

(1) We have seen the time evolution operator $U(t_0, t) \equiv \exp(-iH(t - t_0)/\hbar)$ and its matrix representation in x -space, $K(x', t; x, t_0)$. Here we will study the *imaginary-time* evolution operator and its propagator. Specifically, we consider the operator $\exp(-\beta H)$ (β is real) and its matrix representation $K(x', x; \beta) \equiv \langle x' | \exp(-\beta H) | x \rangle$ for a one-dimensional system with the Hamiltonian

$$H = \frac{p^2}{2m} + V(x).$$

For convenience let us set $\hbar = m = 1$.

1. Show that

$$K(x', x; \beta) = \sum_n e^{-\beta E_n} \phi_n^*(x') \phi_n(x),$$

where E_n is an energy eigenvalue and $\phi_n(x)$ is the corresponding eigenfunction. The sum is taken over the complete set of n .

2. Show that the operator $\exp(-\beta H)$ projects out the ground state $|\phi_0\rangle$ from *any* initial state that is not orthogonal to the ground state. That is, given an arbitrary $|\psi^{(0)}\rangle$ that satisfies $\langle \psi^{(0)} | \phi_0 \rangle \neq 0$, we have

$$\lim_{\beta \rightarrow \infty} \exp[-\beta(H - E_0)] |\psi^{(0)}\rangle \propto |\phi_0\rangle.$$

3. Show that, for a short imaginary-time $\Delta\tau$ (> 0),

$$K(x', x; \Delta\tau) \doteq \frac{1}{\sqrt{2\pi\Delta\tau}} \exp\left[-\frac{(x' - x)^2}{2\Delta\tau} - \Delta\tau V(x)\right].$$

The approximately equal sign, which indicates we have dropped higher order terms in $\Delta\tau$, becomes exact in the limit of infinitesimal $\Delta\tau$. Please indicate where the approximation occurs in the proof.

4. Now we construct a method to obtain the ground-state wave function. Suppose we choose the constant β in (2) to be finite but large enough so that the projection gives $|\phi_0\rangle$ for practical purposes. Suppose we then choose $\Delta\tau = \beta/L$, where L is a large enough integer so that the error in the approximation in (3) is small. We choose a $\psi^{(0)}(x)$ which is our best guess of the ground-state wave function. Using (3), express the projection $|\phi_0\rangle \doteq C \exp(-\beta H) |\psi^{(0)}\rangle$ in real space in terms of a path integral. (Do not worry about the constant C .)

Computational methods based on these results have proven extremely powerful for studying many-body quantum-mechanical systems.