1. **Getting to know the delta "function"**
Let's define the Dirac delta "function" $\delta(x)$ by the property

$$\int f(x)\delta(x)\,\mathrm{d}x = f(0), \tag{1}$$

for "well-behaved" functions f.

(a) Consider the family of box functions

$$B_a(x) = \begin{cases} \frac{1}{2a} & -a < x < a, \\ 0 & \text{else.} \end{cases} \tag{2}$$

Show that in the $a \to 0$ limit, B_a goes to the delta function.
(Hint: Taylor expand f around 0)

(b) Show that the Gaussian with $\mu = 0$ goes to the delta function as $\sigma \to 0$.
(Hint: use a change of variables to show that $\langle x^n \rangle = C_n \sigma^n$, for some constant C_n which you need to evaluate only for $n = 0$)

(c) What are the values of $\delta(x)$ for $x \neq 0$, $x = 0$? Is it a well-defined function?

(d) Consider the family of functions

$$\delta_L(x) = \frac{1}{2\pi}\int_{-L}^{L} e^{ikx}\,\mathrm{d}k\,. \tag{3}$$

Do the integral to find a closed form for $\delta_L(x)$. Show that in the limit $L \to \infty$, δ_L goes to the delta function.

(e) Show that the Fourier transform of a Gaussian is a Gaussian, and hence show that

$$\int_{-\infty}^{\infty} e^{ikx}\,\mathrm{d}k = 2\pi\delta(x). \tag{4}$$

(f) The Heaviside step function is

$$\Theta(x) = \begin{cases} 1 & x > 0, \\ 0 & x < 0. \end{cases} \tag{5}$$

Show that $\delta(x) = \frac{\mathrm{d}\Theta(x)}{\mathrm{d}x}$.
(Hint: integrate by parts, assuming that "well-behaved" f go to zero at $\pm\infty$)

(g) Show that

$$\int f(x)\frac{\mathrm{d}^n\delta(x)}{\mathrm{d}x^n}\,\mathrm{d}x = (-1)^n\frac{\mathrm{d}^n f}{\mathrm{d}x^n}(0). \tag{6}$$

(h) Show that

$$\delta(f(x)) = \sum_{x_0 \text{ s.t. } f(x_0)=0} \frac{\delta(x - x_0)}{|f'(x_0)|}, \tag{7}$$

where $'$ denotes (spatial) derivative, i.e. $f'(x) = \frac{\mathrm{d}f(x)}{\mathrm{d}x}$.
(Hint: change variables inside the integral)

2. **Bra-ket notation, integration kernels, Fourier transform**
Given a discrete orthonormal basis $\{|e_i\rangle\}$, we can write any vector $|v\rangle$ as a linear combination of basis vectors $|v\rangle = \sum_i v_i |e_i\rangle$, where v_i are the components of $|v\rangle$ in this basis. Similarly, we can write any operator in a "matrix" representation, $\hat{A} = \sum_{i,j} A_{ij} |e_i\rangle\langle e_j|$, where A_{ij} are the components or matrix elements of $\hat{A}$ in this basis and $|v\rangle\langle w|$ is the outer product of $|v\rangle$ and $|w\rangle$, the operator that maps $|u\rangle \mapsto \langle w|u\rangle |v\rangle$. For a continuous orthonormal basis, e.g. $\{|x\rangle \,|\, x \in \mathbb{R}\}$, the analogous representations are $|\psi\rangle = \int \psi(x) |x\rangle \, \mathrm{d}x$ and $\hat{A} = \int \mathrm{d}x \, \mathrm{d}y \, A(x,y) |x\rangle\langle y|$, where the integration kernel $A(x,y)$ plays the role of the matrix elements, so $[\hat{A}\Psi](x) = \int \mathrm{d}y \, A(x,y)\Psi(y)$.

   (a) Orthonormality in the discrete case means $\langle e_i|e_j\rangle = \delta_{ij}$. Check that this allows us to find the components of a vector using the inner product, $v_i = \langle e_i|v\rangle$. What is the orthonormality condition for continuous bases, and how do we find the components $\psi(x)$ from $|\psi\rangle$ and $|x\rangle$?

   (b) Given an operator $\hat{A}$ and a basis, how would you find the components A_{ij} or $A(x,y)$? Show that the i^{th} component of $\hat{A}|v\rangle$ is $\sum_j A_{ij} v_j$ and similarly the x-component of $\hat{A}|\psi\rangle$ is $\int \mathrm{d}y \, A(x,y)\psi(y)$.

   (c) Show that the matrix of $\hat{A}^\dagger$ is the conjugate transpose of the matrix of $\hat{A}$, $(A^\dagger)_{ij} = A^*_{ji}$. Find the kernel of $\hat{A}^\dagger$, $[A^\dagger](x,y)$ in terms of $A(x,y)$.

   (d) Show that the matrix elements of the identity operator are δ_{ij}. Find its kernel.

   (e) An operator $\hat{A}$ is diagonalisable iff it has a complete eigenbasis, i.e. there is a basis in which where every basis vector is an eigenvector, e.g. $\hat{A}|e_i\rangle = A_i |e_i\rangle$ for a discrete basis. Show that the matrix of such an operator has elements $A_{ij} = A_i \delta_{ij}$. What does its kernel look like?

   (f) The continuous Fourier transform $\hat{F}$ maps f to $[\hat{F}f](k) = \frac{1}{\sqrt{2\pi}} \int \mathrm{d}x \, e^{-ikx} f(x)$. What is the kernel of $\hat{F}$? Show that it is unitary. (Recall that an operator $\hat{U}$ is unitary iff it is invertible and preserves the inner product, or, equivalenty, $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = 1$.)

   (g) Show that if $\{|x\rangle\}$ is an orthonormal basis and $\hat{U}$ is unitary, $\{\hat{U}^\dagger|x\rangle\}$ is also an orthonormal basis. Hence define the Fourier basis $\{|k\rangle = \hat{F}^\dagger|x\rangle = \frac{1}{\sqrt{2\pi}} \int e^{ikx} |x\rangle\}$. What is the Fourier-space kernel $A(k',k)$ of an operator in terms of its real-space kernel $A(x,y)$?

   (h) When $|x\rangle$ represent position eigenstates, $|k\rangle$ represent momentum eigenstates. Find the kernels of the position and momentum operators $\hat{x}, \hat{p}$ in the position basis $\{|x\rangle\}$ and in the momentum basis $\{|k\rangle\}$. (If you wanted to define $|p\rangle$ so that $\hat{p}|p\rangle = p|p\rangle$ instead of $\hat{p}|k\rangle = \hbar k |k\rangle$, how would you do it to ensure normalisation?)

   (i) Find the kernel of the translation operator $[\hat{T}_a\Psi](x) = \Psi(x-a)$ in position space and momentum space. Hence show that to shift a wavefunction to the right in position space by x_0 we simply multiply the momentum space wavefunction by e^{-ikx_0}, and deduce that to shift momentum by $p_0 = \hbar k_0$ we simply multiply the real space wavefunction by $e^{ik_0 x}$.

   (j) If an operator $\hat{A}$ is translation invariant, that means it looks the same no matter how we translate it, i.e. $\hat{T}^\dagger\hat{A}\hat{T} = \hat{A}$, for any translation operator $\hat{T}$. What does this mean in terms of its matrix elements and/or kernel? Show that if an operator is translation invariant, it is diagonal in momentum space.

3. **Classical computers aren't completely useless**

   (a) If you're unfamiliar with numerical computing, or with Python, please see this tutorial made by the Physics department. If you're on the fence about whether or not to learn numerical computing, see this quick tour of some of the cool ways we can solve physics problems using computers. To open the Jupyter notebooks, either download them and install Jupyter, or use an online environment such as Berkeley DataHub (instructions on the GitHub pages linked above) or on Google Colab (change the URL domain from `github.com` to `githubtocolab.com`).

   (b) Carefully read the "discretising continuous systems" section of this notebook. Play around with the code and try different potentials if you'd like.

   (c) Suppose we're in a finite periodic interval (e.g. a circle) of length L. Let's approximate the continuous interval by a grid/lattice of N evenly spaced points with positions $x_i = i\frac{L}{N} = ia$ for $i = 0, 1, \ldots, N-1$, where a is the grid spacing. Write down the $N \times N$ matrix representing the position operator in the $|x_i\rangle$ basis. Write down the matrix representing $V(\hat{x})$ for any given potential $V(x)$.

   (d) Approximating the second derivative by finite differences, $\frac{\partial^2 f}{\partial x^2}(x_i) \approx \frac{f(x_{i+1})+f(x_{i-1})-2f(x_i)}{a^2}$ (with $x_N = x_0$ and $x_{-1} = x_{N-1}$ because of the periodicity), write down the matrix representing the kinetic energy operator $\frac{\hat{p}^2}{2m}$ in the position basis.

   (e) The position space wavefunction of a Gaussian wavepacket with mean position x_0, mean momentum p_0 and position standard deviation σ is $G(x) \propto e^{-(x-x_0)^2/4\sigma^2 + ip_0x/\hbar}$. In our finite circular grid, approximate it as $|G\rangle = A\sum_i G(x_i)\,|x_i\rangle$. For a circular grid with $N = 200$, set up a Gaussian wavefunction with $x_0 = \frac{3L}{10}, p_0 = \frac{10h}{L}, \sigma = \frac{L}{40}$, computing the normalisation constant A numerically. Plot the wavefunction (you could plot all three of $\operatorname{Re}\psi, \operatorname{Im}\psi, |\psi|$ on the same plot, or plot $|\psi|^2$ using colour to denote phase).

   (f) Set up the free particle Hamiltonian and diagonalise it. What are the energy eigenvalues? Plot the probability of measuring each possible value of energy. (Measure energy in units of $\frac{h^2}{mL^2}$.) Compute the expected energy $\langle E\rangle$ and compare with the classical value.

   (g) Apply the time evolution matrix $\hat{T}(t) = e^{-i\hat{H}t/\hbar}$ to plot the Gaussian wavefunction at later times. You can also make an animation (see the "likelihood fitting" section of this notebook for an example). Does it behave as you expect? Does the energy distribution change with time? (Measure time in units of $\frac{mL^2}{h}$.)

   (h) Now let's add two potential barriers of height V_0 and width $\frac{L}{10}$ to create two equal intervals separated by finite potential walls, set $V(x) = V_0$ for $0 < x < \frac{L}{10}$ and $\frac{L}{2} < x < \frac{3L}{5}$ and $V(x) = 0$ everywhere else. Choose $V_0 = \frac{p_0^2}{m}$, about double the energy of the Gaussian wavepacket. Repeat the above and compare with a classical particle. Plot the probability of finding the particle in the other region as a function of time.

   (i) Repeat for larger values of N. We expect to recover the continuous case as $N \to \infty$. Do your plots change much as you increase N? Does $N = 200$ approximate the continuum well?

If you're stuck and would like some hints, or if you'd like to play around with the code without writing it all yourself, you can look at my solution in this notebook. To submit your work, compile it as a PDF (in Jupyter, this can be done from File; Download as; PDF via HTML) and merge it with the rest of your submission (there are several websites that do this).