Imaginary-Time Evolution and the Berry Phase

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As in real-time evolution, a discrete eigenstate also acquires a Berry phase in the adiabatic limit under imaginary-time evolution.

Consider the imaginary-time evolution generated by an imaginary-time-dependent Hermitian Hamiltonian $H(\tau)$. The Schrodinger equation is

$$\frac{d}{d\tau} |\psi(\tau)\rangle = -H(\tau) |\psi(\tau)\rangle . \tag{1}$$

Assume that the eigenvalues of $H(\tau)$ are discrete, and write the instantaneous eigenstates as

$$H(\tau) |n(\tau)\rangle = E_n(\tau) |n(\tau)\rangle , \quad n = 1, 2, \dots . \tag{2}$$

We impose the normalization and orthogonality condition $\langle n|m\rangle = \delta_{nm}$. It follows that

$$\langle m(\tau)| \frac{dH}{d\tau}(\tau) |n(\tau)\rangle = \frac{dE_n}{d\tau}(\tau)\delta_{nm} + (E_n(\tau) - E_m(\tau)) \langle m(\tau)| \frac{dn}{d\tau}(\tau)\rangle . \tag{3}$$

In particular,

$$\langle n(\tau)| \frac{dH}{d\tau}(\tau) |n(\tau)\rangle = \frac{dE_n}{d\tau}(\tau) \tag{4}$$

is the Hellmann–Feynman formula. Also, when $E_n(\tau) \neq E_m(\tau)$,

$$\langle m(\tau)| \frac{dn}{d\tau}(\tau)\rangle = \frac{\langle m(\tau)| \frac{dH}{d\tau}(\tau) |n(\tau)\rangle}{E_n(\tau) - E_m(\tau)} . \tag{5}$$

Expand the wave function as

$$|\psi(\tau)\rangle = \sum_n c_n(\tau) |n(\tau)\rangle . \tag{6}$$

Substituting this into the Schrodinger equation gives

$$\frac{d}{d\tau} c_n(\tau) = -E_n(\tau) c_n(\tau) - \sum_m \langle n(\tau)| \frac{dm}{d\tau}(\tau)\rangle c_m(\tau). \tag{7}$$

Assuming $E_n(\tau) \neq E_m(\tau)$ for $m \neq n$, we obtain

$$\frac{d}{d\tau} c_n(\tau) = -E_n(\tau) c_n(\tau) - \langle n(\tau)| \frac{dn}{d\tau}(\tau)\rangle c_n(\tau) - \sum_{m \neq n} \frac{\langle n(\tau)| \frac{dH}{d\tau}(\tau) |m(\tau)\rangle}{E_m(\tau) - E_n(\tau)} c_m(\tau). \tag{8}$$

If the imaginary-time evolution of the system is sufficiently slow compared with the energy differences $E_m(\tau) - E_n(\tau)$, the third term can be ignored, and hence

$$\frac{d}{d\tau} c_n(\tau) = -E_n(\tau) c_n(\tau) - \langle n(\tau)| \frac{dn}{d\tau}(\tau)\rangle c_n(\tau). \tag{9}$$

Therefore

$$c_n(\tau) = e^{-\int_0^\tau E_n(\tau')d\tau'} e^{-\int_0^\tau \langle n(\tau')|\frac{dn}{d\tau}(\tau')\rangle d\tau'} c_n(\tau = 0). \tag{10}$$

If $H(\tau)$ is Hermitian, the first factor does not affect the $U(1)$ phase of the wave function. Since

$$\langle n|dn\rangle^* = \langle dn|n\rangle = -\langle n|dn\rangle\,, \tag{11}$$

the second factor is a $U(1)$ phase factor. In particular, for a closed path $H(T) = H(0)$, one obtains the Berry phase:

$$c_n(T) = e^{-\int_0^T E_n(\tau)d\tau} e^{-\oint\langle n|dn\rangle} c_n(\tau = 0). \tag{12}$$