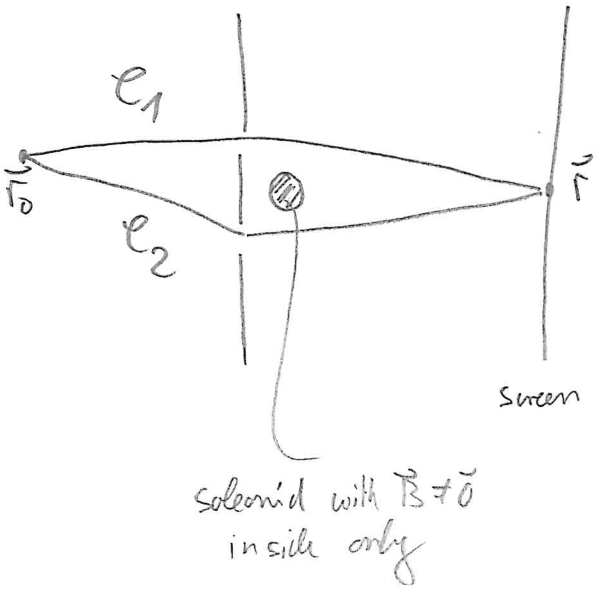
$$\rightsquigarrow \quad H\psi_B = \frac{1}{2m}\left(\vec{p}-\frac{e}{c}\vec{A}\right)^2\psi_B + V\psi_B = i\hbar\partial_t\psi_B$$

Gauge transformation by $-\Lambda$

$$\rightsquigarrow \quad H'\psi_0' = \left(\frac{1}{2m}\vec{p}^2 + V\right)\psi_0' = i\hbar\partial_t\psi_0' \quad \text{with } \psi_0' = e^{-\frac{ie}{\hbar c}\Lambda}\psi_B$$

$$\psi_B(\vec{r},t) = \psi_0'(\vec{r},t)\exp\left\{\frac{i\hbar}{ec}\int_{\vec{r}_0}^{\vec{r}} d\vec{x}\cdot\vec{A}(\vec{x})\right\}$$

- **Aharonov-Bohm effect**



$$\psi_{1B}(\vec{r},t) = \psi_{10}(\vec{r},t)\exp\left\{\frac{ie}{\hbar c}\int_{C_1} d\vec{x}\cdot\vec{A}(\vec{x})\right\}$$

$$\psi_{2B}(\vec{r},t) = \psi_{20}(\vec{r},t)\exp\left\{\frac{ie}{\hbar c}\int_{C_2} d\vec{x}\cdot\vec{A}(\vec{x})\right\}$$

↑ $\vec{B}\neq 0$ in solenoid ↑ $\vec{B}=0$ in solenoid

Phase difference between two paths due to vector potential

$$\int_{\mathcal{C}_1} d\vec{r}\cdot\vec{A}(\vec{r}) - \int_{\mathcal{C}_2} d\vec{r}\cdot\vec{A}(\vec{r}) = \oint_{\mathcal{C}_1-\mathcal{C}_2} d\vec{r}\cdot\vec{A}(\vec{r}) =$$

$$= \int_{\text{Area enclosed}} d\vec{f}\cdot(\vec{\nabla}\times\vec{A}) = \int d\vec{f}\cdot\vec{B} =: \Phi \quad \text{flux in solenoid}$$

$$\rightsquigarrow \Delta\varphi_B := \frac{e}{\hbar c}\Phi = 2\pi\frac{\Phi}{\Phi_0} \quad \text{with } \Phi_0 := 2\pi\frac{\hbar c}{e} = 4.135\times 10^{-7}\,G\,cm^2$$

flux quantum

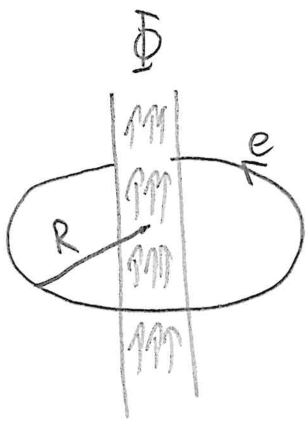
Switching on magnetic field in solenoid results in shift of interference pattern when $\Phi \neq n\Phi_0$ → <u>Aharonov-Bohm effect</u>

Predicted 1959

First experiment 1960 by Chambers

⇒ In QM the potentials are relevant not e.m. fields !

- Idealised Setup : Electric charge e moves on ring with radius R around a magnetic flux tube



$$\vec{A}(\vec{r}) = \frac{\Phi}{2\pi\rho}\vec{e}_\varphi \quad \text{in cylinder coordinates}$$

$$H = \frac{1}{2mR^2}\left(\frac{\hbar}{i}\partial_\varphi - \frac{e}{c}\frac{\Phi}{2\pi}\right)^2$$

$$\rightsquigarrow E_l = \frac{\hbar^2}{2mR^2}\left(l - \frac{e}{c\hbar}\frac{\Phi}{2\pi}\right)^2 = \frac{\hbar^2}{2mR^2}\left(l - \frac{\Phi}{\Phi_0}\right)^2$$

$$\psi_l(\varphi) = \frac{1}{\sqrt{2\pi}}e^{il\varphi}, \quad l\in\mathbb{Z}$$

Propagator:

$$K(\varphi'',\varphi',t) = \sum_{\ell} e^{-\frac{i}{\hbar}E_\ell t}\, \psi_\ell(\varphi'')\, \psi_\ell^*(\varphi')$$

angular momentum repr.

$$= \frac{1}{2\pi} \sum_{\ell} e^{i(\varphi''-\varphi')\ell} \exp\left\{-\frac{i\hbar t}{2mR^2}\left(\ell - \frac{\Phi}{\Phi_0}\right)^2\right\}$$

: Homework

winding number repr.

$$= \sum_{n\in\mathbb{Z}} \exp\left\{i(\varphi''-\varphi'+2\pi n)\frac{\Phi}{\Phi_0}\right\} K_n(\varphi'',\varphi',t)$$

with zero-field partial propagator

$$K_n(\varphi'',\varphi',t) = \sqrt{\frac{mR^2}{2\pi i\hbar t}}\, \exp\left\{\frac{i}{\hbar}\frac{mR^2}{2t}(\varphi''-\varphi'+2\pi n)^2\right\}$$