Quasi-free One-dimensional problems

Consider a box of size a with high walls.

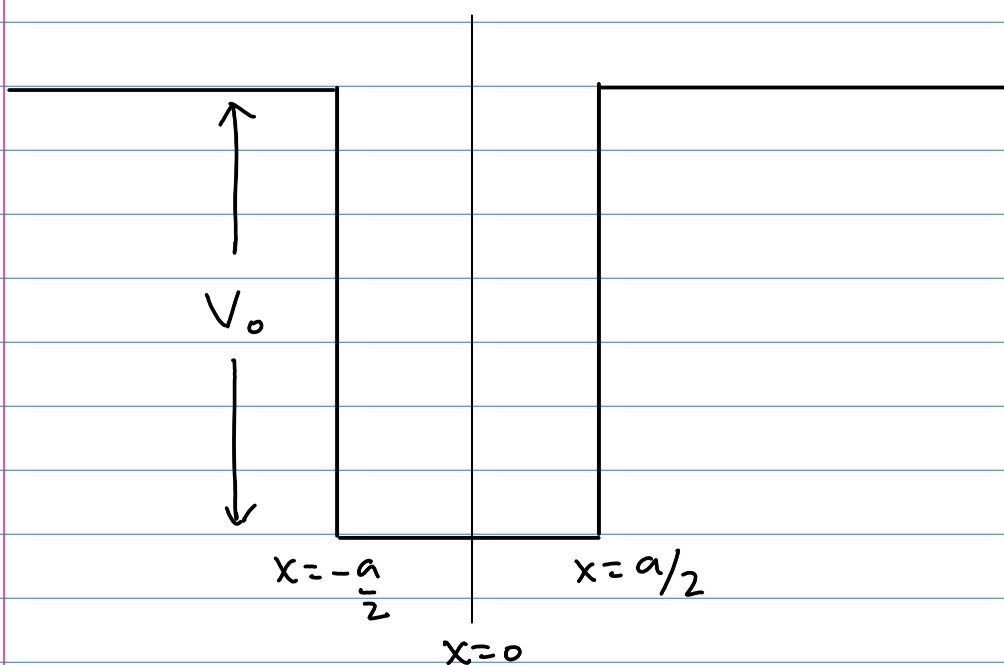
$$\boxed{\mathcal{H} = \frac{\mathbb{P}^2}{2M} + V(\mathbb{X})} \tag{1}$$

where

$$\boxed{V(x) = \begin{cases} 0 & -\frac{a}{2} < x < \frac{a}{2} \\ V_0 & |x| > a/2 \end{cases}} \tag{2}$$

The standard particle in a box corresponds to the limit $V_0 \to \infty$

We want to look for normalizable bound states with energy $\mathcal{E}$ $\boxed{0 < \mathcal{E} < V_0}$ (3)



It is easiest to solve the problem in the x-basis with wavefunctions

Suppose the energy of the eigenstate is ε

$$-\frac{\hbar^2}{2M}\frac{d^2\psi}{dx^2} = \varepsilon\psi \qquad |x| < \frac{a}{2} \qquad \text{Regim I}$$

(4)

$$-\frac{\hbar^2}{2M}\frac{d^2\psi}{dx^2} = (\varepsilon - V_0)\psi \qquad |x| > a/2 \qquad \text{Regim II}$$

Let $k^2 = \frac{2M\varepsilon}{\hbar^2} > 0$ (5) and $\kappa^2 = \frac{2M}{\hbar^2}(V_0 - \varepsilon) > 0$ (6)

because $0 < \varepsilon < V_0$

Then in Regim I

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx} \quad (7)$$

In Region II

$$\psi_{II}(x) = Ce^{\kappa x} + De^{-\kappa x} \quad (8)$$

In order to be normalizable we need (9)

$$\psi_{II}(x) = C_1 e^{-\kappa x} \quad x > \frac{a}{2} \qquad \text{or} \qquad C_2 e^{\kappa x} \quad x < -\frac{a}{2}$$

What happens at the boundary? The wave f^n should be continuous. Also, integrate the Schrödinger eq^n between $\frac{a}{2} - \eta$ and $\frac{a}{2} + \eta$

$$\frac{d^2\psi}{dx^2} = -\frac{2M}{\hbar^2}(\varepsilon - V(x)) \quad (10)$$

$$\Rightarrow \boxed{\int_{\frac{a}{2}-\eta}^{\frac{a}{2}+\eta} dx \, \frac{d^2\psi}{dx^2} = \frac{d\psi}{dx}\Big|_{\frac{a}{2}+\eta} - \frac{d\psi}{dx}\Big|_{\frac{a}{2}-\eta} = -\frac{2M}{\hbar^2} \, 2\varepsilon\eta\, \psi\left(\tfrac{a}{2}\right) + V_0 \eta \psi(a/2)} \quad (11)$$

As long as V_0 is finite we can take the limit $\eta \to 0$ so the RHS vanishes and the derivative of ψ has to be continuous

$$\boxed{\begin{aligned} &\lim_{\eta\to 0} \frac{d\psi}{dx}\Big|_{\frac{a}{2}+\eta} = \lim_{\eta\to 0} \frac{d\psi}{dx}\Big|_{\frac{a}{2}-\eta} \\ &\text{and} \quad \lim_{\eta\to 0} \psi\left(\tfrac{a}{2}+\eta\right) = \lim_{\eta\to 0} \psi\left(\tfrac{a}{2}-\eta\right) \end{aligned}} \quad (12)$$

So at $\frac{a}{2}$ we get

$$\boxed{\begin{aligned} &A e^{ik\frac{a}{2}} + B e^{-ik\frac{a}{2}} = C_1 e^{-\kappa a/2} \\ \text{and} \quad &ik\left(A e^{ik\frac{a}{2}} - B e^{-ik\frac{a}{2}}\right) = -\kappa C_1 e^{-\kappa a/2} \end{aligned}} \quad (13)$$

At $-\frac{a}{2}$ we get

$$\boxed{\begin{aligned} &A e^{-ik\frac{a}{2}} + B e^{ik\frac{a}{2}} = C_2 e^{-\kappa a/2} \\ &ik\left(A e^{-ik\frac{a}{2}} - B e^{ik\frac{a}{2}}\right) = +\kappa C_2 e^{-\kappa\frac{a}{2}} \end{aligned}} \quad (14)$$

Define $\boxed{\xi = \frac{\kappa a}{2} \quad \text{and} \quad \varphi = \frac{ka}{2}}$ (15)

From (13) $$C_1 = e^{\xi}\left[Ae^{i\varphi} + Be^{-i\varphi}\right]$$

$$= -\frac{ik}{k} e^{\xi}\left[Ae^{i\varphi} - Be^{-i\varphi}\right]$$

Therefore
$$Ae^{i\varphi}\left(1+\frac{ik}{k}\right) = -Be^{-i\varphi}\left(1-\frac{ik}{k}\right)$$

or
$$\boxed{B = -e^{2i\varphi}\frac{(k+ik)}{(k-ik)}A} \quad (16)$$

From (14) $$C_2 = e^{\xi}\left(Ae^{-i\varphi} + Be^{i\varphi}\right)$$

$$= +\frac{ik}{k}\left(Ae^{-i\varphi} - Be^{i\varphi}\right)e^{\xi}$$

$$\Rightarrow \quad Ae^{-i\varphi}\left(1-\frac{ik}{k}\right) = -Be^{i\varphi}\left(1+\frac{ik}{k}\right)$$

$$\Rightarrow \quad \boxed{B = -e^{-2i\varphi}\frac{k-ik}{k+ik}A} \quad (17)$$

Consistency between (16) and (17) requires

$$e^{2i\varphi}\frac{k+ik}{k-ik} = e^{-2i\varphi}\frac{k-ik}{k+ik}$$

$$e^{4i\varphi} = \left(\frac{k-ik}{k+ik}\right)^2 \Rightarrow \boxed{e^{2i\varphi} = \pm\frac{k-ik}{k+ik}} \quad (18)$$

Define $$\boxed{\theta = \tan^{-1}\left(\frac{k}{k}\right) = \tan^{-1}\left(\sqrt{\frac{\varepsilon}{V_0-\varepsilon}}\right)} \quad (19)$$

$$e^{2i\varphi} = \pm e^{-2i\theta}$$

For $e^{2i\varphi} = +e^{-2i\theta}$ $\qquad \varphi_{n+} = n\pi - \theta \qquad n$ integer

For $e^{2i\varphi} = -e^{-2i\theta}$ $\qquad \varphi_{n-} = (n+\frac{1}{2})\pi - \theta \qquad n$ integer

Let's write these out fully. We will call the allowed wavevectors

$$\boxed{\begin{aligned} k_{n+} &= \sqrt{\frac{2M\varepsilon_{n+}}{\hbar^2}} \qquad k_{n-} = \sqrt{\frac{2M\varepsilon_{n-}}{\hbar^2}} \\ \varphi_{n+} &= \frac{a}{2}\sqrt{\frac{2M\varepsilon_{n+}}{\hbar^2}} = n\pi - \tan^{-1}\sqrt{\frac{\varepsilon_{n+}}{V_0-\varepsilon_{n+}}} \\ \varphi_{n-} &= \frac{a}{2}\sqrt{\frac{2M\varepsilon_{n-}}{\hbar^2}} = (n+\tfrac{1}{2})\pi - \tan^{-1}\sqrt{\frac{\varepsilon_{n-}}{V_0-\varepsilon_{n-}}} \end{aligned}} \quad (20)$$

These are nonlinear self-consistency conditions which can only be solved numerically.

For example, for $\boxed{V_0 = \frac{\hbar^2}{2M}\frac{400}{a^2}}$ (21), we can say

$$\frac{k_{n+}a}{2} = n\pi - \tan^{-1}\left[\frac{k_{n+}a}{(400-(k_{n+}a)^2)^{1/2}}\right]$$

$$\frac{k_{n-}a}{2} = (n+\tfrac{1}{2})\pi - \tan^{-1}\left[\frac{k_{n-}a}{(400-(k_{n-}a)^2)^{1/2}}\right]$$

$$\boxed{k_{+1} = \frac{5.7220}{a} \qquad k_{+2} = \frac{11.5093}{a} \qquad k_{-0} = \frac{2.8568}{a} \qquad k_{-1} = \frac{8.6043}{a}} \quad (22)$$

Once we know k, we can go back to get B in terms of A, then get C_1 and C_2 in terms of A. Finally we fix A by normalizing the wavefunction

From 13 $\quad C_1 = e^{\xi}\left(Ae^{i\varphi} + Be^{-i\varphi}\right)$

$$= e^{\xi} A e^{i\varphi}\left[1 - \frac{\kappa + ik}{\kappa - ik}\right] = \boxed{\frac{-2ik}{\kappa} e^{\frac{\kappa a}{2}} A e^{i\varphi} = C_1} \quad (23)$$

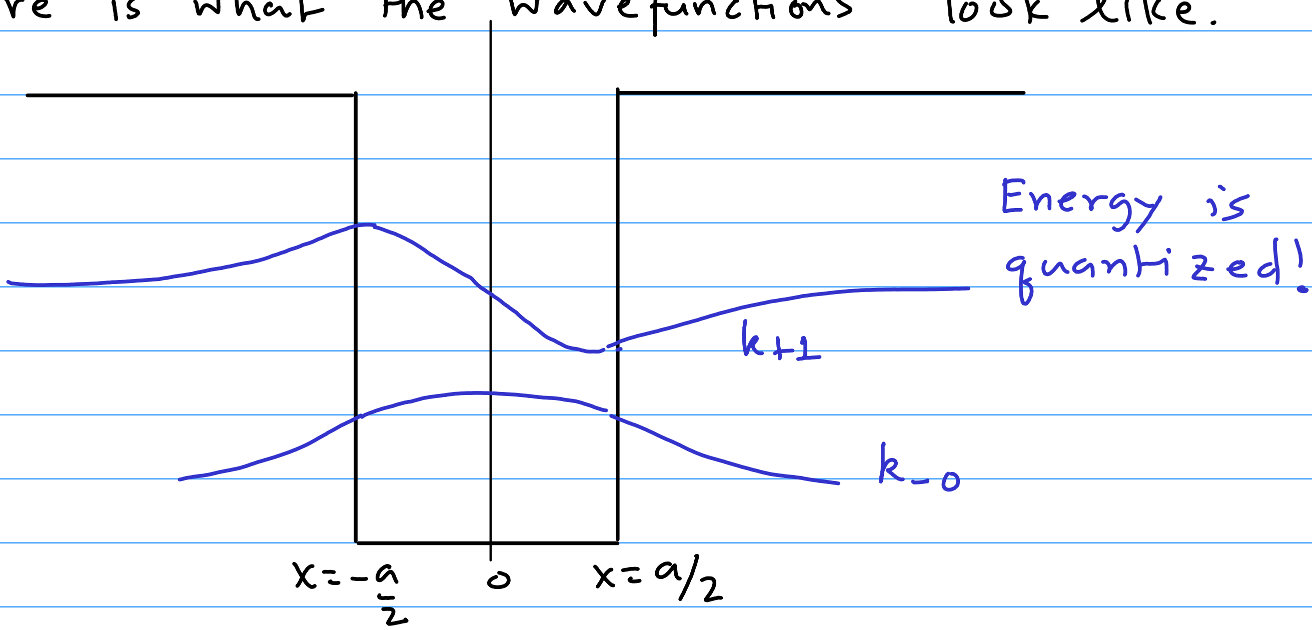
Similarly $\quad \boxed{C_2 = \frac{2ik}{\kappa} e^{\kappa a/2} A e^{-i\varphi}} \quad (24)$

The total probability in Region II is

$$2\int_{a/2}^{\infty} dx\, |A|^2 \frac{k^2}{\kappa^2} e^{-\kappa(x - a/2)}$$

$$\boxed{P_{\text{forbidden}} = \frac{2|A|^2 k^2}{\kappa^3}} \quad (25)$$

Here is what the wavefunctions look like.



The particle has a nonzero amplitude to be in the classically forbidden region $|x| > a/2$

As $\frac{V_0}{\varepsilon}$ gets larger the tails in the forbidden region get shorter and shorter and the total probability of being there decreases like

$$\sim \frac{\varepsilon}{V_0^{3/2}}$$

In the (singular) limit $V_0 \to \infty$ we can simplify because $\vartheta = 0$

$$\boxed{\begin{aligned} \varphi_{n+} &= n\pi \qquad && n = 1, 2, \cdots \\ \varphi_{n-} &= \left(n + \tfrac{1}{2}\right)\pi \qquad && n = 0, 1, \cdots \end{aligned}} \qquad (26)$$

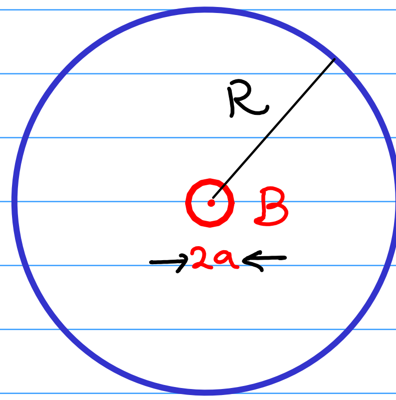
The exponential tails vanish in this limit and the wavefunction vanishes for $|x| > a/2$.

This is what you usually study in your undergraduate.

The Aharanov-Bohm Effect

Consider an electron (charge = $-e$) moving in a 1D ring. There is a solenoid of radius a which pierces the ring at the center. Assume that the solenoid is long enough that there is no field outside it.

So there is no field in the region where the electron lives.



Classically, the electron does not care about the solenoid, and its motion is independent of whether the solenoid has a field or not.

In QM, there is a surprise, first pointed out by Aharanov & Bohm in 1959.

As we know from our discussion of the Lagrangian and Hamiltonian of a charged particle talking to an EM field

$$\boxed{\mathcal{H} = \frac{(\vec{p} - q\vec{A})^2}{2M} + q A_0} \quad (27)$$

A_0 = scalar potential

$$\boxed{\vec{E} = -\vec{\nabla} A_0 - \frac{\partial \vec{A}}{\partial t} \qquad \vec{B} = \vec{\nabla} \times \vec{A}} \quad (28)$$

You probably know that one has the freedom to choose different "gauges" which result in the same $\vec{E}$ and $\bar{B}$ fields. For any arbitrary function $\chi(\vec{x},t)$ we can define

$$\boxed{A_{0,new} = A_{0,old} - \frac{\partial \chi}{\partial t} \qquad \vec{A}_{new} = \vec{A}_{old} + \vec{\nabla}\chi} \quad (29)$$

It is easy to check that $\vec{E}$ & $\bar{B}$ remain unchanged under this transformation of $\bar{A}$ and A_0.

So in E&M one argues that $\bar{A}$ and A_0 are not physical, only $\bar{E}$ and $\bar{B}$ are physical

Coming back to the Aharanov – Bohm (AB) problem let's choose the convenient gauge

$$\boxed{\vec{A} = \hat{e}_\varphi \begin{cases} \dfrac{B_0 \rho}{2} & \rho = \sqrt{x^2+y^2} < a \\[2ex] \dfrac{B_0 a^2}{2\rho} & \rho > a \end{cases}} \quad (30)$$

where we work in cylindrical coordinates ρ, φ, z. The unit vectors in cartesian components are

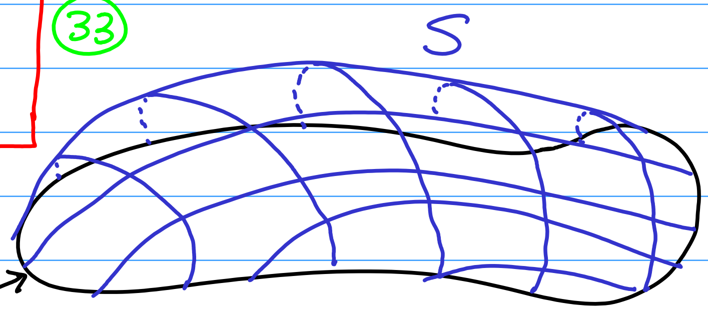
$$\boxed{\hat{e}_\rho = \cos\varphi\,\hat{i} + \sin\varphi\,\hat{j} \qquad e_\varphi = -\sin\varphi\,\hat{i} + \cos\varphi\,\hat{j}} \quad (31)$$

$$\boxed{\begin{aligned} \vec{B} = \vec{\nabla}\times\vec{A} &= B_0\,\hat{e}_z && \rho < a \\ &= 0 && \rho > a \end{aligned}} \quad (32)$$

Can we find a gauge where $\vec{A}=0$ everywhere outside the solenoid?

This cannot happen, as seen from the following simple argument. From Stokes' Theorem we know that if there is an open surface S with boundary ∂S (read as "boundary S")

$$\boxed{\oint_{\partial S} \vec{A}(\vec{x})\cdot d\vec{x} = \int_S \vec{\nabla}\times\vec{A}\cdot\hat{n}\, da} \quad (33)$$



where $\hat{n}$ is the local normal to S, with orientation decided by the right-hand rule.

Taking S to be a disk A radius $\rho>a$ we see that

$$\boxed{\oint_{\rho=\text{const}} \vec{A}(\rho)\cdot\hat{e}_\varphi\, \rho\, d\varphi = \int_S \vec{B}\cdot\hat{n}\, da = \pi a^2 B_0} \quad (34)$$

So $\bar{A}$ cannot be made to vanish outside the solenoid.

It is also easy to check that the loop integral of $\vec{A}$ (over ∂S) is gauge-invariant.

Let's get back to the problem at hand.

This is a problem with constraints forcing the electron to move in the ring

Classically the constraints are

$$\boxed{z=0, \qquad \rho = R} \quad (35)$$

The electron's position is (36)

$$\boxed{\begin{aligned} \vec{x} &= R(\cos\varphi\,\hat{i} + \sin\varphi\,\hat{j}) \\ \dot{\vec{x}} &= R\dot{\varphi}\,(-\sin\varphi\,\hat{i} + \cos\varphi\,\hat{j}) = R\dot{\varphi}\,\hat{e}_\varphi \end{aligned}}$$

Since $R > a$

$$\boxed{\vec{A}(\bar{x},t) = \frac{B_0 a^2}{2R}\,\hat{e}_\varphi} \quad (37)$$

(38)

$$\Rightarrow \boxed{L = \frac{1}{2} M \dot{\vec{x}}^2 + q\,\dot{\vec{x}}\cdot\vec{A} = \frac{1}{2} M R^2 \dot{\varphi}^2 - \frac{e B_0 a^2}{2}\dot{\varphi}}$$

$$\boxed{P_\varphi = \frac{\partial L}{\partial \dot{\varphi}} = M R^2 \dot{\varphi} - \frac{e B_0 a^2}{2}} \quad (39)$$

(40)

$$\boxed{\mathcal{H} = P_\varphi \dot{\varphi} - L = \frac{1}{2} M R^2 \dot{\varphi}^2 = \frac{\left(P_\varphi + \frac{e B_0 a^2}{2}\right)^2}{2 M R^2}}$$

Now we carry out canonical quantization

$$\boxed{P_\varphi \to \mathbb{P}_\varphi \qquad \varphi \to \boldsymbol{\varphi}} \quad (41)$$

Let's work in the real space basis

$$\boxed{\psi(\varphi) = \langle \varphi | \psi \rangle} \quad (42)$$

$$\boxed{P_\varphi \psi(\varphi) = -i\hbar \frac{\partial}{\partial \varphi} \psi(\varphi)} \quad (43)$$

Let us introduce the total magnetic flux Φ

$$\boxed{\Phi = \pi B a^2} \quad (44)$$

$$\boxed{\begin{aligned} \mathcal{H} \psi(\varphi) &= \frac{1}{2MR^2} \left(-i\hbar \frac{\partial}{\partial \varphi} + \frac{e\Phi}{2\pi} \right)^2 \psi(\varphi) \\ &= \frac{-\hbar^2}{2MR^2} \left[\frac{\partial}{\partial \varphi} + \frac{ie\Phi}{h} \right]^2 \psi(\varphi) \end{aligned}} \quad (45)$$

Since φ is an angle it is dimensionless. So $\frac{e\Phi}{h}$ must also be dimensionless. This allows us to introduce the flux quantum

$$\boxed{\Phi_0 = \frac{h}{e}} \quad (46)$$

$$\boxed{\mathcal{H} \psi(\varphi) = \frac{-\hbar^2}{2MR^2} \left(\frac{\partial}{\partial \varphi} + i \frac{\Phi}{\Phi_0} \right)^2 \psi(\varphi)} \quad (47)$$

The smoothness of the wavef^n means that we are forced to have

$$\boxed{\psi(\varphi + 2\pi) = \psi(\varphi)} \quad (48)$$

We can easily find the eigenfunctions of $\mathcal{H}$

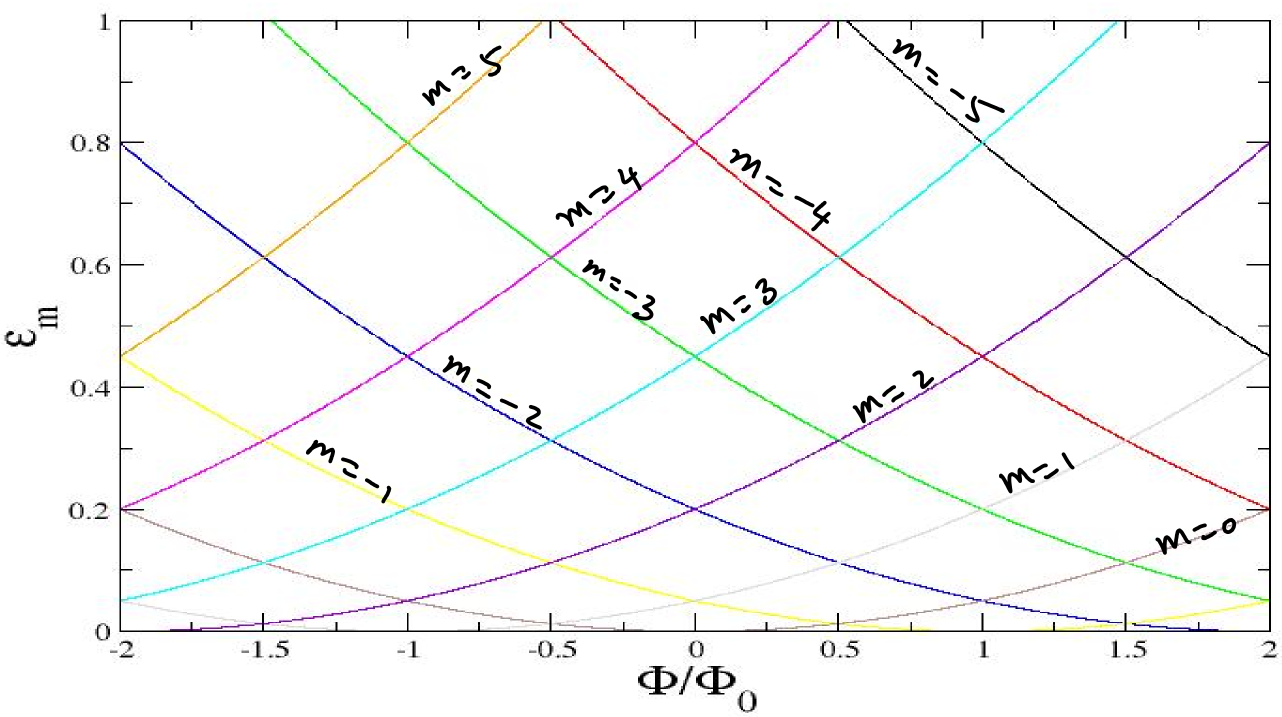
$$\boxed{\psi_m(\varphi) = \frac{e^{im\varphi}}{\sqrt{2\pi R}}} \quad (49)$$

$$\mathcal{H}\psi_m(\varphi) = \frac{\hbar^2}{2MR^2}\left[m + \frac{\Phi}{\Phi_0}\right]^2 \psi_m(\varphi)$$

$$\boxed{\varepsilon_m = \frac{\hbar^2}{2MR^2}\left[m + \frac{\Phi}{\Phi_0}\right]^2} \quad (50)$$

The spectrum, which is something very physical, depends on Φ!

So, even though the electron's wavefunction is never in a region where $B \neq 0$, it "knows" about the solenoid.



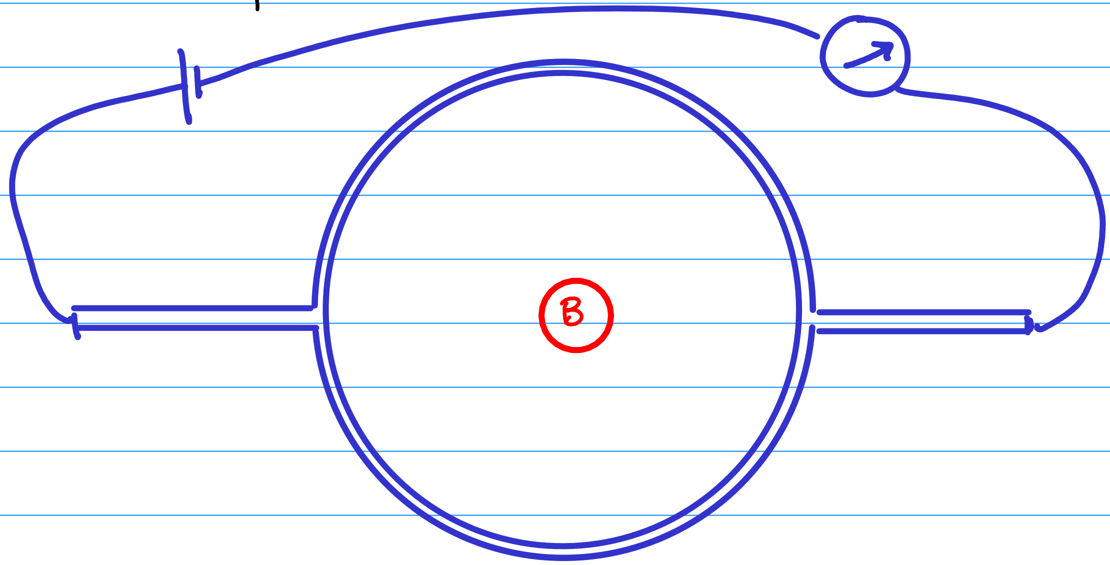
A striking feature of the spectrum is its periodicity under

$$\boxed{\Phi \to \Phi + \Phi_0} \quad (51)$$

The dependence of the spectrum on Φ can in principle be directly measured. However, there is another interesting physical consequence known as "persistent currents".

The ground state can have nonzero current. Since this is the lowest state, it cannot decay. This was seen in the 80's in μm-sized copper rings.

The AB effect can also be detected as electron interference when the ring is connected to leads and a current is made to flow



The current oscillates as a function of the flux through the ring.

Before we leave this topic, let's discuss how gauge transformations affect the wavefunction. Consider the time-dependent Schrödinger eqn in 3D in the real-space basis

$$\boxed{\begin{gathered}\vec{x}\,|\vec{x}\rangle = \vec{x}\,|\vec{x}\rangle \\ \langle\vec{x}|\vec{x}'\rangle = \delta^3(\vec{x}-\vec{x}') \qquad \mathbb{1} = \int d^3x\, |\vec{x}\rangle\langle\vec{x}| \\ \psi(\vec{x}) = \langle\vec{x}|\psi\rangle \qquad \vec{p}\,\psi(\vec{x}) = -i\hbar\vec{\nabla}\psi(\vec{x})\end{gathered}} \tag{52}$$

$$\boxed{i\hbar\frac{\partial}{\partial t}\psi(\vec{x},t) = \left[\frac{\left(\vec{p}-q\vec{A}(\vec{x},t)\right)^2}{2M} + qA_0(\vec{x},t)\right]\psi(\vec{x},t)} \tag{53}$$

Let us make a phase transformation on ψ in a space time dependent way

$$\boxed{\psi_{old}(\vec{x},t) = e^{\frac{iq}{\hbar}\chi(\vec{x},t)}\,\psi_{new}(\vec{x},t)} \tag{54}$$

$$\boxed{i\hbar\frac{\partial}{\partial t}\psi_{old} = e^{\frac{iq}{\hbar}\chi(\vec{x},t)}\left\{i\hbar\frac{\partial\psi_{new}}{\partial t} - q\frac{\partial\chi}{\partial t}\psi_{new}\right\}} \tag{55}$$

$$\vec{p}\,\psi_{old} = -i\hbar\vec{\nabla}\left(e^{\frac{iq}{\hbar}\chi(\vec{x},t)}\psi_{new}(\vec{x},t)\right)$$

$$= e^{\frac{iq\chi(\vec{x},t)}{\hbar}}\left\{-i\hbar\vec{\nabla}\psi_{new} + q(\vec{\nabla}\chi)\psi_{new}\right\}$$

$$\boxed{\vec{p}\,\psi_{old} = e^{\frac{iq\chi}{\hbar}}\left(\vec{p}+q\vec{\nabla}\chi\right)\psi_{new}} \tag{56}$$

The Schrödinger eq^n becomes, after cancelling $\exp(iq\chi/\hbar)$ from both sides

$$\boxed{i\hbar \frac{\partial}{\partial t}\psi_{new} - q\left(\frac{\partial \chi}{\partial t}\right)\psi_{new} = \frac{1}{2M}\left(\bar{\mathbb{P}} - q\bar{A} + q\bar{\nabla}\chi\right)^2 \psi_{new} + qA_0\psi_{new}} \quad (57)$$

Define

$$\boxed{\begin{aligned} \vec{\bar{A}}_{new} &= \bar{A} - \bar{\nabla}\chi \\ A_{0,new} &= A_0 + \frac{\partial \chi}{\partial t} \end{aligned}} \quad (58)$$

A gauge transformation!

to get

$$\boxed{i\hbar \frac{\partial \psi_{new}}{\partial t} = \left[\frac{(\bar{\mathbb{P}} - q\bar{A}_{new})^2}{2M} + qA_{0,new}\right]\psi_{new}} \quad (59)$$

So a spacetime dependent phase transformation of ψ can be absorbed into a gauge transformation of $\bar{A}, A_0$, leaving the form of the Hamiltonian unchanged

You can see that the physical fields $\bar{E}$ and $\bar{B}$ felt by ψ_{new} are the same as those felt by ψ_{old}. So the physics remains unchanged under gauge transformations.

Here is a different, and perhaps more convincing way to see this.

First we need some new technology.

The Schrödinger eq^n is itself an equation of motion. One can ask whether it can arise as an Euler-Lagrange eq^n from extremizing an action.

The answer is yes, but it is a bit more complicated than the Lagrangian for a particle. We are now looking for a functional S that takes in a function of $\bar{x}, t$ $(\psi(\bar{x},t))$ and spits out a real number, the action.

Clearly, it must have integrals over both $\bar{x}$ and t. Here is the action that leads to the Schrödinger eq^n

$$\boxed{S = \int_{t_1}^{t_2} dt \int d^3x \left\{ \frac{i\hbar}{2}\left[\psi^*(\bar{x},t)\frac{\partial}{\partial t}\psi(\bar{x},t) - \left(\frac{\partial}{\partial t}\psi^*(\bar{x},t)\right)\psi(\bar{x},t)\right] - \psi^*(\bar{x},t)\frac{\left(-i\hbar\vec{\nabla} - q\vec{A}(\bar{x},t)\right)^2}{2M}\psi(\bar{x},t) - qA_0(\bar{x},t)\psi^*(\bar{x},t)\psi(\bar{x},t) \right\}} \quad (60)$$

In the jargon of theoretical physics, the object in $\{\ \}$ is called the Lagrangian density $\mathcal{L}$ because one gets the Lagrangian by integrating $\mathcal{L}$ over space.

S should be extremized subject to boundary conditions

$$\boxed{\psi(\vec{x}, t=t_1) = \Phi_1(\bar{x}) \qquad \psi(\bar{x}, t=t_2) = \Phi_2(\bar{x})} \quad (61)$$

where $\Phi_{1,2}$ are given complex functions

To obtain the Euler-Lagrange eq^n assume that we have the $\psi_0(\bar{x},t)$ that extremizes $\mathcal{S}$

Let $\boxed{\psi(\bar{x},t) = \psi_0(\bar{x},t) + \delta\psi(\bar{x},t)}$ (62) $\boxed{\delta\psi = 0 \text{ at } t_1, t_2}$ (63)

$$\mathcal{S}[\psi(\bar{x})] = \int_{t_1}^{t_2} dt \int d^3\bar{x} \left\{ \frac{i\hbar}{2}\left[(\psi_0^* + \delta\psi^*)\,\partial_t(\psi_0 + \delta\psi) - \left(\partial_t(\psi_0^* + \delta\psi^*)\right)(\psi_0 + \delta\psi) \right] \right.$$
$$\left. - (\psi_0^* + \delta\psi^*)\frac{\left[-i\hbar\vec{\nabla} - q\bar{A}(\bar{x},t)\right]^2}{2M}(\psi_0 + \delta\psi) - qA_0(\psi_0^* + \delta\psi)(\psi_0 + \delta\psi) \right\}$$

We want $\delta\mathcal{S}$ to 1st order in $\delta\psi, \delta\psi^*$

$$\boxed{\begin{aligned} \delta\mathcal{S} = \int_{t_1}^{t_2} dt \int d^3\vec{x} \Big\{ & \frac{i\hbar}{2}\left[\psi_0^*\,\delta\dot{\psi} + \delta\psi^*\,\dot{\psi}_0 - \dot{\psi}_0^*\,\delta\psi - \delta\dot{\psi}^*\,\psi_0 \right] \\ & - \delta\psi^*\frac{\left[-i\hbar\vec{\nabla} - q\vec{A}\right]^2}{2M}\psi_0 - \psi_0^*\frac{\left[-i\hbar\vec{\nabla} - q\vec{A}\right]^2}{2M}\delta\psi \\ & - qA_0\,\psi_0^*\,\delta\psi - qA_0\,\delta\psi^*\,\psi_0 \Big\} \end{aligned}}$$ (64)

Now $\delta\psi$ has a real part and an imaginary part at every $\bar{x},t$. So varying $\mathrm{Re}(\delta\psi)$ and $\mathrm{Im}(\delta\psi)$ is equivalent to varying $\delta\psi, \delta\psi^*$ independently.

The most convenient thing to do is vary with respect to ψ^*. Look at the coefficient of $\delta\psi^*$ in $\delta\mathcal{S}$

$$\delta S = \int_{t_1}^{t_2} dt \int d^3x \left\{ \frac{i\hbar}{2}\left(\delta\psi^* \dot{\psi}_0 - \delta\dot{\psi}^* \psi_0 \right) \right.$$

$$\left. - \delta\psi^* \left\{ \frac{(-i\hbar\bar{\nabla} - q\bar{A})^2}{2M}\psi_0 + qA_0\psi_0 \right\} + \text{terms without } \delta\psi^* \right. \quad (65)$$

Integrate the 2nd term by parts

$$\int_{t_1}^{t_2} dt \int d^3x \left(-\frac{i\hbar}{2} \delta\dot{\psi}^* \psi_0 \right) = -\frac{i\hbar}{2} \int d^3x \left[\delta\psi^*(\bar{x},t_2)\,\psi_0(\bar{x},t_2) - \delta\psi^*(\bar{x},t_1)\,\psi_0(\bar{x},t_1) \right]$$

$$+ \int_{t_1}^{t_2} dt \int d^3x \ \frac{i\hbar}{2}\, \delta\psi^* \dot{\psi}_0$$

The boundary terms vanish because
$\delta\psi|_{t_1} = \delta\psi|_{t_2} = \delta\psi^*|_{t_1} = \delta\psi^*|_{t_2} = 0$

$$\boxed{\delta S = \int_{t_1}^{t_2} dt \int d^3x \left\{ \delta\psi^*(\bar{x},t) \left[i\hbar \frac{\partial\psi_0}{\partial t} - \frac{(-i\hbar\bar{\nabla} - q\bar{A})^2}{2M}\psi_0 - qA_0\psi_0 \right] + \text{terms without } \delta\psi^* \right\} = 0} \quad (66)$$

The only way this can vanish for arbitrary (but small) $\delta\psi^*(\bar{x},t)$ is if the term in the [ ] vanishes for all $\bar{x},t$

$$\Rightarrow \boxed{ i\hbar \frac{\partial\psi_0}{\partial t} = \frac{(-i\hbar\bar{\nabla} - q\bar{A})^2}{2M}\psi_0 + qA_0\psi_0 } \quad (67)$$

which is the Schrödinger eqn.

Varying with respect to $\delta\psi$ instead of $\delta\psi^*$ gives the complex conjugate of the Schrödinger eq^n.

Now let's go back to the gauge transformation.

We will show that S is invariant under the combined set of transformations

$$\boxed{\begin{aligned} \psi(\bar{x},t) &= e^{\frac{iq\chi(\bar{x},t)}{\hbar}} \tilde{\psi}(\bar{x},t) \\ \vec{A} &= \tilde{\vec{A}} + \bar{\nabla}\chi \\ A_0 &= \tilde{A}_0 - \frac{\partial \chi}{\partial t} \end{aligned}} \quad (68)$$

To see this, rewrite S more conveniently as

$$S = \int dt \int d^3\bar{x} \left\{ \frac{i\hbar}{2} \left[\psi^* \left(\partial_t + i\frac{q}{\hbar}A_0\right)\psi - \left(\left(\partial_t - i\frac{q}{\hbar}A_0\right)\psi^*\right)\psi \right] - \psi^* \frac{\left[-i\hbar\bar{\nabla} - q\bar{A}\right]^2}{2M}\psi \right\}$$

First express ψ in terms of $\tilde{\psi}$

$$(69) \quad \boxed{\begin{aligned} \left(\partial_t + i\frac{qA_0}{\hbar}\right)\tilde{\psi} e^{\frac{iq\chi}{\hbar}} &= e^{\frac{iq\chi}{\hbar}} \left(\partial_t + i\frac{q}{\hbar}\left(A_0 + \frac{\partial \chi}{\partial t}\right)\right)\tilde{\psi} \\ \left(\partial_t - i\frac{qA_0}{\hbar}\right)\tilde{\psi}^* e^{-\frac{iq\chi}{\hbar}} &= e^{-\frac{iq\chi}{\hbar}} \left(\partial_t - \frac{iq}{\hbar}\left(A_0 + \frac{\partial \chi}{\partial t}\right)\right)\tilde{\psi}^* \\ \left(-i\hbar\bar{\nabla} - q\bar{A}\right)\tilde{\psi} e^{\frac{iq\chi}{\hbar}} &= e^{\frac{iq\chi}{\hbar}} \left(-i\hbar\bar{\nabla} - q\left(\bar{A} - \bar{\nabla}\chi\right)\right)\tilde{\psi} \end{aligned}}$$

So
$$\boxed{\mathcal{S} = \int dt \int d^3x \left\{ \frac{i\hbar}{2} \left[\tilde{\psi}^* \left(\partial_t - \frac{iq}{\hbar} \left(A_0 + \frac{\partial \chi}{\partial t} \right) \right) \tilde{\psi} - \left(\left(\partial_t + \frac{iq}{\hbar} \left(A_0 + \frac{\partial \chi}{\partial t} \right) \right) \tilde{\psi}^* \right) \tilde{\psi} \right] - \tilde{\psi}^* \frac{\left[-i\hbar \vec{\nabla} - q(\vec{A} - \vec{\nabla}\chi) \right]^2}{2M} \tilde{\psi} \right\}} \quad (70)$$

Now looking at the last two eq^{n}s of (68) we see that

$$\boxed{\mathcal{S} = \int dt \int d^3x \left\{ \frac{i\hbar}{2} \left[\tilde{\psi}^* \left(\partial_t - \frac{iq}{\hbar} \tilde{A}_0 \right) \tilde{\psi} - \left(\left(\partial_t + \frac{iq}{\hbar} \tilde{A}_0 \right) \tilde{\psi}^* \right) \tilde{\psi} \right] - \tilde{\psi}^* \frac{\left[-i\hbar \vec{\nabla} - q \tilde{\vec{A}} \right]^2}{2M} \tilde{\psi} \right\} \quad (71)}$$

The action has the same form in $\tilde{\psi}, \tilde{\vec{A}}, \tilde{A}_0$ as it did in $\psi, \vec{A}, A_0$.

Gauge transformations are invariances of the action. Since the action controls the physics (classical as well as quantum, as we will see when we do path integrals) the physics is invariant under gauge transformations.