Advanced Quantum Physics
Week 10

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From classical to quantum physics

Several effects that we have discussed in previous sections involved the coupling of the magnetic field with magnetic moments, but we have never precisely derived the Hamiltonian that describes the motion of a charged quantum particle in a magnetic field. Classically, we know that the force on a charged particle is specified by the Lorentz law

$$\vec{F} = q\left(\vec{E} + \vec{v} \times \vec{B}\right),$$

where $\vec{v}$ is the velocity of a particle with charge q in the electromagnetic field described by the vectors $\vec{E}$ and $\vec{B}$. We would like to find the Hamiltonian for this system. Until now, we have used Hamiltonians of the form

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + \hat{V}(\vec{r}),$$

where $V(\vec{r})$ is a scalar potential. The Lorentz force can however not be derived from such a Hamiltonian. Indeed, classically, the force would be derived from the gradient of the potential $V(\vec{r})$. This is a quantity that cannot depend on the velocity. So we will have to construct a different kind of Hamiltonian to describe the motion of charged particles. Our strategy will be to go back to the classical Lagrangian and Hamiltonian of a charged particle in a magnetic field and then use the correspondence principle to derive the quantum Hamiltonian. Let us start by summarizing some of the main results from analytical mechanics.

Lagrange mechanics

In Newtonian mechanics, the state of a system (we suppose it is just a single particle) is given by the position $\vec{r}$ and velocity $\vec{v}$ of the particle at a given time t and by the forces that act on it. This allows to find the position and velocity at later times. Analytical mechanics started with the work of Lagrange in the 18th century. He developed a formalism that is

based on scalar properties to describe the dynamics of a system rather than the vectors used in Newtonian mechanics. His idea was to phrased the problem differently and ask what *trajectory* the particle follows if it is at position $\vec{r}_1$ at time t_1 and at position $\vec{r}_2$ at a later time t_2.

Principle of least action

In order to find the trajectory of the particle, Lagrange introduced the quantity S, the action, that is minimized along the physical trajectory of the particle. More precisely, in Lagrangian mechanics, a mechanical system is fully characterized by the Lagrangian $\mathcal{L}(q, \dot{q}, t)$, a function of the coordinate q, its time derivative $\dot{q}$ and the time t. For example, a particle in a one-dimensional potential is described by a Lagrangian

$$\mathcal{L} = \frac{1}{2}m\dot{q}^2 - V(q,t)$$

For any trajectory $q(t)$ that the particle follows between times t_1 and t_2, one can define the action

$$\mathcal{S} = \int_{t_1}^{t_2} \mathcal{L}(q, \dot{q}, t)dt$$

The principle of least action states that the physical trajectory of the particle is the one that minimizes (or extremalizes) the action S.

Euler-Lagrange equations

Mathematically, saying that the action S is extremal means that infinitesimal changes to the trajectory do not change the action at first order. More specifically, let us consider a modification $\delta q(t)$ of a path $Q(t)$

$$q(t) = Q(t) + \delta q(t) \qquad \dot{q}(t) = \dot{Q}(t) + \delta\dot{q}(t) \qquad \delta\dot{q}(t) = \frac{d}{dt}\delta q(t)$$

This new path still has the same start and end points, so we assume that $\delta q(t_1) = \delta q(t_2) = 0$. The corresponding variation of the action is

$$\begin{aligned}\delta\mathcal{S} = \delta\int_{t_1}^{t_2} \mathcal{L}(q, \dot{q}, t)dt &= \int_{t_1}^{t_2} \left(\frac{\partial\mathcal{L}}{\partial q}\delta q(t) + \frac{\partial\mathcal{L}}{\partial\dot{q}}\delta\dot{q}(t)\right)dt \\ &= \int_{t_1}^{t_2} \left[\frac{\partial\mathcal{L}}{\partial q} - \frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\dot{q}}\right)\right]\delta q(t)dt\end{aligned}$$

If the action is extremal $\delta S = 0$ for all $\delta q(t)$. The physical trajectory is therefore the one that satisfies the *Euler-Lagrange* equation

$$\frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\dot{q}}\right) = \frac{\partial\mathcal{L}}{\partial q}$$

The equation above generalizes easily to more degrees of freedom $\{q_i, \dot{q}_i\}$. There is then a Euler-Lagrange equation for every pair $q_i, \dot{q}_i$. For N coordinates, one therefore has to

solve a set of N coupled second-order equations. Applying this formula, for example, to a particle in a one-dimensional potential as above, we obtain the expected equation of motion

$$m\ddot{q}(t) = -\frac{d}{dx}V(x)$$

Energy for isolated systems

In an isolated system, the Lagrangian has no explicit time dependence and we have $\partial\mathcal{L}/\partial t = 0$. The full time derivative of the Lagrangian is then given by

$$\frac{d\mathcal{L}}{dt}(q,\dot{q}) = \dot{q}(t)\frac{\partial\mathcal{L}}{\partial q} + \ddot{q}(t)\frac{\partial\mathcal{L}}{\partial\dot{q}}$$

Along the physical trajectory, we have

$$\begin{aligned}\frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\dot{q}}\right) = \frac{\partial\mathcal{L}}{\partial q} \quad &\Rightarrow \quad \frac{d\mathcal{L}}{dt}(q,\dot{q}) = \dot{q}(t)\frac{d}{dt}\left(\frac{\partial\mathcal{L}}{\partial\dot{q}}\right) + \frac{d\dot{q}}{dt}\frac{\partial\mathcal{L}}{\partial\dot{q}} = \frac{d}{dt}\left(\dot{q}(t)\frac{\partial\mathcal{L}}{\partial\dot{q}}\right) \\ &\Rightarrow \quad \frac{d}{dt}\left(\dot{q}(t)\frac{\partial\mathcal{L}}{\partial\dot{q}} - \mathcal{L}(q,\dot{q})\right) = 0\end{aligned}$$

We therefore see that the quantity

$$E = \dot{q}(t)\frac{\partial\mathcal{L}}{\partial\dot{q}} - \mathcal{L}(q,\dot{q})$$

is a constant of motion. It is the energy of the system. In the simple example above we recover $E = m\dot{q}^2/2 + V(x)$.

Hamilton mechanics

Hamilton introduced a different description of mechanical system that has some advantages over the formulation of Lagrange. He introduced the *conjugate momentum* p of the coordinate q defined by

$$p = \frac{\partial\mathcal{L}}{\partial\dot{q}}$$

In simple cases p is the same as the linear momentum $p = m\dot{q}$ but this will not always be true. The Euler-Lagrange equation implies that

$$\dot{p} = \frac{\partial\mathcal{L}}{\partial q}$$

Using the conjugate momentum, the state of the system can be described by the *Hamiltonian*

$$\mathcal{H}(q,p,t) = p\,\dot{q} - \mathcal{L}(q,\dot{q},t)$$

In this expression, it is assumed that $\dot{q}$ is written in terms of of q and p.

Canonical equations of Hamilton and Jacobi

We can find the equations of motion of the system by taking the total differential of $\mathcal{H}$

$$\begin{aligned} d\mathcal{H} &= p\,d\dot{q} + \dot{q}\,dp - \frac{\partial \mathcal{L}}{\partial q}dq - \frac{\partial \mathcal{L}}{\partial \dot{q}}d\dot{q} - \frac{\partial \mathcal{L}}{\partial t}dt \\ &= \dot{q}\,dp - \dot{p}\,dq - \frac{\partial \mathcal{L}}{\partial t}dt \end{aligned}$$

This yields the following equations of motion, the *canonical equations* of Hamilton and Jacobi

$$\dot{p} = -\frac{\partial \mathcal{H}}{\partial q} \qquad \dot{q} = \frac{\partial \mathcal{H}}{\partial p}$$

For N coordinates, this is a set of $2N$ first-order equations, in contrast to the N second-order equations within the Lagrange formulation.

Poisson brackets

Let us consider two functions A and B of q, p and t. We introduce the *Poisson brackets* of A and B defined as

$$\{A, B\} = \frac{\partial A}{\partial q}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial q}$$

It is clear that $\{A, B\} = -\{B, A\}$. We also always have $\{q, p\} = 1$ or more generally $\{q_i, q_j\} = \{p_i, p_j\} = 0$ and $\{q_i, p_j\} = \delta_{ij}$. The full time derivative of a function $A(q, p, t)$ is

$$\frac{dA}{dt} = \frac{\partial A}{\partial q}\dot{q} + \frac{\partial A}{\partial p}\dot{p} + \frac{\partial A}{\partial t}$$

If we use the canonical equations we find

$$\frac{dA}{dt} = \{A, \mathcal{H}\} + \frac{\partial A}{\partial t}$$

With this expression, the canonical equations simply become

$$\dot{q} = \{q, \mathcal{H}\} \qquad \dot{p} = \{p, \mathcal{H}\}$$

The correspondence principle

It is striking how the equation for dA/dt derived above resembles the Ehrenfest theorem we have seen earlier in quantum mechanics

$$\frac{d}{dt}\langle a\rangle(t) = \frac{1}{i\hbar}\langle\Psi(t)|[\hat{A}, \hat{\mathcal{H}}]|\Psi(t)\rangle + \langle\Psi(t)|\frac{\partial \hat{A}}{\partial t}|\Psi(t)\rangle$$

The same is true for the canonical commutation relations

$$[\hat{x}_i, \hat{p}_j] = \delta_{ij}$$

The similarity of the structure of the Hamiltonian classical mechanics and quantum mechanics was one of the great discoveries of Dirac. He formulated a correspondence principle telling how a classical theory should be turned into a quantum theory. The resulting quantization rule is that the Poisson brackets should be replaced by the commutators of the corresponding observables, divided by $i\hbar$

$$\{A, B\} \to \frac{1}{i\hbar}[\hat{A}, \hat{B}]$$

This prescription is very useful to find the quantum mechanical formulation of complex systems with many degrees of freedom, constraints, etc. We will now use it to describe the quantum physics of a charged particle in a magnetic field.

Charged particle in a magnetic field

A charged particle moving in a electromagnetic field given by $\vec{E}$ and $\vec{B}$ at a velocity $\vec{v}$ will feel a force

$$\vec{F} = q\left(\vec{E} + \vec{v} \times \vec{B}\right)$$

This force cannot by derived from a potential and a usual Hamiltonian of the form $\hat{\mathcal{H}} = \hat{p}^2/2m + V(\vec{r})$ cannot be used. Classically, one can however construct a Lagrangian for this problem. The Maxwell equations

$$\vec{\nabla} \cdot \vec{B} = 0 \qquad \vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

allow to express the fields $\vec{E}$ and $\vec{B}$ using a scalar potential Φ and a vector potential $\vec{A}$:

$$\vec{B} = \vec{\nabla} \times \vec{A} \qquad \vec{E} = -\vec{\nabla}\Phi - \frac{\partial \vec{A}}{\partial t}$$

Using these potentials, the following Lagrangian correctly describes the motion of a charged particle

$$\mathcal{L} = \frac{1}{2}m\dot{r}^2 + q\dot{\vec{r}} \cdot \vec{A}(\vec{r}, t) - q\Phi(\vec{r}, t).$$

Indeed the Euler-Lagrange equations then yield

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{r}_i}\right) = \frac{\partial \mathcal{L}}{\partial r_i} \quad \Rightarrow \quad \frac{d}{dt}\left(m\dot{r}_i + qA_i(\vec{r}, t)\right) = q\dot{\vec{r}} \cdot \frac{\partial \vec{A}(\vec{r}, t)}{\partial r_i} - q\frac{\partial \Phi(\vec{r}, t))}{\partial r_i}$$

Expanding the time derivative we obtain

$$m\ddot{r}_i + q\left(\frac{\partial A_i(\vec{r}, t)}{\partial t} + \sum_j \frac{\partial A_i(\vec{r}, t)}{\partial r_j}\dot{r}_j\right) = q\sum_j \frac{\partial A_j(\vec{r}, t)}{\partial r_i}\dot{r}_j - q\frac{\partial \Phi(\vec{r}, t))}{\partial r_i}$$

Remembering that $\vec{a} \times \vec{\nabla} \times \vec{b} = \vec{\nabla}(\vec{a} \cdot \vec{b}) - (\vec{\nabla} \cdot \vec{a})\vec{b}$, we now have an expression for the equation of motion

$$m\ddot{r}_i = q\sum_j \left(\frac{\partial A_j(\vec{r}, t)}{\partial r_i}\dot{r}_j - \frac{\partial A_i(\vec{r}, t)}{\partial r_j}\dot{r}_j\right) - q\left(\frac{\partial \Phi(\vec{r}, t))}{\partial r_i} - \frac{\partial A_i(\vec{r}, t)}{\partial t}\right)$$

$$m\frac{d\vec{v}}{dt} = q\left(\vec{v} \times \vec{B} + \vec{E}\right)$$

We see that we recover the Lorentz force. From here, we can go ahead and construct the Hamiltonian. The canonical conjugate of the position $\vec{r}$ is

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{r}_i} = m\dot{r}_i + qA_i(\vec{r}, t) \quad \Rightarrow \quad \vec{p} = m\dot{\vec{r}} + q\vec{A}(\vec{r}, t)$$

Note that $\vec{p}$ is not the velocity of the particle $\vec{p} \neq m\dot{\vec{r}}$. We can now write the classical Hamiltonian

$$\mathcal{H} = \frac{1}{2m}\left(\vec{p} - q\vec{A}(\vec{r}, t)\right)^2 + q\Phi(\vec{r}, t)$$

For an isolated system, the energy is conserved and is given by

$$E = \dot{\vec{r}}(t) \cdot \frac{\partial \mathcal{L}}{\partial \dot{\vec{r}}} - \mathcal{L}(\vec{r}, \dot{\vec{r}}) = \frac{1}{2}m\dot{r}^2 + q\Phi(\vec{r}, t)$$

Minimal coupling

In the section above, we have shown that the substitution

$$\vec{p} \to \vec{p} - q\vec{A}(\vec{r},t) \quad E \to E + q\Phi(\vec{r},t)$$

yields a classical Hamiltonian that describes the motion of a charged particle. This substitution is often called the *minimal substitution*. In order to find this rule, we have constructed a Lagrangian that yields the correct Lorentz force law. But there is a more elegant way to obtain that Lagrangian that does not require the knowledge of the Lorentz force. The construction goes beyond the scope of this lecture, but one can show that imposing the local gauge invariance of the theory leads to quite strong constraints on the form of the Lagrangian. The formula above is the simplest form (in the sense that it only couples the vector potential to the charge and not to higher moments, hence the minimal coupling name) that is compatible with local gauge invariance. This is very powerful, because the local gauge invariance constraint actually yields the Lorentz force law!

Quantum Hamiltonian

Now that we have found the classical Hamiltonian, we can use the correspondence principle to find the quantum Hamiltonian describing a charged particle in an electromagnetic field

$$\hat{\mathcal{H}} = \frac{1}{2m}\left(\hat{\vec{p}} - q\hat{\vec{A}}(\vec{r},t)\right)^2 + q\hat{\Phi}(\vec{r},t)$$

In the classical picture we clearly have the Poisson bracket $\{x_i, p_j\} = \delta_{ij}$. It follows that the momentum operator $\hat{\vec{p}}$ obeys the standard commutation relation

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$$

We see that we still can still write the momentum operator as $\vec{p} = -i\hbar\vec{\nabla}$. However, the velocity operator is given by

$$\hat{\vec{v}} = \frac{1}{m}\left(\hat{\vec{p}} - q\hat{\vec{A}}(\vec{r},t)\right)$$

It is interesting to observe that different components of the velocity do not commute in general!

Normal Zeeman effect

Let us consider the example of a hydrogen atom in a constant magnetic field. We can choose a gauge such that $\vec{A} = \vec{B} \times \vec{r}/2$ and $\Phi = 0$. The Hamiltonian is given by

$$\hat{\mathcal{H}} = \frac{1}{2m}\left(\hat{\vec{p}} - q\hat{\vec{A}}(\vec{r},t)\right)^2 + \hat{V}(\vec{r}),$$

where $V(\vec{r}) = -\frac{q^2}{4\pi\epsilon_0 r}$. The Hamiltonian can be rewritten as

$$\hat{\mathcal{H}} = \left[\frac{\hat{p}^2}{2m} + \hat{V}(\vec{r})\right] - \frac{q}{2m}\left(\hat{\vec{p}}\cdot\hat{\vec{A}} + \hat{\vec{A}}\cdot\hat{\vec{p}}\right) + \frac{q^2}{2m}\hat{A}^2$$

In this Hamiltonian, the first term describes the usual hydrogen atom in the absence of a magnetic field. The second term is called the *paramagnetic term*. Given our choice of gauge, we have $\hat{\vec{p}}\cdot\hat{\vec{A}} = \hat{\vec{A}}\cdot\hat{\vec{p}}$ and the term can be written

$$\hat{\mathcal{H}}_{\rm para} = -\frac{q}{2m}\left(\vec{B}\times\hat{\vec{r}}\right)\cdot\hat{\vec{p}} = -\frac{q}{2m}\left(\hat{\vec{r}}\times\hat{\vec{p}}\right)\cdot\vec{B} = -\gamma_0\hat{\vec{L}}\cdot\vec{B} = -\hat{\vec{\mu}}\cdot\vec{B},$$

where $\gamma_0 = q/2m$. This is the form of the coupling that we were using when we described the coupling of a magnetic moment with the external magnetic field. The paramagnetic term will split the $(2\ell+1)$-fold degenerate energy levels according to the different eigenvalues of $\hat{L}_z$. The third term is called the *diamagnetic term*. This term can very often be neglected. For a magnetic field along z it would be written

$$\hat{\mathcal{H}}_{\rm dia} = \frac{q^2}{2m}\hat{A}^2 = \frac{q^2}{8m}\left(\hat{r}^2B^2 - (\hat{\vec{r}}\cdot\vec{B})^2\right) = \frac{q^2B^2}{8m}(x^2+y^2)$$

In the hydrogen atom we typically have $\langle x^2+y^2\rangle \simeq a_0^2$ and $\langle L_z\rangle \simeq \hbar$. The ratio of the paramagnetic and the diamagnetic term is then of the order

$$\frac{(q^2/8m)a_0^2B^2}{(q/2m)\hbar B} \simeq 10^{-6}B$$

For magnetic fields smaller than 1 tesla the diamagnetic term is therefore negligible. Note that in situation where the particle orbits become macroscopic, such as in the case of free electron in a uniform magnetic field (leading to the Landau levels), the diamagnetic term cannot be ignored.

Gauge invariance and the Aharonov-Bohm effect

Physical properties should only depend on the value of the electric and magnetic fields $\vec{E}$ and $\vec{B}$. There is however a degree of freedom in choosing the potentials Φ and $\vec{A}$. Indeed, the following *gauge transformation* defines new potentials that yield the same fields $\vec{E}$ and $\vec{B}$

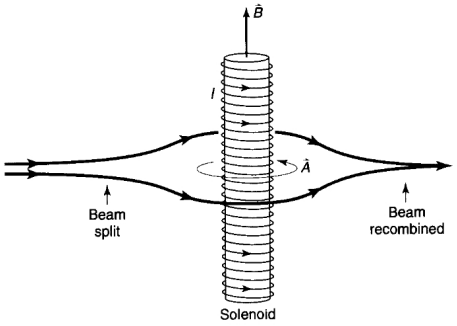
$$\vec{A}' = \vec{A} + \vec{\nabla}\chi(\vec{r},t) \qquad \Phi' = \Phi - \frac{\partial\chi}{\partial t}$$

This may look surprising as these new potentials define a different Hamiltonian. However, one can show that if $\psi(\vec{r},t)$ is a solution for the original Hamiltonian, then the following state will be a solution for the modified Hamiltonian after the gauge transformation

$$\psi(\vec{r},t) \to \psi'(\vec{r},t) = e^{iq\chi(\vec{r},t)/\hbar}\psi(\vec{r},t)$$

These two wavefunctions only differ by a phase. They do therefore lead to the same values for any physical observable.

There is however an experiment, proposed by Aharonov and Bohm, that shows a manifestation of the gauge invariance of the wavefunction. In spirit, it is very close to the two-slit Young experiment. The experiment is illustrated in the figure below



Electrons from a coherent source can follow two paths (that we will denote by P and P') around a solenoid with a non-zero magnetic field and then meet at the same point. The solenoid is long enough that the magnetic field is vanishing outside the solenoid. So we have $\vec{B} = 0$ along the two paths P and P'. A vanishing magnetic field does however not imply that the vector potential $\vec{A}$ is zero. Indeed, any $\vec{A} = \vec{\nabla}\chi$ will yield a vanishing magnetic field. Let us now investigate how the wavefunction is modified by the presence of the vector potential. The Schrödinger equation has the form

$$\hat{\mathcal{H}} = \frac{1}{2m}\left(\hat{\vec{p}} - q\hat{\vec{A}}(\vec{r},t)\right)^2 + \hat{V}(\vec{r})$$

We introduce the wavefunction

$$\Psi(\vec{r},t) = e^{i\varphi(\vec{r})}\Psi'(\vec{r},t) \qquad \varphi(\vec{r}) = \frac{q}{\hbar}\int_0^{\vec{r}} \vec{A}(\vec{r}')\cdot d\vec{r}'$$

The function $\varphi(\vec{r})$ is the line integral of a conservative vector field (that is the gradient of a function). Its value therefore does not depend on the chosen path. The gradient of $\Psi(\vec{r},t)$ is given by

$$\vec{\nabla}\Psi = e^{i\varphi(\vec{r})}(i\vec{\nabla}\varphi(\vec{r}))\Psi' + e^{i\varphi(\vec{r})}\vec{\nabla}\Psi'$$

But $\vec{\nabla}\varphi(\vec{r}) = (q/\hbar)\vec{A}(\vec{r})$ and we have

$$\left(-i\hbar\vec{\nabla} - q\hat{\vec{A}}\right)\Psi = -i\hbar e^{i\varphi(\vec{r})}\vec{\nabla}\Psi'$$
$$\left(-i\hbar\vec{\nabla} - q\hat{\vec{A}}\right)^2\Psi = -\hbar^2 e^{i\varphi(\vec{r})}\nabla^2\Psi'$$

Using this result, we can rewrite the Schrödinger equation for the wavefunction Ψ'

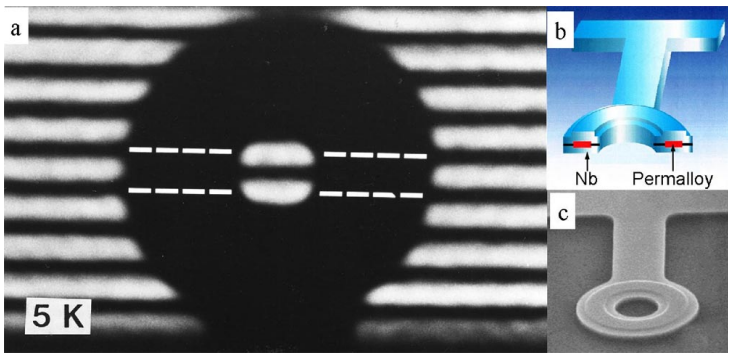
$$i\hbar\partial_t\Psi' = \left[-\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(\vec{r})\right]\Psi'$$

This shows that the wavefunction in the presence of the vector potential $\vec{A}$ is the same as the one in the absence of $\vec{A}$ but multiplied by a phase $\exp(i\varphi)$. If we come back to the experiment, we expect that there will be a phase difference between the wavefunction for the paths P and P' given by

$$\Delta\varphi = \frac{q}{\hbar}\int_P \vec{A}\cdot d\vec{r} - \frac{q}{\hbar}\int_{P'} \vec{A}\cdot d\vec{r} = \frac{q}{\hbar}\otimes\vec{A}\cdot d\vec{r} = \frac{q}{\hbar}\int_A \vec{B}\cdot d^2\vec{r}$$

We have used Stokes' theorem to express the phase difference as $q/\hbar$ multiplying the magnetic flux enclosed by the loop formed by the two paths. In the presence of a magnetic field the wavefunctions will acquire a non-vanishing relative phase leading to interference fringes.

The first experiment showing the Aharonov-Bohm effect was carried out by Tonomura and collaborators in 1986, see the figure below.



They fabricated a doughnut-shaped ferromagnet covered with a niobium superconductor to confine the magnetic field inside the doughnut (Meissner effect). Interference fringes were observed between electrons going through the hole of the doughnut and those passing outside. It can be shown that the magnetic flux inside a superconductor is quantized and must be a multiple of $h/2e$. For a odd number of flux quanta the electrons acquire a phase shift which is exactly π. This explains why the fringes are displaced by half a spacing!

The experimental observation of the Aharonov-Bohm effect shows that the vector potential $\vec{A}$ may be more than just a mathematical tool to manipulate electromagnetic fields. The wavefunction of a particle is sensitive to the vector potential in the region where the particle is found, while it is sensitive to the magnetic field in regions where the particle is excluded. In that sense, vector potentials allow to continue to manipulate a local theory.