Notes: Particle in a Box By Random Walk

— Phys690 HW5 (Fall '03)

The goal is to solve for the ground state of a particle in a box. We set $\hbar = m = 1$. The Hamiltonian is $H = -\frac{1}{2}\frac{d^2}{dx^2} + V(x)$, where $V(x)$ is 0 when x is on $(-1, 1)$ and ∞ otherwise.

Note that this is essentially the drunkard problem (HW2) in disguise. Recall that the solution to

$$-\frac{\partial}{\partial t}\psi(x,t) = H\psi(x,t)$$

leads to the ground state of H at large t: $\psi(x, t \to \infty) \to \psi_0(x)$. On the other hand, the probability distribution of the drunkard is described by

$$\frac{\partial}{\partial t}\psi(x,t) = \frac{1}{2}\frac{d^2}{dx^2}\psi(x,t),$$

the same equation. Given the boundary condition $\psi(x = \pm 1, t) = 0$, the solution to this equation is unique. That is, the probability distribution of the drunkard at large t, which is a smooth function that vanishes at the two bars, *is* the ground-state wave function of a particle in a box! Our strategy to solve the quantum mechanical problem is therefore to simulate the motion of many drunkards in order to obtain their distribution at large time. Of course, because of trapping at the bars, there is a finite probability of losing the drunkard. We would have to multiply $\psi(x,t)$ by a constant to make up for that loss, so as to ensure a constant normalization.

Now we need to figure out how to simulate the drunkard motion. The zeroth-order description is that it is just diffusion (Gaussian). But boundary effect must be properly accounted for. In the lattice version the drunkard must be one step away to be able to "land" in the bar (trapping). The situation in the continuum version is less straightforward: there is always a *finite* probability that the drunkard will land at the bar, no matter where he is. We need to modify the diffusion probability (Gaussian) to take this effect into consideration. Below is a more formal description.

We need to repeatedly operate $\exp(-\tau H)$ on an initial wave function. (τ is small.) Recall that $\exp(-\tau H) \equiv g(x, x')$ is called the *short-time* Green's function. It can be approximated by:

$$g(x,x') = \begin{cases} g_0(x,x') - g_0(x, Ix'), & \text{if } x \,\&\, x' \text{ inside box} \\ 0, & \text{otherwise} \end{cases}, \tag{1}$$

where g_0 is the free-particle Green's function: $g_0(x,x') = 1/\sqrt{2\pi\tau}\,\exp[-(x-x')^2/2\tau]$, and Ix' denotes the mirror image of x' with respect to the closer side of the box. It is easily verified that $g(x,x')$ indeed: (i) satisfies $-\partial g/\partial\tau = Hg$, (ii) is $\delta(x - x')$ at $\tau = 0$ and, (iii) (approximately) satisfies the boundary condition at the sides. Note that, except for near the two sides, $g(x,x')$ is essentially the free Green's function $g_0(x,x')$.

We want to propagate

$$\psi(x) = e^{\tau E_0}\int g(x,x')\psi(x')\,dx'. \tag{2}$$

The *constant* $e^{\tau E_0}$ ensures normalization when ψ is the ground-state wave function, *i.e.*, when the propagation has reached equilibrium. We can rewrite Eq. (2) as:

$$\psi(x) = e^{\tau E_0}\int K(x,x')\; g_0(x,x')\; \psi(x')\,dx', \tag{3}$$

where

$$K(x,x') = \begin{cases} 1 - \frac{g_0(x,Ix')}{g_0(x,x')} \equiv 1 - P(x,x'), & \text{if } x' \text{ and } x \text{ inside box} \\ 0, & \text{otherwise} \end{cases}. \tag{4}$$

Inside the integral in Eq. (3), from right to left, the three factors: (a) $\psi(x')$ can be viewed as probability density for x', (b) $g_0(x,x')$ can be viewed as probability density for x conditional on x' and, (c) $K(x,x')$ is between 0 and 1 and can be used as a probability.

As a variant of the method we discussed in class, we introduce another way to treat branching. We use a *fixed* number of walkers to represent ψ. The three steps in the help page on '`step`' correspond to (a), (b), and (c) in the above paragraph. In the last step, we accept x with probability K (note that `exp(-imgdist)` in the code is P in Eq. (4)). If we reject, we must start all over again from (a). We do not normalize `exp(-imgdist)`, because $g(x, x')$ (or K) is *not* normalized with respect to x. The key is to keep *randomly* picking a walker out of the current pool until we have obtained exactly the desired number of new walkers. The advantage is that no E_T is needed; the disadvantage is that this scheme introduces a systematic bias in the final result that becomes more pronounced as the number of walkers `n_wlks` decreases.