where the ϕ_n are the eigenstates of H. For simplicity, we set $\hbar = 1$ in the following. As before, we substitute $\tau = it$ into (16.94) and obtain

$$G(x, x_0, \tau) = \sum_n \phi_n(x)\phi_n(x_0)\, e^{-\tau E_n}. \tag{16.95}$$

We first consider the ground state. In the limit $\tau \to \infty$, we have

$$G(x, x, \tau) \to \phi_0(x)^2\, e^{-\tau E_0} \quad (\tau \to \infty). \tag{16.96}$$

From the form of (16.96) and (16.92), we see that we need to compute G and hence S to estimate the properties of the ground state.

To compute S, we convert the integral in (16.91) to a sum. The Lagrangian for a single particle of unit mass in terms of τ becomes

$$L = -\frac{1}{2}\left(\frac{dx}{d\tau}\right)^2 - V(x) = -E. \tag{16.97}$$

We divide the imaginary time interval τ into N equal steps of size $\Delta\tau$ and write E as

$$E(x_j, \tau_j) = \frac{1}{2}\frac{(x_{j+1} - x_j)^2}{(\Delta\tau)^2} + V(x_j), \tag{16.98}$$

where $\tau_j = j\Delta\tau$, and x_j is the corresponding displacement. The action becomes

$$S = -i\Delta\tau \sum_{j=0}^{N-1} E(x_j, \tau_j) = -i\Delta\tau \left[\sum_{j=0}^{N-1} \frac{1}{2}\frac{(x_{j+1} - x_j)^2}{(\Delta\tau)^2} + V(x_j)\right], \tag{16.99}$$

and the probability amplitude for the path becomes

$$e^{iS} = e^{\Delta\tau[\sum_{j=0}^{N-1} \frac{1}{2}(x_{j+1} - x_j)^2/(\Delta\tau)^2 + V(x_j)]}. \tag{16.100}$$

Hence, the propagator $G(x, x_0, N\Delta\tau)$ can be expressed as

$$G(x, x_0, N\Delta\tau) = A\int dx_1 \cdots dx_{N-1}\, e^{\Delta\tau[\sum_{j=0}^{N-1} \frac{1}{2}(x_{j+1} - x_j)^2/(\Delta\tau)^2 + V(x_j)]}, \tag{16.101}$$

where $x \equiv x_N$, and A is an unimportant constant.

From (16.101) we see that $G(x, x_0, N\Delta\tau)$ has been expressed as a multidimensional integral with the displacement variable x_j associated with the time τ_j. The sequence $x_0, x_1, \ldots, x_N$ defines a possible path, and the integral in (16.101) is over all paths. Because the quantity of interest is $G(x, x, N\Delta\tau)$ (see (16.96)), we adopt the periodic boundary condition $x_N = x_0$. The choice of x in the argument of G is arbitrary for finding the ground state energy, and the use of the periodic boundary conditions implies that no point in the closed path is unique. It is thus possible (and convenient) to rewrite (16.101) by letting the sum over j go from 1 to N:

$$G(x_0, x_0, N\Delta\tau) = A\int dx_1 \cdots dx_{N-1}\, e^{-\Delta\tau[\sum_{j=1}^{N} \frac{1}{2}(x_j - x_{j-1})^2/(\Delta\tau)^2 + V(x_j)]}, \tag{16.102}$$

where we have written x_0 instead of x because the x_j that is not integrated over is $x_N = x_0$.

The result of this analysis is to convert a quantum mechanical problem for a single particle into a statistical mechanics problem for N "atoms" on a ring connected by nearest neighbor "springs" with spring constant $1/(\Delta\tau)^2$. The label j denotes the order of the atoms in the ring.

Note that the form of (16.102) is similar to the form of the Boltzmann distribution. Because the partition function for a single quantum mechanical particle contains terms of the form $e^{-\beta E_n}$, and (16.95) contains terms proportional to $e^{-\tau E_n}$, we make the correspondence $\beta = \tau = N\Delta\tau$. We shall see in the following how we can use this identity to simulate a quantum system at a finite temperature.

We can use the Metropolis algorithm to simulate the motion of N "atoms" on a ring. Of course, these atoms are a product of our analysis just as were the random walkers we introduced in diffusion Monte Carlo and should not be confused with real particles. A possible path integral algorithm can be summarized as follows:

1. Choose N and $\Delta\tau$ such that $N\Delta\tau \gg 1$ (the zero temperature limit). Also choose δ, the maximum trial change in the displacement of an atom, and `mcs`, the total number of Monte Carlo steps per atom.
2. Choose an initial configuration for the displacements x_j that is close to the approximate shape of the ground state probability amplitude.
3. Choose an atom j at random and a trial displacement $x_j \to x_j + (2r - 1)\delta$, where r is a uniform random number in the unit interval. Compute the change ΔE in the energy E, where ΔE is given by

$$\begin{aligned}\Delta E = &\frac{1}{2}\left[\frac{x_{j+1} - x_j}{\Delta\tau}\right]^2 + \frac{1}{2}\left[\frac{x_j - x_{j-1}}{\Delta\tau}\right]^2 + V(x_j) \\ &- \frac{1}{2}\left[\frac{x_{j+1} - x_j}{\Delta\tau}\right]^2 - \frac{1}{2}\left[\frac{x_j - x_{j-1}}{\Delta\tau}\right]^2 - V(x_j).\end{aligned} \tag{16.103}$$

   If $\Delta E < 0$, accept the change; otherwise, compute the probability $p = e^{-\Delta\tau\Delta E}$ and a random number r in the unit interval. If $r \le p$, then accept the move; otherwise, reject the trial move.
4. Divide the possible x values into equal size bins of width Δx. Update $P(x)$; that is, let $P(x = x_j) \to P(x = x_j) + 1$, where x is the displacement of the atom chosen in step 3 after step 3 is completed. Do this update even if the trial move was rejected.
5. Repeat steps 3 and 4 until a sufficient number of Monte Carlo steps per atom has been obtained. (Do not take data until the memory of the initial path is lost and the system has reached "equilibrium.")

Normalize the probability density $P(x)$ by dividing by the product of N and `mcs`. The ground state energy E_0 is given by

$$E_0 = \sum_x P(x)[T(x) + V(x)], \tag{16.104}$$

where $T(x)$ is the kinetic energy as determined from the virial theorem

$$\langle 2T(x)\rangle = \left\langle x\frac{dV}{dx}\right\rangle, \tag{16.105}$$