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Let ρ be the density operator for a 1D system. Define

$$\langle x|\rho|x_0\rangle = \text{the } \underline{\text{density}}\ \underline{\text{matrix}} \equiv \rho(x,x_0).$$

Notice that it is a correlation function for ψ:

$$\rho(x,x_0) = \overline{\psi(x)\,\psi(x_0)^*}^{\,\text{stat}} \leftarrow \text{means statistical average.}$$

In case of thermal equilibrium, $\rho = \frac{1}{Z} e^{-\beta H}$, $\beta = 1/kT$,

so

$$\rho(x,x_0) = \frac{1}{Z(\beta)} \underbrace{\langle x|e^{-\beta H}|x_0\rangle}.$$

Call $e^{-\beta H}$ "the Boltzmann operator".

looks like $\langle x|e^{-itH/\hbar}|x_0\rangle$, in fact is same if $\boxed{t = -i\beta\hbar}$

So analytically continue the path integral in complex time.

Let

$$\varepsilon = \frac{t}{N} = -i\frac{\beta\hbar}{N}, = -i\eta \quad \text{where } \eta = \frac{\beta\hbar}{N}.$$

Then:

$$\langle x|e^{-\beta H}|x_0\rangle = \lim_{N\to\infty}\left(\frac{m}{2\pi\eta\hbar}\right)^{N/2} \int dx_1 \ldots dx_{N-1}$$

$$\times \exp\left\{-\frac{\eta}{\hbar}\sum_{j=1}^{N}\left[\frac{m(x_j - x_{j-1})^2}{2\eta^2} + V(x_{j-1})\right]\right\}$$

or, write this in more compact notation in terms of a path $x(u)$, where $0 \le u \le \beta\hbar$, $x(0) = x_0$, $x(\beta\hbar) =$ final x.

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Then

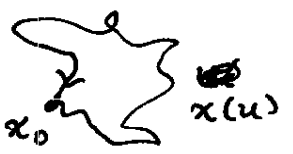
$$\langle x| e^{-\beta H} |x_0\rangle = C \int d[x(u)] \; e^{-\frac{1}{\hbar}\int_0^{\hbar\beta} \left[\frac{m}{2}\left(\frac{dx}{du}\right)^2 + V(x)\right] du}$$

Functional in exponent is u-integral of Hamiltonian $T+V$ (not Lagrangian $T-V$). Or, better point of view, it is time (u) integral of Lagrangian in <u>inverted</u> potential ($V \to -V$).

Suppose we are only interested in the partition fn. $Z(\beta)$:

$$Z(\beta) = \mathrm{tr}\, e^{-\beta H} = \int dx_0 \quad \langle x_0| e^{-\beta H} |x_0\rangle.$$

The integrand is the matrix element of the Boltzmann operator with initial, final points set equal. So path integral for integrand is sum over all paths $x(u)$ that begin and end at x_0:



It is a sum over closed paths.

Suppose $\beta\hbar$ is small (high temperature limit). Then path cannot deviate very far from x_0 in small "time" $\beta\hbar$, because that would imply large velocity, hence strong damping from $\frac{m}{2}\left(\frac{dx}{du}\right)^2$ term. So contributing paths stay close to x_0. Thus $V(x) \approx V(x_0)$,

$$\int_0^{\hbar\beta} V(x)\, du \approx \int_0^{\hbar\beta} V(x_0)\, du = \hbar\beta V(x_0),$$

and we can remove a factor $e^{-\beta V(x_0)}$ from the path integral.

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So,

$$\langle x_0 | e^{-\beta H} | x_0 \rangle \approx e^{-\beta V(x_0)} \underbrace{C' \int d[x(u)]\, e^{-\frac{1}{\hbar}\int_0^{\hbar\beta} \frac{m}{2}\left(\frac{dx}{du}\right)^2}}.$$

but this is the free particle propagator,

$$\langle x | e^{-itH/\hbar} | x_0 \rangle = \sqrt{\frac{m}{2\pi i \hbar t}}\; e^{\frac{i}{\hbar}\frac{m(x-x_0)^2}{2t}},$$

with $t = -i\hbar\beta$ and $x = x_0$, or,

$$= \sqrt{\frac{m}{2\pi\hbar^2\beta}}.$$

Thus,

$$\boxed{Z(\beta) = \sqrt{\frac{m}{2\pi\hbar^2\beta}} \int dx_0\; e^{-\beta V(x_0)}}$$

This result is most easily derived from classical statistical mechanics. It was known to Boltzmann.

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Vector potentials and scalar potential in classical mechanics can be thought of as auxiliary fields useful for computing the physical fields $\vec{E}$ and $\vec{B}$:

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

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

$\vec{E}$ and $\vec{B}$ are physical because they can be measured by measuring forces on particles. We will mostly work with $\vec{A}$, but similar considerations apply to ϕ (see the book). The existence of $\vec{A}$ follows from the mathematical theorem:

> If a vector field (call it $\vec{B}$) satisfies $\nabla\cdot\vec{B}=0$ on a contractible region, then there exists another vector field (call it $\vec{A}$) such that $\vec{B} = \nabla\times\vec{A}$. (Poincaré lemma).

Since by Maxwell's eqn, $\nabla\cdot\vec{B}=0$, $\vec{A}$ such that $\vec{B}=\nabla\times\vec{A}$ exists in ordinary space. It is, however, not unique;

$$\vec{A}' = \vec{A} + \nabla f$$

transforms $\vec{A}$ into new $\vec{A}'$ s.t. $\nabla\times\vec{A}' = \nabla\times\vec{A} = \vec{B}$. So $\vec{A}$ has both a physical part (the part that determines $\vec{B}$) and a nonphysical part (the part that changes under a gauge transformation). The physics ($\vec{E}$ and $\vec{B}$), however, is gauge-invariant at the classical level.

It is also gauge-invariant at the quantum level, that is, no physical result depends on the choice of gauge for $\vec{A}$, but the

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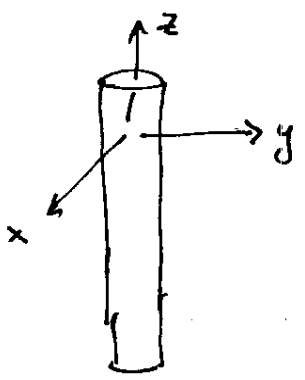
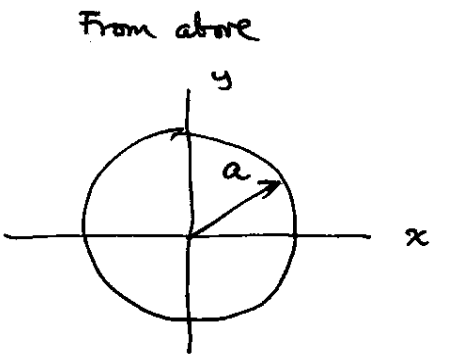
conclusion is more subtle in this case because the Hamiltonian uses $\vec{A}$ explicitly, and the wavefunction depends on the choice of gauge:

$$\left.\begin{aligned} \vec{A}' &= \vec{A} + \nabla f \\ \psi' &= e^{\frac{i}{\hbar}\frac{q}{c}f}\,\psi \end{aligned}\right\} \text{ old and new } \vec{A}, \psi$$

Nevertheless, magnetic fields in QM give rise to nonclassical phenomena, including the fact that a magnetic field can have a <u>nonlocal</u> effect on the dynamics of charged particles.

An example is the <u>Aharanov-Bohm effect</u>, in which we consider the motion of a charged particle exterior to a long solenoid.





a = radius of solenoid

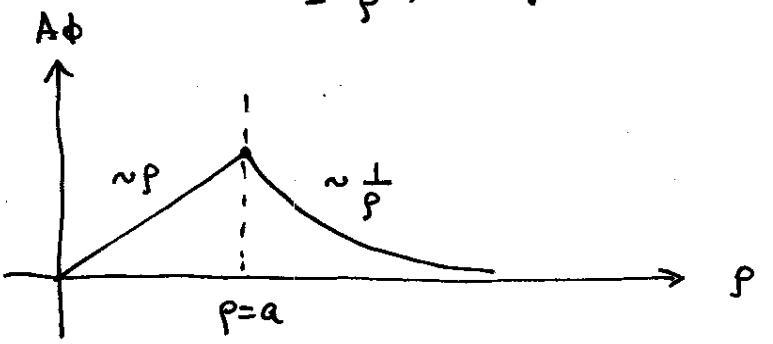
$\rho = \sqrt{x^2+y^2}$.

$$\vec{B} = \begin{cases} B\hat{z}, & \rho < a \\ 0, & \rho > a. \end{cases}$$

Need $\vec{A}$ for QM. $\vec{A}$ not unique, but one choice is

$$\vec{A} = A_\phi \hat{\phi}$$

$$A_\phi = \begin{cases} \frac{B}{2}\rho, & \rho < a \\ \frac{B}{2}\frac{a^2}{\rho}, & \rho > a. \end{cases}$$



In the exterior region, $\vec{B}=0$ but $\vec{A}\neq 0$. We will consider a particle that is free in the exterior region but prevented by hard walls at $\rho=a$ from entering the region where $\vec{B}\neq 0$. In classical mech., the orbits ~~are~~ in $\rho>a$ region are straight lines, unaffected by the solenoid. In QM, the wave fn. ψ vanishes at bdry $\rho=a$.

In the region $\rho>a$, we cannot set $\vec{A}=0$, even though $\vec{B}=0$, nor can we achieve $\vec{A}=0$ by a gauge transformation. This is because the external region is not contractible (actually, not simply connected). You <u>could</u> break the external region into two simply connected subregions, gauge away $\vec{A}$ in each, and then solve the free particle Schrödinger eqn. in each. Then you would have to do gauge transformations in overlap regions to match solutions. Instead...

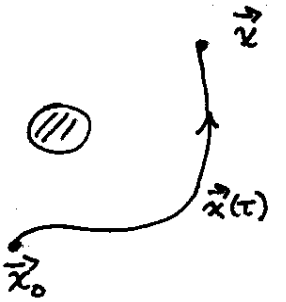
We will use path integrals. We have

$$\langle \vec{x} | U(t) | \vec{x}_0 \rangle = \int d[x(\tau)] \; e^{\frac{i}{\hbar}\int_0^t L \, d\tau} ,$$

where

$$L = \frac{m}{2}|\dot{\vec{x}}|^2 + \frac{q}{c}\dot{\vec{x}}\cdot\vec{A}(\vec{x})$$

$$= \underset{\substack{\uparrow \\ \left(\text{free particle Lagr.}\right)}}{L_0} + L_{mag}.$$



and where the path integral is taken over all paths that go from $\vec{x}_0$ to $\vec{x}$ in time t, without entering region $\rho < a$.

The magnetic contribution to the action is

$$\frac{q}{c}\int_0^t \dot{\vec{x}}(\tau)\cdot\vec{A}(\vec{x}(\tau))\,d\tau = \frac{q}{c}\int_{\vec{x}_0}^{\vec{x}} \vec{A}(\vec{x}')\cdot d\vec{x}' .$$

It depends on the path geometrically connecting $\vec{x}_0$ and $\vec{x}$, but not on the τ-parameterization or the final time t. In fact, it only depends on the path in a limited way, since any two paths that can be continuously deformed into one another give the same magnetic action. That's because $\vec{B}=0$ in the exterior region.

Consider 2 paths $\vec{x}_0 \to \vec{x}$ <u>equivalent</u> if they can be continuously deformed into one another. Then two paths are equivalent if and only if they have the same <u>winding number</u>,

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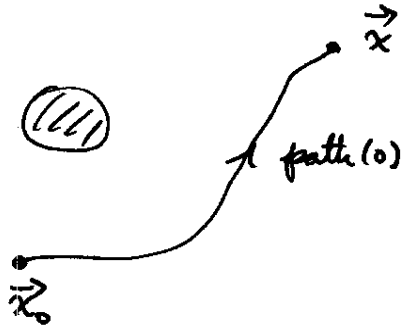
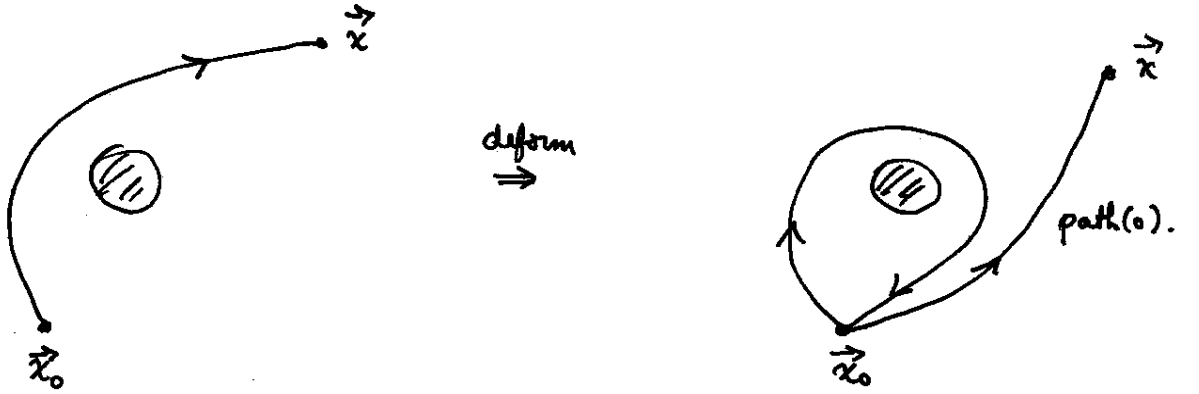
defined as follows. Choose (arbitrarily) one path connecting $\vec{x}_0 \to \vec{x}$, call it <u>path(0)</u> or <u>the reference path</u>.



Take any other path $\vec{x}_0 \to \vec{x}$ and continuously deform it into another path starting at $\vec{x}_0$, going around the solenoid n times in a ~~clock~~ counterclockwise direction, returning to $\vec{x}_0$, then proceeding along path(0) to $\vec{x}_1$. For example:



~~Here the pa~~ The number of times the path goes around the solenoid n is the <u>winding number</u> of the path. In the example above, $n=-1$ (since it went around once in a clockwise direc.).

~~The~~ Any two paths with the same winding number give the same magnetic action. So, the magnetic action depends on the winding number, not ~~on the~~ otherwise on the path itself.

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Define the <u>n-th class of paths</u> (homotopy class) as the set of paths with winding number n. Then from the definition, if path $\in$ class (n), then

$$\frac{q}{c}\int_{\substack{\vec{x}_0 \\ \text{path} \in \text{class}(n)}}^{\vec{x}} \vec{A}\cdot d\vec{\ell} = \frac{nq}{c}\Phi + \frac{q}{c}\int_{\substack{\vec{x}_0 \\ \text{path}(0)}}^{\vec{x}} \vec{A}\cdot d\vec{\ell},$$

where

$$\Phi = \oint_{\text{solenoid}} \vec{A}\cdot d\vec{\ell} = B\pi a^2 = \text{flux inside solenoid.}$$

The first term above depends on n (the class #) but not on $\vec{x}, \vec{x}_0$ or otherwise on the path. The 2nd term depends on the endpts $\vec{x}_0, \vec{x}$, but not on the class. Now write:

$$\int_{\text{all paths.}} d[x(\tau)] = \sum_{n=-\infty}^{+\infty} \int_{\text{paths} \in \text{class}(n)} d[x(\tau)] .$$

Then:

$$\boxed{\langle \vec{x} | U(t) | \vec{x}_0 \rangle = e^{\frac{i}{\hbar}\frac{q}{c}\int_{\substack{\vec{x}_0 \\ \text{path}(0)}}^{\vec{x}} \vec{A}\cdot d\vec{\ell}} \sum_{n=-\infty}^{+\infty} e^{\frac{inq}{\hbar c}\Phi} \times \int_{\substack{\text{paths} \in \\ \text{class}(n)}} d[x(\tau)]\, e^{\frac{i}{\hbar}\int_0^t L_0\, d\tau} .}$$

Mostly Aharanov-Bohm effect today. 10/9/07

The action in the final path integral is just $\int L_0 \, d\tau$, the free particle action. This differs from the free particle propagator by the phase factors $e^{\frac{inq}{\hbar c}\Phi}$ and the overall phase $e^{\frac{iq}{\hbar c}\int_{path(\omega)} \vec{A}\cdot d\vec{l}}$.

Notice that if

$$\frac{q}{\hbar c}\Phi = 2m\pi \qquad \text{some integer } m,$$

then all phase factors $e^{\frac{inq}{\hbar c}\Phi} = 1$, and the sum + integral turns into an unrestricted path integral over all paths, using the free particle Lagrangian. In this case one can also gauge away the overall phase, so the particle in the exterior region is not affected by the magnetic flux. This occurs when

$$\Phi = \text{integer} \times \Phi_0,$$

where $\Phi_0 = \frac{2\pi\hbar c}{e} = \frac{hc}{e} =$ <u>flux quantum</u>.

The flux in the solenoid is not quantized in multiples of Φ_0, it can take on any value, but when Φ is an integer multiple of Φ_0, then the motion in region $\rho > a$ is the same as for $\Phi = 0$. For non-integer multiples of Φ/Φ_0, there are phases introduced that shift energy levels, wave functions, interference patterns, etc.