on the sign of $V(x)$. The walkers do not interact with each other because the Schrödinger equation (16.61) is linear in Ψ. Note that it is $\Psi\Delta x$ and *not* $\Psi^2\Delta x$ that corresponds to the probability distribution of the random walkers. This probabilistic interpretation requires that Ψ be nonnegative and real.

We now use this probabilistic interpretation of (16.61) to develop an algorithm for determining the ground state wave function and energy. The general solution of Schrödinger's equation can be written for imaginary time τ as (see (16.10))

$$\Psi(x,\tau) = \sum_n c_n \phi_n(x)\, e^{-E_n\tau}. \tag{16.62}$$

For sufficiently large τ, the dominant term in the sum in (16.62) comes from the term representing the eigenvalue of lowest energy. Hence, we have

$$\Psi(x,\tau\to\infty) = c_0\,\phi_0(x)\, e^{-E_0\tau}. \tag{16.63}$$

From (16.63) we see that the spatial dependence of $\Psi(x,\tau\to\infty)$ is proportional to the ground state eigenstate $\phi_0(x)$. If $E_0 > 0$, we also see that $\Psi(x,\tau)$ and hence the population of walkers will eventually decay to zero unless $E_0 = 0$. This problem can be avoided by measuring E_0 from an arbitrary reference energy V_{ref}, which is adjusted so that an approximate steady state distribution of random walkers is obtained.

Although we could attempt to fit the τ-dependence of the computed probability distribution of the random walkers to (16.63) and thereby extract E_0, it is more convenient to compute E_0 directly from the relation

$$E_0 = \langle V\rangle = \frac{\sum n_i V(x_i)}{\sum n_i}, \tag{16.64}$$

where n_i is the number of walkers at x_i at time τ. An estimate for E_0 can be found by averaging the sum in (16.64) for several values of τ once a steady state distribution of random walkers has been reached. To derive (16.64), we rewrite (16.61) and (16.63) by explicitly introducing the reference potential V_{ref}:

$$\frac{\partial\Psi(x,\tau)}{\partial\tau} = \frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,\tau)}{\partial x^2} - [V(x) - V_{\text{ref}}]\Psi(x,\tau), \tag{16.65}$$

and

$$\Psi(x,\tau) \approx c_0\phi_0(x)\, e^{-(E_0 - V_{\text{ref}})\tau}. \tag{16.66}$$

We first integrate (16.65) with respect to x. Because $\partial\Psi(x,\tau)/\partial x$ vanishes in the limit $|x|\to\infty$, $\int(\partial^2\Psi/\partial x^2)\,dx = 0$, and hence

$$\int\frac{\partial\Psi(x,\tau)}{\partial\tau}\,dx = -\int V(x)\,\Psi(x,\tau)\,dx + V_{\text{ref}}\int\Psi(x,\tau)\,dx. \tag{16.67}$$

If we differentiate (16.66) with respect to τ, we obtain the relation

$$\frac{\partial\Psi(x,\tau)}{\partial\tau} = (V_{\text{ref}} - E_0)\Psi(x,\tau). \tag{16.68}$$

We then substitute (16.68) for $\partial\Psi/\partial\tau$ into (16.67) and find

$$\int(V_{\text{ref}} - E_0)\Psi(x,\tau)\,dx = -\int V(x)\Psi(x,\tau)\,dx + V_{\text{ref}}\int\Psi(x,\tau)\,dx. \tag{16.69}$$

If we cancel the terms proportional to V_{ref} in (16.69), we find that

$$E_0\int\Psi(x,\tau)\,dx = \int V(x),\Psi(x,\tau)\,dx, \tag{16.70}$$

or

$$E_0 = \frac{\int V(x)\Psi(x,\tau)\,dx}{\int\Psi(x,\tau)\,dx}. \tag{16.71}$$

The desired result (16.64) follows by making the connection between $\Psi(x)\,\Delta x$ and the density of walkers between x and $x + \Delta x$.

Although the derivation of (16.64) is somewhat involved, the random walk algorithm is straightforward. A simple implementation of the algorithm is as follows:

1. Place a total of N_0 walkers at the initial set of positions x_i, where the x_i need not be on a grid.
2. Compute the reference energy $V_{\text{ref}} = \sum_i V_i/N_0$.
3. Randomly move the first walker to the right or left by a fixed step length Δs. The step length Δs is related to the time step $\Delta\tau$ by $(\Delta s)^2 = 2D\Delta\tau$. ($D = 1/2$ in units such that $\hbar = m = 1$.)
4. Compute $\Delta V = V(x) - V_{\text{ref}}$ and a random number r in the unit interval. If $\Delta V > 0$ and $r < \Delta V\Delta\tau$, then remove the walker. If $\Delta V < 0$ and $r < -\Delta V\Delta\tau$, then add another walker at x. Otherwise, just leave the walker at x. This procedure is accurate only in the limit of $\Delta\tau \ll 1$. A more accurate procedure consists of computing $P_b = e^{-\Delta V\Delta\tau} - 1 = n + f$, where n is the integer part of P_b, and f is the fractional part. We then make n copies of the walker, and if $f > r$, we make one more copy.
5. Repeat steps 3 and 4 for each of the N_0 walkers and compute the mean potential energy (16.71) and the actual number of random walkers. The new reference potential is given by

$$V_{\text{ref}} = \langle V\rangle - \frac{a}{N_0\Delta\tau}(N - N_0), \tag{16.72}$$

where N is the new number of random walkers, and $\langle V\rangle$ is their mean potential energy. The average of V is an estimate of the ground state energy. The parameter a is adjusted so that the number of random walkers N remains approximately constant.

6. Repeat steps 3–5 until the estimates of the ground state energy $\langle V\rangle$ have reached a steady state value with only random fluctuations. Average $\langle V\rangle$ over many Monte Carlo steps to compute the ground state energy. Do a similar calculation to estimate the distribution of random walkers.

The `QMWalk` class implements this algorithm for the harmonic oscillator potential. Initially, the walkers are randomly distributed within a distance `initialWidth` of the origin.