The adiabatic approximation and Berry's phase[1]

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27 April 2012

I offer here some background for Chapter 5 of J. J. Sakurai, *Modern Quantum Mechanics*.

1 The problem

We consider a system with a hamiltonian $H(t)$ that changes slowly in time. We suppose that the eigenvalues of H at any time t are discrete and are not degenerate. Thus any time t, the hamiltonian has a complete set of eigenstates with

$$H(t)\big|n;t\big\rangle = E_n(t)\big|n;t\big\rangle \quad . \tag{1}$$

The phase of $\big|n;t\big\rangle$ is not determined by the eigenvalue equation, but you should think of the phase as varying only slowly with t.

Now suppose that at time $t = 0$ the system starts in a state $\big|\alpha;0\big\rangle$ and evolves according to the time-dependent Schrödinger equation:

$$i\frac{d}{dt}\big|\alpha;t\big\rangle = H(t)\big|\alpha;t\big\rangle \quad . \tag{2}$$

I claim that if $\big|\alpha;0\big\rangle$ is one of the eigenstates of $H(0)$, then $\big|\alpha;t\big\rangle$ will be a phase factor times the corresponding eigenstate of $H(t)$ as long as $H(t)$ is slowly varying. Here "slowly varying" means that the time scale τ characteristic of changes in H is large compared to the inverse of energy differences $E_n(t) - E_m(t)$.

2 The differential equation

Let us expand $\big|\alpha;t\big\rangle$ in the energy eigenstates:

$$\big|\alpha;t\big\rangle = \sum_n c_n(t) e^{i\theta_n(t)}\big|n;t\big\rangle \quad , \tag{3}$$

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where

$$\theta_n(t) = -\int_0^t dt'\ E_n(t') \quad . \tag{4}$$

We are interested in how the expansion coefficients $c_n(t)$ evolve. We expect them to evolve slowly because we have put the main time dependence in the dynamical phase factor $\exp(i\theta_n(t))$.

Applying the Schrödinger equation, we have

$$\begin{split}\sum_n E_n(t) c_n(t) e^{i\theta_n(t)} \big|n;t\big\rangle = \sum_n \big\{ i\dot{c}_n(t) e^{i\theta_n(t)} \big|n;t\big\rangle \\ + E_n(t) c_n(t) e^{i\theta_n(t)} \big|n;t\big\rangle + c_n(t) e^{i\theta_n(t)}\, i\frac{d}{dt}\big|n;t\big\rangle \big\} \ .\end{split} \tag{5}$$

That is

$$0 = \sum_n \big\{ \dot{c}_n(t) e^{i\theta_n(t)} \big|n;t\big\rangle + c_n(t) e^{i\theta_n(t)}\, \frac{d}{dt}\big|n;t\big\rangle \big\} \ . \tag{6}$$

Taking the inner product with $\big\langle m;t\big|$ gives

$$0 = \dot{c}_m(t) e^{i\theta_m(t)} + \sum_n c_n(t) e^{i\theta_n(t)}\, \big\langle m;t\big|\frac{d}{dt}\big|n;t\big\rangle \ . \tag{7}$$

Thus

$$\dot{c}_m(t) = \ - c_m(t) \, \big\langle m;t\big|\frac{d}{dt}\big|m;t\big\rangle - \sum_{n\neq m} c_n(t) e^{i(\theta_n(t)-\theta_m(t))}\, \big\langle m;t\big|\frac{d}{dt}\big|n;t\big\rangle \ . \tag{8}$$

The factor multiplying $-c_m(t)$ in the first term in Eq. (8) is purely imaginary. To see that, note that

$$\begin{split} 0 &= \frac{d}{dt}\big\langle m,t\big|m;t\big\rangle \\ &= \big\langle m,t\big|\frac{d}{dt}\big|m;t\big\rangle + \left(\frac{d}{dt}\big\langle m,t\big|\right)\big|m;t\big\rangle \\ &= \big\langle m,t\big|\frac{d}{dt}\big|m;t\big\rangle + \left(\big\langle m,t\big|\frac{d}{dt}\big|m;t\big\rangle\right)^* \quad . \end{split} \tag{9}$$

This factor is of some importance, so we give it a name:

$$\langle m,t|\frac{d}{dt}|m;t\rangle = -i\,\dot\gamma(t) \quad , \tag{10}$$

where

$$\gamma_m(t) = i\int_0^t dt'\ \langle m;t|\frac{d}{dt}|m;t\rangle \quad . \tag{11}$$

The second term in Eq. (8) can be rewritten by differentiating the energy eigenvalue equation,

$$0 = [\dot H(t) - \dot E_n(t)\big|n;t\rangle + [H(t) - E_n(t)]\frac{d}{dt}\big|n;t\rangle \quad . \tag{12}$$

Taking the inner product with $\langle m;t\big|$ for $m \neq n$ gives

$$0 = \langle m;t\big|\dot H(t)\big|n;t\rangle + \langle m;t\big|[H(t) - E_n(t)]\frac{d}{dt}\big|n;t\rangle \quad , \tag{13}$$

or

$$0 = \langle m;t\big|\dot H(t)\big|n;t\rangle + \langle m;t\big|[E_m(t) - E_n(t)]\frac{d}{dt}\big|n;t\rangle \quad , \tag{14}$$

Thus

$$\langle m;t|\frac{d}{dt}|n;t\rangle = \frac{\langle m;t\big|\dot H(t)\big|n;t\rangle}{E_n(t) - E_m(t)} \quad . \tag{15}$$

Using this result, we have

$$\dot c_m(t) = ic_m(t)\dot\gamma(t) - \sum_{n\neq m} c_n(t)e^{i(\theta_n(t)-\theta_m(t))}\,\frac{\langle m;t\big|\dot H(t)\big|n;t\rangle}{E_n(t) - E_m(t)} \ . \tag{16}$$

This is the exact evolution equation for $c_m(t)$. When $H(t)$ is slowly varying, we can drop the second term. Why? We are supposing that $H(t)$ varies on a time scale τ that is long compared to $1/(E_n - E_m)$. The second term is evidently proportional to $1/\tau$, so it is small. But we want to use the evolution equation to find $c_m(t)$ after a time T over which H has changed substantially. That is, we want to find $c_m(t)$ after a time $T \sim \tau$. Since $\tau/\tau = 1$, it is not immediately evident that the second term can be neglected. However

$$c_m(T) = \int_0^T dt\ c_m(t) + c_m(0) \quad . \tag{17}$$

When we integrate the second term over t, the phase factor $\exp(i(\theta_n(t) - \theta_m(t)))$ oscillates inside the integral, so that the contribution from the second term is very small. The first term has no phase factor, so it has the potential to contribute to a finite change in $c_m(t)$.

Thus we have approximately

$$\dot{c}_m(t) = i c_m(t) \dot{\gamma}_m(t) \quad . \tag{18}$$

The solution of this is

$$c_m(t) = e^{i\gamma_m(t)} c_m(0) \quad . \tag{19}$$

The result (19) shows that if the system starts in a particular eigenstate N, so that $c_N(0) = 1$ and $c_m(0) = 0$ for $m \neq N$, then as the hamiltonian slowly canges the system remains in the eigenstate $\big|N; t\big\rangle$ that evolves from the starting eigenstate. The coefficient $c_N(t)$ can, however, acquire a phase.

3 Berry's phase

Let's consider the phase $\gamma_m(t)$ in more detail. Suppose that the hamiltonian depends on several parameters $R_1, R_2, \dots$ and that these parameters are changed over time, resulting in the slow change in the hamiltonian over time. Then the energy eigenstates also depend on $\boldsymbol{R}$ and their time dependence is the result of their $\boldsymbol{R}$ dependence:

$$\frac{d}{dt}\big|n; \boldsymbol{R}(t)\big\rangle = \boldsymbol{\nabla}_R \big|n; \boldsymbol{R}(t)\big\rangle \cdot \frac{d\boldsymbol{R}(t)}{dt} \quad . \tag{20}$$

Thus the phase γ_m is

$$\gamma_m(T) = i \int_0^t dt\ \frac{d\boldsymbol{R}(t)}{dt} \cdot \big\langle m; \boldsymbol{R}(t)\big|\boldsymbol{\nabla}_R\big|m; \boldsymbol{R}(t)\big\rangle \quad . \tag{21}$$

This can be rewritten as an integral over the path C that the parameters follow:

$$\gamma_m(T) = i \int_C d\boldsymbol{R}\ \cdot \big\langle m; \boldsymbol{R}\big|\boldsymbol{\nabla}_R\big|m; \boldsymbol{R}\big\rangle \quad . \tag{22}$$

Now note that the phase $\gamma_m(T)$ seems as though it should be pretty arbitrary. Suppose that I redefine the phase of $\big|m; \boldsymbol{R}\big\rangle$ so that

$$\big|m; \boldsymbol{R}\big\rangle \to e^{-i\lambda(\boldsymbol{R})}\big|m; \boldsymbol{R}\big\rangle \quad . \tag{23}$$

Here the extra phase $\lambda(\boldsymbol{R})$ can be anything that I like. Then

$$\boldsymbol{\nabla}_R \big| m; \boldsymbol{R} \big\rangle \to e^{-i\lambda(\boldsymbol{R})} \boldsymbol{\nabla}_R \big| m; \boldsymbol{R} \big\rangle - i \left(\boldsymbol{\nabla}_R \lambda(\boldsymbol{R}) \right) e^{-i\lambda(\boldsymbol{R})} \big| m; \boldsymbol{R} \big\rangle \tag{24}$$

and

$$\big\langle m; \boldsymbol{R} \big| \boldsymbol{\nabla}_R \big| m; \boldsymbol{R} \big\rangle \to \big\langle m; \boldsymbol{R} \big| \boldsymbol{\nabla}_R \big| m; \boldsymbol{R} \big\rangle - i \boldsymbol{\nabla}_R \lambda(\boldsymbol{R}) \ . \tag{25}$$

Then the phase changes by

$$\gamma_m(T) \to \gamma_m(T) + \int_C d\boldsymbol{R} \ \cdot \boldsymbol{\nabla}_R \lambda(\boldsymbol{R}) \ . \tag{26}$$

That is,

$$\gamma_m(T) \to \gamma_m(T) + \lambda(\boldsymbol{R}(T)) - \lambda(\boldsymbol{R}(0)) \ . \tag{27}$$

We see that if we simply change the parameters from one setting to another, then the phase $\gamma_m(T)$ can be anything. However, if if we change the parameters from $R(0)$ and go along a path in the parameter space, finally coming back to the parameters we started with, then $\lambda(\boldsymbol{R}(T)) - \lambda(\boldsymbol{R}(0)) = 0$ and the phase is not arbitrary. The phase $\gamma_m(T)$ then depends on the geometry of the path in parameter space. It is called Barry's phase.