Lecture 12

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1 Path integral in statistical physics

The last aspect of path integrals I would like to discuss is its connection to statistical physics. The fundamental object in statistical physics is called the partition function, defined as $\mathcal{Z} = \sum_\alpha \langle\alpha|e^{-\beta\mathcal{H}}|\alpha\rangle = \mathrm{tr} e^{-\beta\mathcal{H}}$, which describes a statistical mechanical system at inverse temperature $\beta = \frac{1}{k_B T}$ where k_B is the Boltzmann constant and T is temperature. Comparing to the expression for the quantum mechanical propagator $\langle f|e^{-\frac{i}{\hbar}\mathcal{H}T}|i\rangle$, we see that the two expressions seem related by the replacement $T = -i\hbar\beta$ i.e. a system at finite temperature looks like a dynamical quantum system propagating in imaginary time. This correspondence can be implemented in a transparent in the path integral formalism. The reason is that for integrals, we can always deform the integration contour as long as we do not encounter any singularity. Thus, in many cases we can actually deform the contour in a path integral to relate a quantum mechanical propagator to a statistical partition function in imaginary time. Such deformation to imaginary time is called Wick rotation $t \mapsto -i\tau$. It changes the action into

$$iS = -\int_0^{\hbar\beta} d\tau \left\{\frac{1}{2}m\dot{x}^2 + V(x)\right\} = -S_E \tag{1}$$

Importantly, the relative sign between kinetic and potential term is now positive and we get the total energy integrated over time in the exponential instead of the action. Such quantity is called the Euclidean action. Beyond its usefulness in relating quantum mechanical models to statistical mechanical models, Wick rotation can also be useful in evaluating quantum mechanical path integrals, particularly for problems where the classical equations of motion has no solution for real time which usually happens for tunneling problems. Such problems usually have some stationary (or saddle point) solutions in imaginary time. Note also that the Berry phase term we discussed last lecture remains purely imaginary under this transformation i.e. it represents a phase both in real and imaginary time and it serves the same role of ensuring the theory is only consistent for integer or half-integer values of the spin.

2 The adiabatic approximation and Berry phase

Let us now get back to the first term in the action for the spin path integral. This term turns out to represent a very important effect in quantum mechanics called the Berry phase. To understand how the Berry phase appears in a more general context, consider a Hamiltonian that changes in time. For sufficiently slow changes, we can apply a result called the adiabatic theorem to significantly simplify the analysis of the problem. The adiabatic theorem is the statement that for suffficiently slow changes in the Hamiltonian, a state that was the eigenstate of the initial Hamiltonian at time $t = 0$, remains an instantaneous eigenstate at finite time t. The statement makes intuitive sense. For example, consider the spin Hamiltonian $\mathcal{H} = \gamma\boldsymbol{B}\cdot\boldsymbol{S}$. If we take $\boldsymbol{B}$ to be time-dependent and start with $\boldsymbol{B}(t=0) = B\hat{z}$ then slowly rotate $\boldsymbol{B}$ away from the z-plane, we expect a system initially in the ground state $|\alpha, t=0\rangle = |z+\rangle$ to slowly rotate to follow the direction of $\boldsymbol{B}(t)$.

Now consider for simplicitly a Hamiltonian that changes in time such that $\mathcal{H}(T) = \mathcal{H}(0)$ and assume the change is sufficiently slow such that the adiabatic theorem is valid (this will be made more precise below). The adiabatic theorem tells us that if we start in the ground state at $t = 0$, we end up at the ground state at $t = T$. However, remember that a state in quantum mechanics is specified by a ray in the Hilbert space. This means that going back to the same state means that

$$|\psi, T\rangle = e^{i\gamma}|\psi, 0\rangle \tag{2}$$

For a long time, it was thought that the phase factor γ is unimportant and can be dropped. However, it turned out that it is physically measurable. The reason is that this is really a phase difference. To see this, imagine taking an electron that could take two possible paths, one that involves the slowly changing Hamiltonian and one that doesn't. The interference pattern between these paths will be sensitive to the phase γ. This is precisely what happens in the Aharonov-Bohm effect which will be discussed in the next lecture.

To derive the explicit form of the phase γ and clarify what we mean by slow changes in the Hamiltonian, let us introduce the simultaneous eigenkets and eigenvalues of a Hamiltonian $\mathcal{H}(t)$ as

$$\mathcal{H}(t)|\psi_n(t)\rangle = E_n(t)|\psi_n(t)\rangle \tag{3}$$

We emphasize here that $|\psi_n(t)\rangle$ does not correspond to any unitary time evolution associated with the Hamiltonian. Instead, it represents the eigenbasis of the Hamiltonian $\mathcal{H}(t)$. Now consider the time-dependent Schrödinger equation for a general ket $|\alpha, t\rangle$:

$$i\hbar\frac{d}{dt}|\alpha, t\rangle = \mathcal{H}(t)|\alpha, t\rangle \tag{4}$$

Since $|\psi_n(t)\rangle$ is a complete basis, we can expand any state as:

$$|\alpha, t\rangle = \sum_n c_n(t)|\psi_n(t)\rangle \tag{5}$$

It is important to note here that both the coefficients $c_n(t)$ and the basis states $|\psi_n(t)\rangle$ depend on t. The first through the time evolution governed by the Schrödinger equation and the second through the time dependence of the Hamiltonian. Substituting in the Schrödinger equation, we get

$$i\hbar\sum_n[\dot{c}_n(t)|\psi_n(t)\rangle + c_n(t)\frac{d}{dt}|\psi_n(t)\rangle] = \sum_n c_n(t)E_n(t)|\psi_n(t)\rangle \tag{6}$$

Multiplying both sides by $\langle\psi_m(t)|$ and using the orthonormality of the eigenkets: $\langle\psi_m(t)|\psi_n(t)\rangle = \delta_{nm}$, we get

$$\dot{c}_m(t) = -\frac{i}{\hbar}E_m(t)c_m(t) - \sum_n c_n(t)\langle\psi_m(t)|\frac{d}{dt}\psi_n(t)\rangle \tag{7}$$

Note that the second term vanishes if the Hamiltonian is time-independent. To simplify the second term on the right hand side, we take the time derivative of Eq. 3:

$$\dot{\mathcal{H}}(t)|\psi_n(t)\rangle + \mathcal{H}(t)\frac{d}{dt}|\psi_n(t)\rangle = \dot{E}_n(t)|\psi_n(t)\rangle + E_n(t)\frac{d}{dt}|\psi_n(t)\rangle \tag{8}$$

Again acting with $\langle\psi_m(t)|$ on both sides, we get

$$\langle\psi_m(t)|\dot{\mathcal{H}}(t)|\psi_n(t)\rangle = \dot{E}_n(t)\delta_{nm} + [E_n(t) - E_m(t)]\langle\psi_m(t)|\frac{d}{dt}|\psi_n(t)\rangle \tag{9}$$

Thus, for $n \neq m$, we get

$$\langle\psi_m(t)|\frac{d}{dt}\psi_n(t)\rangle = \frac{\langle\psi_m(t)|\dot{\mathcal{H}}(t)|\psi_n(t)\rangle}{E_n(t) - E_m(t)} \tag{10}$$

Substituting in (7) and separating the terms $n = m$ and $n \neq m$, we get

$$\dot{c}_m(t) = -[\frac{i}{\hbar}E_m(t) + \langle\psi_m(t)|\frac{d}{dt}\psi_m(t)\rangle]c_m(t) - \sum_{n\neq m} c_n(t)\frac{\langle\psi_m(t)|\dot{\mathcal{H}}(t)|\psi_n(t)\rangle}{E_n(t) - E_m(t)} \tag{11}$$

The adiabatic approximation corresponds to neglecting the last term in the expression above. This is justified if the Hamiltonian changes slowly which means that its matrix elements $\langle\psi_m(t)|\dot{\mathcal{H}}(t)|\psi_n(t)\rangle$ for $n \neq m$ are small compared to the gap $E_n(t) - E_m(t)$ [1]. Once we ignore this term, we see that if $c_m(0) = 0$, then $c_m(t) = 0$ which means that if we start at an eigenstate at $t = 0$, we always remain in that eigenstate for all time t.

For a given m, we can solve Eq. 11 to get

$$c_m(t) = e^{i\gamma_n(t) - \frac{i}{\hbar}\int_0^t dt' E_m(t)} c_m(0) \tag{12}$$

The second term in the exponent is the expected dynamical phase which simply generalizes the factor $e^{-\frac{i}{\hbar}E_m T}$ to the time-dependent case. The first term, however, is different. It is explicitly given by

$$\gamma_n(t) = i\int_0^t dt'\langle\psi_n(t)|\frac{d}{dt}\psi_n(t)\rangle \tag{13}$$

This term is called the Berry phase. Notice that this term has the same form as the first term that appears in the path integral action for the spin problem with $|\psi_n(t)\rangle$ replaced by $|\hat{n}(t)\rangle$. The Berry phase is manifestly real since

$$\langle\psi_n(t)|\frac{d}{dt}\psi_n(t)\rangle = \frac{d}{dt}\langle\psi_n(t)|\psi_n(t)\rangle - \langle\frac{d}{dt}\psi_n(t)|\psi_n(t)\rangle = -\langle\psi_n(t)|\frac{d}{dt}\psi_n(t)\rangle^* \tag{14}$$

which means that $\langle\psi_n(t)|\frac{d}{dt}\psi_n(t)\rangle$ is purely imaginary.

The Berry phase features prominently in problems where the Hamiltonian depends on a set of continuous parameters R^a and we consider a trajetory in parameter space R^a as a function of time. For instance, we can think of the Hamiltonian for a 3D particle in a potential which confines the particle in a box (the potential is infinite outside the box). We can then move this box as a function of time which effectively implements moving the confining potential of the electron slowly in space. Another application is in band theory. Here, we have a Hamiltonian with discrete translation symmetry whose eigenstates are labelled by an analog of momentum called crystal momentum, that is defined modulo $2\pi/a$ (a is the lattice constat) in each direction. This means that crystal momentum parametrizes a torus. We can consider state at momentum at crystal momentum $k^a(t)$ which depends on time.

If the Hamiltonian only depends on time through the parameters $R^a(t)$, the same will be the case for $|\psi_n(t)\rangle$. We will denote by $\boldsymbol{R}$, the vector whose components are the parameters R^a such that

$$\mathcal{H}(\boldsymbol{R})|\psi_n(\boldsymbol{R})\rangle = E_n(\boldsymbol{R})|\psi_n(\boldsymbol{R})\rangle \tag{15}$$

Then we can write the Berry phase as

$$\gamma = i\int_0^t dt'\dot{R}^a\langle\psi_n(\boldsymbol{R})|\frac{\partial}{\partial R^a}|\psi_n(\boldsymbol{R})\rangle = i\int_{\boldsymbol{R}=\boldsymbol{R}(0)}^{\boldsymbol{R}=\boldsymbol{R}(t)} dR^a\langle\psi_n(\boldsymbol{R})|\frac{\partial}{\partial R^a}|\psi_n(\boldsymbol{R})\rangle = \int_{\boldsymbol{R}=\boldsymbol{R}(0)}^{\boldsymbol{R}=\boldsymbol{R}(t)} d\boldsymbol{R}\cdot\mathcal{A}(\boldsymbol{R}) \tag{16}$$

Here, we used the convention where repeated upper/lower indices are summed over. This illustrates that the Berry phase is in general a geometric phase that depends on the path in parameter space not on how fast it is traversed. The quantity $\mathcal{A}$ is called the Berry connection:

$$\mathcal{A}_a(\boldsymbol{R}) = i\langle\psi_n(\boldsymbol{R})|\frac{\partial}{\partial R^a}|\psi_n(\boldsymbol{R})\rangle \tag{17}$$

[1] The quantitiy $\frac{\langle\psi_m(t)|\dot{\mathcal{H}}(t)|\psi_n(t)\rangle}{E_n(t)-E_m(t)} \sim \frac{1}{\tau}$ has units of inverse time. To neglect it, τ needs to be long compared to the characteristic time scale of the state of interest given by the inverse of the difference in the first term on the right hand side in (11) in the level of interest compared to the closest energy level

The quantity $\mathcal{A}_a$ shares several features with the more familiar electromagnetic vector potential. First, note that Eq. 15 which defines the instantaneous eigenstates does not fix the overall phase of the wavefunction $|\psi_n(\boldsymbol{R})\rangle$ [2]. This means that we have the freedom to multiply the ket $|\psi_n(\boldsymbol{R})\rangle$ by any **$\boldsymbol{R}$-dependent phase** $e^{-i\varphi(\boldsymbol{R})}$. Under such transformation, the Berry connection changes as

$$\mathcal{A}_a(\boldsymbol{R}) \mapsto \mathcal{A}_a(\boldsymbol{R}) + \partial_a \varphi(\boldsymbol{R}) \tag{18}$$

which is precisely how the electromagnetic vector potential changes under gauge transformation. This suggests defining the gauge invariant quantity

$$\mathcal{F}_{ab} = \partial_a \mathcal{A}_b - \partial_b \mathcal{A}_a \tag{19}$$

which is called the Berry curvature. If the parameter space spanned by $\boldsymbol{R}$ is two-dimensional, the Berry curvature has a simple form since it reduces to a scalar $F_{ab}(\boldsymbol{R}) = \epsilon_{ab}\Omega(\boldsymbol{R})$ (here ϵ_{ab} is the antisymmetric tensor).

The Berry phase associated with any close path $\mathcal{C}$ can be written in terms of the flux of the Berry curvature across any 2D surface $\mathcal{S}$ enclosing this path

$$\gamma = i \oint_{\mathcal{C}} dR^a \mathcal{A}_a = i \int_{\mathcal{S}} d\mathcal{S}^{ab} \mathcal{F}_{ab} \tag{20}$$

We emphasize here that the Berry phase is obtained by a one-dimensional line integral of the Berry connection or a two-dimensional surface integral of the Berry curvature **irrespective of the dimension of the parameter space**. Another way to say this is that the Berry connection is a one-form and the Berry curvature is a two-form.

This leads naturally to the question: can there be sources for the Berry curvature? the answer turns out to be yes. Sources of the Berry curvature are points in the parameter space where the energy eigenvalues become degenerate such that the adiabatic approximation becomes invalid and the Berry curvature becomes singular. However, similar to the argument we employed last time, the Berry curvature associated with such sources has to be constrained to yield a well-defined theory. To see this, consider any closed 2D surface $\mathcal{M}$ and consider the Berry phase along any closed path $\mathcal{C}$. Similar to what we did last lecture, we can write this as the surface integral of Berry curvature in two possible ways corresponding to the two surfaces on $\mathcal{M}$ whose boundary is $\mathcal{C}$. These two choices should give the same phase up to integer multiples of 2π. This means that the integral of the Berry curvature across all $\mathcal{M}$ should be quantized

$$\int_{\mathcal{M}} d\mathcal{S}^{ij} \mathcal{F}_{ij} = 2\pi C \tag{21}$$

The integer C is called the Chern number. This means that sources of the Berry curvature has to have integer charge.

One of the most prominent application of these ideas is in topological band theory. For example, in two spatial dimensions, the crystal momentum lives on the two-dimensional torus. The Berry curvature is simply a scalar on this torus whose integral over the entire torus is quantized in integer multiples of 2π. The Chern number in this case has very clear physical manifestation. It yields the Hall conductance of the system measured in units e^2/h and is responsible for the perfect quantization plateaus observed in the quantum Hall effect.

Let us now consider a concrete example for the Berry phase calculation, whose details you will be asked to fill in in the pset. Consider the Hamiltonian

$$\mathcal{H}(\boldsymbol{B}) = \frac{\hbar\gamma}{2} \boldsymbol{B} \cdot \boldsymbol{\sigma} \tag{22}$$

[2] this is always the case for wavefunctions defined as the eigenfunctions of some operator

Since the parameter space spanned by $\boldsymbol{B}$ is three-dimensional, we can express the curvature tensor (which is an antisymmetric 3×3 matrix and thus have 3 non-zero parameters) in terms of a 3-component vector that acts as an effective magnetic field in the parameter space

$$\mathcal{B}_i(\boldsymbol{B}) = -\frac{1}{2}\epsilon_{ijk}F^{jk} = \frac{B_i}{2|B|^3} \tag{23}$$

Notice that this field is singular at the origin. This is the point where the two eigenstates of the Hamiltonian are degenerate and the adiabatic approximation fails. This point acts as a source for Berry curvature. Integrating this field over a sphere in the $\boldsymbol{B}$ space gives 2π consistent with our discussion of quantized Chern number.