Please note, all Griffiths problems come from our class text, the second edition.

1. **Griffiths 2.4**

***Problem 2.4** Calculate $\langle x\rangle$, $\langle x^2\rangle$, $\langle p\rangle$, $\langle p^2\rangle$, σ_x, and σ_p, for the nth stationary state of the infinite square well. Check that the uncertainty principle is satisfied. Which state comes closest to the uncertainty limit?

Solution: Using the reflection symmetry around the midpoint of the well,

$$\psi_n(a-x) = A\sin(n\pi - k_n x) = -A\cos(n\pi)\sin(k_n x) = (-1)^{n+1}\psi_n(x), \tag{1}$$

since $\sin(n\pi) = 0$,

$$\begin{aligned}\langle x\rangle &= \langle\psi_n|\hat{x}|\psi_n\rangle = \int_{-\infty}^{\infty} x\psi_n^*(x)\psi_n(x)\,\mathrm{d}x = \int x\psi_n^*(a-x)\psi_n(a-x)\,\mathrm{d}x \\ &= \int (a-x')\psi_n^*(x')\psi_n(x')\,\mathrm{d}x' = a - \langle x\rangle\,,\end{aligned} \tag{2}$$

so $\langle x\rangle = \frac{a}{2}$, as one might expect.

To calculate σ_x, we will need to do an integral. Since $\sin(kx)^2 = \frac{1}{2}(1-\cos(2kx))$, making the substitution $y = 2k_n(x - \frac{a}{2})$,

$$\sigma_x^2 = \left\langle (x-\tfrac{a}{2})^2\right\rangle = \frac{2}{a}\int_0^a \left(x - \frac{a}{2}\right)^2 \sin^2(k_n x)\,\mathrm{d}x = \frac{1}{8ak_n^3}\int_{-n\pi}^{n\pi} y^2(1-\cos(y+n\pi))\,\mathrm{d}y\,, \tag{3}$$

and, integrating by parts,

$$\begin{aligned}&\int_{-n\pi}^{n\pi} y^2\cos(y+n\pi)\,\mathrm{d}y = (-1)^n\int_{-n\pi}^{n\pi} y^2\cos y\,\mathrm{d}y = (-1)^n\int_{-n\pi}^{n\pi} y^2\frac{\partial}{\partial y}\sin y\,\mathrm{d}y \\ &= (-1)^n\left([y^2\sin y]_{-n\pi}^{n\pi} - 2\int_{-n\pi}^{n\pi} y\sin y\,\mathrm{d}y\right) = 2(-1)^{n+1}\int_{-n\pi}^{n\pi} y\frac{\partial}{\partial y}(-\cos y)\,\mathrm{d}y \\ &= 2(-1)^n\left([y\cos y]_{-n\pi}^{n\pi} - \int_{-n\pi}^{n\pi}\cos y\,\mathrm{d}y\right) = 4n\pi(-1)^n\cos(n\pi) = 4n\pi,\end{aligned} \tag{4}$$

and thus finally

$$\sigma_x^2 = \frac{1}{8ak_n^3}\left(\frac{2(n\pi)^3}{3} - 4n\pi\right) = \frac{a^2}{12}\left(1 - \frac{6}{(n\pi)^2}\right). \tag{5}$$

This makes sense: the lower energy modes are more localised away from the high potential, and as the energy goes to infinity, the position distribution approaches a uniform distribution, which has standard deviation $\frac{a}{\sqrt{12}}$.

In a stationary state, since $\langle x\rangle$ is constant the expected momentum $\langle p\rangle = m\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t}$ is zero. For the infinite square well, one can understand it as the stationary states being equal combinations of left and right moving waves, each with $|p| = \hbar k_n = \frac{n\pi\hbar}{a}$, so we also expect that to be σ_p. Indeed,

$$\begin{aligned}\sigma_p^2 = \langle p^2\rangle &= \langle\psi_n|\hat{p}^2|\psi_n\rangle = \langle\psi_n|\hat{p}^\dagger\hat{p}|\psi_n\rangle = \int_{-\infty}^{\infty}\left|-i\hbar\frac{\partial\psi_n}{\partial x}(x)\right|^2\mathrm{d}x \\ &= \frac{2\hbar^2k_n^2}{a}\int_0^a\cos(k_n x)^2\,\mathrm{d}x = \frac{\hbar^2k_n^2}{a}\int_0^a(1+\cos(2k_n x))\,\mathrm{d}x = \hbar^2k_n^2.\end{aligned} \tag{6}$$

$$\sigma_x\sigma_p = \frac{n\pi\hbar}{\sqrt{12}}\sqrt{1-\frac{6}{(n\pi)^2}} = \frac{\hbar}{2}\sqrt{\frac{(n\pi)^2}{3}-2}, \tag{7}$$

which increases with n, so the ground state has the lowest uncertainty, which is greater than $\frac{\hbar}{2}$ since $\pi^2 > 6$.

2. **Infinite square well** (based on Griffiths 2.8, 2.38, 2.39)

(a) Suppose you have a particle "at rest", equally likely to be found anywhere in the well, at $t = 0$. What should its mean momentum be? Is its wavefunction uniquely determined by the given information? What is the simplest wavefunction that describes the particle?

Solution: We want $|\Psi(x)|^2$ to be constant inside the well, so $\Psi(x) = \frac{1}{\sqrt{a}}e^{if(x)}$ for real $f(x)$, for $0 < x < a$. Different $f(x)$ would correspond to different momentum distributions. For the particle to be at rest, we need $\langle p\rangle = 0$. This is satisfied by $f(x) = 0$, which I think all reasonable people will agree is the simplest choice.

Although, to evaluate this properly, we need to deal with the discontinuities at $x = 0, a$. The derivative of the step function,

$$\Theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases} = \int_{-\infty}^{x} \delta(x')\,\mathrm{d}x', \tag{8}$$

is the delta function, so since $\Psi(x) = \frac{1}{\sqrt{a}}e^{if(x)}\Theta(x)\Theta(a-x)$ (note that we haven't defined the values at $x = 0, a$),

$$\frac{\partial\Psi}{\partial x} = \frac{1}{\sqrt{a}}e^{if(x)}\left(i\frac{\partial f}{\partial x}\Theta(x)\Theta(a-x) + \delta(x)\Theta(a-x) - \Theta(x)\delta(a-x)\right), \tag{9}$$

and thus, since $\Theta(z)^2 = \Theta(z)$,

$$\begin{aligned}\langle p\rangle &= -i\hbar\int_{-\infty}^{\infty}\Psi^*(x)\frac{\partial\Psi}{\partial x}(x)\,\mathrm{d}x \\ &= \frac{-i\hbar}{a}\int e^{-if(x)}\Theta(x)\Theta(a-x)\left(i\frac{\mathrm{d}f}{\mathrm{d}x} + \delta(x) - \delta(a-x)\right)e^{if(x)}\,\mathrm{d}x \\ &= \frac{\hbar}{a}\left(\int_0^a f'(x)\,\mathrm{d}x - i\Theta(0) + i\Theta(0)\right) = \hbar\left(\frac{f(a)-f(0)}{a}\right) = 0,\end{aligned} \tag{10}$$

regardless of how we define $\Theta(0)$ (as long as we are consistent). Thus any $f(x)$ with $f(0) = f(a)$ describes what we know about the particle.

(b) If the particle is indeed in the state you found in part a, and you measured the energy of the particle, what possible values could you obtain and with what probabilities?

Solution: The possible energy eigenvalues are $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$, and the probability of measuring E_n is the modulus-squared overlap of the wavefunction with the corresponding energy eigenfunction,

$$\begin{aligned}\langle\psi_n|\Psi\rangle &= \int_{-\infty}^{\infty}\Psi^*\psi_n\,\mathrm{d}x = \frac{\sqrt{2}}{a}\int_0^a \sin(k_n x)\,\mathrm{d}x = -\frac{\sqrt{2}}{ak_n}[\cos(k_n x)]_0^a \\ &= -\frac{\sqrt{2}}{n\pi}(\cos(n\pi) - \cos(0)) = -\frac{\sqrt{2}}{n\pi}((-1)^n - 1) = \begin{cases} 0 & n \text{ even}, \\ \frac{2\sqrt{2}}{n\pi} & n \text{ odd}, \end{cases}\end{aligned} \tag{11}$$

$$\Pr(E_n) = |\langle\psi_n|\Psi\rangle|^2 = \begin{cases} 0 & n \text{ even}, \\ \frac{8}{(n\pi)^2} & n \text{ odd}. \end{cases} \tag{12}$$

Note that the overlap with the odd states (i.e. those with even n, for which $\psi(x) = -\psi(a-x)$) is zero since our initial wavefunction is even. Incidentally, since we know Ψ is normalised and the ψ_ns are orthonormal,

$$1 = \sum_{n=1}^{\infty} \Pr(E_n) = \frac{8}{\pi^2} \sum_{m=0}^{\infty} \frac{1}{(2m+1)^2}, \tag{13}$$

so we have proven that $\sum_m (2m+1)^{-2} = \frac{\pi^2}{8}$.

(c) What is the expected value of the energy?
Solution:

$$\langle E\rangle = \sum_{n=1}^{\infty} E_n \Pr(E_n) = \frac{\pi^2\hbar^2}{2ma^2}\frac{8}{\pi^2}\sum_{m=0}^{\infty}\frac{(2m+1)^2}{(2m+1)^2} = \frac{4\hbar^2}{ma^2}\sum_{m=0}^{\infty} 1 = \infty. \tag{14}$$

In fact, any discontinuous wavefunction has infinite kinetic energy, regardless of the potential $V(x)$: suppose $\Psi(x) = f(x) + a\Theta(x-b)$, where f is continuous. Then

$$\begin{aligned} \langle p^2\rangle &= \hbar^2 \int \left|\frac{\partial\Psi}{\partial x}\right|^2 \mathrm{d}x = \hbar^2 \int |f'(x) + a\delta(x-b)|^2 \,\mathrm{d}x \\ &= \hbar^2 \int \left(|f'(x)|^2 + 2\operatorname{Re}(a^* f'(x))\delta(x-b) + |a|^2\delta(x-b)^2\right)\mathrm{d}x \\ &= \hbar^2 \left(\int |f'(x)|^2\,\mathrm{d}x + 2\operatorname{Re}(a^* f'(b)) + |a|^2\delta(0)\right) \\ &= \hbar^2(\ldots + |a|^2 \times \infty) = \infty. \end{aligned} \tag{15}$$

(d) Write down the wavefunction at some later time t. (Leave it as an infinite sum.)
Solution:

$$|\Psi(t)\rangle = \sum_{n=1}^{\infty} e^{-iE_n t/\hbar}\langle\psi_n|\Psi(0)\rangle|\psi_n\rangle = \sum_{\text{odd } n}\frac{2\sqrt{2}}{n\pi}e^{-iE_n t/\hbar}|\psi_n\rangle, \tag{16}$$

$$\Psi(x,t) = \sum_{\text{odd } n}\frac{4}{n\pi a}e^{-iE_n t/\hbar}\sin(k_n x). \tag{17}$$

(e) Show that at time $t = 4ma^2/\pi\hbar$, the wavefunction returns to its initial state.
Solution: Note $E_n t = \frac{n^2\pi^2\hbar^2}{2ma^2}\frac{4ma^2}{\pi\hbar} = 2\pi n^2\hbar$, so for any n, $e^{-iE_n t/\hbar} = e^{-2\pi i n^2} = 1$, so any wavefunction returns to its initial state,

$$|\Psi(t)\rangle = \sum_n e^{-iE_n t/\hbar}\langle\psi_n|\Psi(0)\rangle|\psi_n\rangle = \sum_n \langle\psi_n|\Psi(0)\rangle|\psi_n\rangle = |\Psi(0)\rangle. \tag{18}$$

(f) Suppose the well was somehow expanded to double the length, keeping the centre unchanged, without perturbing the wavefunction of the particle. Now, if you measured the energy, what possible values could you obtain and with what probabilities?
Solution: The new allowed energy values have double the length, $a \to 2a$, so $E_n = \frac{n^2\pi^2\hbar^2}{8ma^2}$. The new eigenstates are

$$\psi_n(x) = \frac{1}{\sqrt{a}}\sin\left(\frac{n\pi}{2a}\left(x + \frac{a}{2}\right)\right), \tag{19}$$

for $-\frac{a}{2} \leq x \leq \frac{3a}{2}$. Now

$$\begin{aligned}\langle\psi_n|\Psi\rangle &= \frac{1}{a}\int_0^a \sin\left(\frac{n\pi}{2a}\left(x+\frac{a}{2}\right)\right)\mathrm{d}x = -\frac{2}{n\pi}\left[\cos\left(\frac{n\pi}{2a}\left(x+\frac{a}{2}\right)\right)\right]_0^a \\ &= \frac{2}{n\pi}\left(\cos\left(\frac{n\pi}{4}\right) - \cos\left(\frac{3n\pi}{4}\right)\right) \\ &= \frac{2}{n\pi}\left(\cos\left(\frac{n\pi}{2}-\frac{n\pi}{4}\right) - \cos\left(\frac{n\pi}{2}+\frac{n\pi}{4}\right)\right) \\ &= \frac{4}{n\pi}\sin\left(\frac{n\pi}{4}\right)\sin\left(\frac{n\pi}{2}\right),\end{aligned} \tag{20}$$

where since $\cos(a+b) = \cos a\cos b - \sin a \sin b$, $\cos(a-b) - \cos(a+b) = 2\sin a \sin b$. For even n, we expect this to be zero because the odd/even symmetry still exists, and it is, because $\sin(m\pi) = 0$, for $n = 2m$. Thus we need only evaluate odd $n = 2m+1$, for which

$$\sin\left(\frac{n\pi}{2}\right) = \sin\left(m\pi + \frac{\pi}{2}\right) = \cos(m\pi)\sin\left(\frac{\pi}{2}\right) = (-1)^m, \tag{21}$$

and

$$\sin\left(\frac{n\pi}{4}\right) = \sin\left(\frac{m\pi}{2}+\frac{\pi}{4}\right) = \begin{cases}\frac{1}{\sqrt{2}} & m = 4k \text{ or } m = 4k+1,\\ -\frac{1}{\sqrt{2}} & m = 4k+2 \text{ or } m = 4k+3,\end{cases} \tag{22}$$

so, putting it all together,

$$\langle\psi_n|\Psi\rangle = \begin{cases}\frac{2\sqrt{2}}{n\pi} & n = 8k+1 \text{ or } n = 8k+7,\\ -\frac{2\sqrt{2}}{n\pi} & n = 8k+3 \text{ or } n = 8k+5,\\ 0 & \text{else.}\end{cases} \tag{23}$$

So we now have a sign that we didn't have before, which leaves the probabilities unchanged,

$$\Pr(E_n) = |\langle\psi_n|\Psi\rangle|^2 = \begin{cases}0 & n \text{ even},\\ \frac{8}{(n\pi)^2} & n \text{ odd}.\end{cases} \tag{24}$$

3. **Griffiths 2.31**

Problem 2.31 The Dirac delta function can be thought of as the limiting case of a rectangle of area 1, as the height goes to infinity and the width goes to zero. Show that the delta-function well (Equation 2.114) is a "weak" potential (even though it is infinitely deep), in the sense that $z_0 \to 0$. Determine the bound state energy for the delta-function potential, by treating it as the limit of a finite square well. Check that your answer is consistent with Equation 2.129. Also show that Equation 2.169 reduces to Equation 2.141 in the appropriate limit.

Solution: To get $\delta(x)$, we set $V_0 = \frac{1}{2a}$ and then take $a \to 0$. Thus to get $\alpha\delta(x)$, we must set $V_0 = \frac{\alpha}{2a}$, and therefore

$$z_0 = \frac{a}{\hbar}\sqrt{2mV_0} = \frac{\sqrt{m\alpha a}}{\hbar} \longrightarrow 0. \tag{25}$$

For small z_0, we expect the resulting z to also be small, i.e. $z \to 0$, so eqn 2.156 in Griffiths becomes

$$\tan z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1} = 0, \tag{26}$$

so $z = z_0$. Thus

$$\kappa = \frac{z \tan z}{a} \approx \frac{z_0^2}{a} = \frac{m\alpha}{\hbar^2} = \frac{\sqrt{-2mE}}{\hbar}, \tag{27}$$

so

$$E = -\frac{m\alpha^2}{2\hbar^2}. \tag{28}$$

For a scattering state with finite energy E, the transmission coefficient is

$$\begin{aligned} \frac{1}{T} - 1 &= \frac{V_0^2}{4E(E+V_0)} \sin\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)^2 \\ &\approx \frac{V_0^2}{4E(E+V_0)} \frac{8ma^2(E+V_0)}{\hbar^2} = \frac{2ma^2V_0^2}{\hbar^2 E} = \frac{m\alpha^2}{2\hbar^2 E}, \end{aligned} \tag{29}$$

since the argument of the sine goes to zero.

4. **Delta function well scattering**
Instead of sending a particle from infinity with well-defined momentum p, suppose we had a Gaussian wavepacket, with some small momentum uncertainty σ_p (i.e. large position uncertainty σ_x), with mean momentum p and mean position $-d$ (with $d \gg \sigma_x$, so it's on the left of the well).

   (a) What is the probability that after a very long time, the particle remains near $x = 0$? (You may leave your answer in terms of an integral.)
   (Hint: which energy eigenstates are localised?)
   Solution: After a very long time, the scattering states will have dispersed off to very large distances, so only the bound state remains. Thus the probability of finding the particle near $x = 0$ after a long time is the modulus-squared overlap of its initial wavefunction $|\Psi\rangle$ with that of the bound state $|\psi\rangle$,

$$\text{Pr(particle remains “near” } x = 0) = \text{Pr(particle in bound state)} = |\langle\psi|\Psi\rangle|^2, \tag{30}$$

$$\langle\psi|\Psi\rangle = \int \psi^*(x)\Psi(x)\,\mathrm{d}x = \frac{\sqrt{m\alpha}}{(2\pi\sigma_x^2)^{\frac{1}{4}}\hbar} \int_{-\infty}^{\infty} e^{-m\alpha|x|/\hbar^2} e^{-(x+d)^2/4\sigma_x^2} e^{ipx/\hbar}\,\mathrm{d}x\,. \tag{31}$$

   (b) If this probability is not zero, comment on the apparent contradiction between $R + T = 1$ and your result.
   (Hint: what happens to this probability as we take $d \to \infty$ or $\sigma_p \to 0$?)
   Solution: $R+T = 1$ for a scattering state. If we take the limit of having well-defined momentum (although if we knew its momentum exactly we couldn't know on which side of the well it is), the Gaussian wavepacket approaches a scattering state, and its overlap with the bound state approaches zero. The overlap also approaches zero when we take the limit of the particle coming from infinity, and when the overlap is zero, $R + T = 1$.

   The point here is that when we have both bound states and scattering states, a general wavepacket can scatter off in either direction, or remain bound, if it starts off with some part in the scattering or bound states respectively. When we're doing scattering, we start off mostly in the scattering states, so end up mostly in the scattering states. But a “true” scattering state is completely delocalised, so is impractical; we use it as an idealised example and practically only approach it as a limit.

5. **Periodic potentials** (see B&J§4.8)
Suppose we have a potential which is periodic with period L, i.e. $V(x + L) = V(x)$

(a) Show that if $\psi(x)$ is a stationary state, then $\psi(x+nL)$ is also a stationary state with the same energy, for any integer n.
Solution: Let E be the energy of ψ, so $\hat{H}\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}(x) + V(x)\psi(x) = E\psi(x)$, and let $\phi(x) = \psi(x+nL)$. Since $V(x+nL) = V(x)$ for all integer n,

$$\begin{aligned}\hat{H}\phi(x) &= -\frac{\hbar^2}{2m}\frac{\partial^2\phi}{\partial x^2}(x) + V(x)\phi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}(x+nL) + V(x)\psi(x+nL) \\ &= -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}(x+nL) + V(x+nL)\psi(x+nL) \\ &= \hat{H}\psi(x+nL) = E\psi(x+nL) = E\phi(x).\end{aligned} \tag{32}$$

Another way to say this is that the translation operators $\hat{T}_n$, which map $\psi(x) \mapsto \psi(x+nL)$, commute with the Hamiltonian $\hat{T}_n\hat{H} = \hat{H}\hat{T}_n$, i.e. these translations are symmetries of the Hamiltonian. As a result,

$$\hat{H}\left|\phi\right\rangle = \hat{H}\hat{T}_n\left|\psi\right\rangle = \hat{T}_n\hat{H}\left|\psi\right\rangle = E\hat{T}_n\left|\psi\right\rangle = E\left|\phi\right\rangle. \tag{33}$$

(b) Given any stationary state $\psi(x)$, construct a set of stationary states $\phi_k(x)$ with the same energy, with the property that $\phi_k(x+L) = e^{ikL}\phi_k(x)$. Check that you can recover ψ from the ϕ_ks.
(Hint: use a linear combination $\phi_k(x) = \sum_{n=-\infty}^{\infty} c_n\psi(x+nL)$ with appropriately chosen coefficients c_n.)
Solution:

$$\phi_k(x) = \sum_{n=-\infty}^{\infty} e^{-inkL}\psi(x+nL), \tag{34}$$

$$\begin{aligned}\phi_k(x+L) &= \sum_{n=-\infty}^{\infty} e^{-inkL}\psi(x+(n+1)L) = e^{ikL}\sum_{n=-\infty}^{\infty} e^{-i(n+1)kL}\psi(x+(n+1)L) \\ &= e^{ikL}\sum_{m=-\infty}^{\infty} e^{-imkL}\psi(x+mL) = e^{ikL}\phi_k(x),\end{aligned} \tag{35}$$

$$\begin{aligned}\int_0^{\frac{2\pi}{L}} \phi_k(x)\,\mathrm{d}k &= \sum_{n=-\infty}^{\infty}\psi(x+nL)\int_0^{\frac{2\pi}{L}} e^{-inkL}\,\mathrm{d}k = \frac{1}{L}\sum_{n=-\infty}^{\infty}\psi(x+nL)\int_0^{2\pi} e^{-in\theta}\,\mathrm{d}\theta \\ &= \frac{2\pi}{L}\sum_n \psi(x+nL)\delta_{n,0} = \frac{2\pi}{L}\psi(x).\end{aligned} \tag{36}$$

(c) Define $u_k(x) = e^{-ikx}\phi_k(x)$ and show that u_k is periodic, i.e. $u_k(x+L) = u_k(x)$. Hence we may choose an energy eigenbasis in which the stationary states are $\phi_k(x) = e^{ikx}u_k(x)$. This is known as *Bloch's theorem.*
Solution:

$$u_k(x+L) = e^{-ik(x+L)}\phi_k(x+L) = e^{-ik(x+L)}e^{ikL}\phi_k(x) = e^{-ikx}\phi_k(x) = u_k(x). \tag{37}$$

A better approach to this proof is that since $\hat{T}_n = (\hat{T}_1)^n$ commutes with $\hat{H}$, they must have a common eigenbasis. Since the translation operator is unitary, its eigenvalues must have modulus one, i.e. $\hat{T}_1\left|\psi\right\rangle = e^{i\theta}\left|\psi\right\rangle$ for any eigenstate $\left|\psi\right\rangle$. Then define ψ to be ϕ_k for $k = \frac{\theta}{L}$ and u_k as above.