Quantum Mechanics II: Week 2

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Aarhus University — September 4, 2018

Brief recap of lecture

At the lecture I covered how to represent quantum mechanical concepts on a computer. Starting from a discussion of the abstract state $|\alpha\rangle$ we saw that to obtain *wave functions* in for example the x- and p-representation by $\psi_\alpha(x) = \langle x|\alpha\rangle$ and $\phi_\alpha(p) = \langle p|\alpha\rangle$. The two wave function representations turns out to be related through Fourier transforms:

$$\phi_\alpha(p) = \mathcal{F}\left[\psi_\alpha(x)\right], \qquad \psi_\alpha(x) = \mathcal{F}^{-1}\left[\phi_\alpha(p)\right] \tag{0.1}$$

Upon discretizing the x-axis in N points we found that:

a) Wave functions $\psi_\alpha(x)$ turn into vectors $\vec{\psi}_\alpha \in \mathbb{C}^N$ (the same ofcourse goes for $\phi_\alpha(p)$)

b) Operators $\hat{A}$ turn into matrices $\mathbf{A} \in \mathbb{C}^{N\times N}$

The Hamiltonian operator $\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2} + \hat{V}(\hat{x})$ also has to be expressed in either the x- or p-representation.

The matrix elements of $\hat{H}$ in the x-representation is calculated in the usual way by

$$\mathbf{H}_{i,j} = \langle x_i|\hat{H}|x_j\rangle = \langle x_i|\hat{T}|x_j\rangle + \langle x_i|\hat{V}(\hat{x})|x_j\rangle = \langle x_i|\hat{T}|x_j\rangle + V(x_i)\delta(x_i - x_j)$$

where we used the property $\hat{V}(\hat{x}_i)\,|x\rangle = V(x_i)\,|x\rangle$ and orthonormality of the x-basis elements $\langle x_i|x_j\rangle = \delta(x_i - x_j)$ [1]. This means that $\mathbf{V}$ is diagonal in the x-representation.
To find the matrix representation of the kinetic energy, $\mathbf{T}$, we performed Taylor expansions of ψ around $x \pm \Delta x$ to orders Δx^3 and discarded higher order terms (using the notation $\cdots + \mathcal{O}(\Delta x^4)$). We then added the two expansions $\psi(x + \Delta x) + \psi(x - \Delta x)$

$$\psi''(x) \approx \frac{\psi(x - \Delta x) - 2\psi(x) + \psi(x + \Delta x)}{\Delta x^2} + O(\Delta x^4) \tag{0.2}$$

We then imposed the discretization of x such that $x_{i\pm1} = x_i + \Delta x$ and employed hard boundary conditions and found that $\mathbf{T}$ has a tri-diagonal structure.

In total, the Hamiltonian operator represented in the x-representation reads:

$$\mathbf{H} = \mathbf{T} + \mathbf{V} = -\frac{1}{2\Delta x^2}\begin{bmatrix} -2 & 1 & \dots & 0 & 0 \\ 1 & \ddots & \ddots & & \vdots \\ \vdots & \ddots & -2 & \ddots & \vdots \\ 0 & & \ddots & \ddots & 1 \\ 0 & 0 & \dots & 1 & -2 \end{bmatrix} + \begin{bmatrix} V(x_1) & 0 & \dots & \dots & 0 \\ 0 & \ddots & & & \vdots \\ \vdots & & V(x_i) & & \vdots \\ \vdots & & & \ddots & 0 \\ 0 & \dots & \dots & 0 & V(x_N) \end{bmatrix} \tag{0.3}$$

[1] In the discretized language the Dirac delta function becomes a Kronecker delta, $\delta(x_i - x_j) \to \delta_{i,j}$.

Time evolution is performed using the time evolution operator. For example,

$$\psi_\alpha(x, t + \Delta t) = \hat{U}(\Delta t)\psi_\alpha(x, t) = e^{-i\hat{H}\Delta t}\psi_\alpha(x, t) \tag{0.4}$$

or in matrix form

$$\vec{\psi}_\alpha(t + \Delta t) = \mathbf{U}(\Delta t)\vec{\psi}_\alpha(t + \Delta t) = e^{-i\mathbf{H}\Delta t}\vec{\psi}_\alpha(t) \tag{0.5}$$

where the definition for the operator exponential (and similar for the matrix exponential) is

$$\hat{U} = e^{-i\hat{H}\Delta t} = \sum_{k=0}^{\infty} \frac{(-i\hat{H}\Delta t)^k}{k!} \tag{0.6}$$

Using the series expansion above we found

$$e^{-i\hat{H}\Delta t} \approx e^{-i\hat{T}\Delta t}e^{-i\hat{V}\Delta t} + \mathcal{O}(\Delta t^2) \tag{0.7}$$

$$e^{-i\hat{H}\Delta t} \approx e^{-i\frac{\hat{V}}{2}\Delta t}e^{-i\hat{T}\Delta t}e^{-i\frac{\hat{V}}{2}\Delta t} + \mathcal{O}(\Delta t^3) \tag{0.8}$$

The $\hat{V}$ exponential is easy to calculate in the x-representation since it is diagonal, but the $\hat{T}$ exponential is tri-diagonal in the x-representation. However, $\hat{T}$ is diagonal in the p-representation. By performing Fourier transforms, we can have both operators being easily exponentiated in the space in which they are diagonal. This leads to the **split-step Fourier method**, which in the discretized notation becomes:

$$\vec{\psi}(t + \Delta t) = e^{-i\frac{\mathbf{V}(t)}{2}\Delta t}[\mathcal{F}^{-1}[e^{-i\mathbf{T}\Delta t}[\mathcal{F}[e^{-i\frac{\mathbf{V}(t)}{2}\Delta t}[\vec{\psi}(t)]]]]] \tag{0.9}$$

1 Problems

1.1 Theoretical exercises

Question 1 : Higher order terms in the kinetic energy matrix

Perform the Taylor expansion of $\psi(x)$ at points $x \pm \Delta$ as in the lecture, but keep terms up to order $\mathcal{O}(\Delta x^6)$. Assuming hard boundary conditions, find the matrix representation of the kinetic energy matrix $\mathbf{T}$.

Question 2 : Splitting of the operator exponential

At the lecture I claimed without proof that

$$e^{-i\hat{H}\Delta t} \approx e^{-i\frac{\hat{V}}{2}\Delta t}e^{-i\hat{T}\Delta t}e^{-i\frac{\hat{V}}{2}\Delta t} + \mathcal{O}(\Delta t^3)$$

Prove this identity by expanding the exponentials in $e^{-i\hat{H}\Delta t}$ and $e^{-i\frac{\hat{V}}{2}\Delta t}e^{-i\hat{T}\Delta t}e^{-i\frac{\hat{V}}{2}\Delta t}$ respectively. Group the terms by their order in Δt and show that they agree up to order $\mathcal{O}(\Delta t^3)$. (*Hint*: defining $q \equiv -i\Delta t \propto \Delta t$ may reduce clutter)

1.2 Numerical exercises (Quantum Composer)

We did not have time to cover much of the program at the Tuesday lecture, but try to build the scenes from scratch. I have created some solutions you can look at if you get stuck. In particular I describe how one can use Scopes in the program to make it look a lot cleaner. You are also welcome to contact me by email or catch me at my office (see title). Also, I recommend using a mouse for this program.

Question 3 : Spectra of different potentials

Previously in your studies you have looked at the harmonic oscillator potential and the infinite square well. The potentials and associated analytical eigen energies solutions are

$$V_{ho}(x) = 0.5\omega^2 x^2, \qquad E_n = \omega(n + \frac{1}{2}) \sim n, \qquad n = 0, 1, 2, \ldots \tag{1.1}$$

$$V_{well}(x) = \begin{cases} 0, & \text{if} \quad -\frac{L}{2} \leq x \leq \frac{L}{2} \\ \infty, & \text{otherwise} \end{cases}, \qquad E_n = \frac{n^2\pi^2}{2L^2} \sim n^2, \qquad n = 1, 2, 3, \ldots \tag{1.2}$$

(a) Set up a scene that calculates the first 5 eigenstates and eigenenergies of $H = T + V_{ho}$.

(1) Create a 'Spatial Dimension' node and a 'Potential' node and connect them.

(2) The default potential is already '$0.5 * a * x^2$'. To represent the frequency value ω, use a 'Scalar' node and attach it to the 'a' input of the 'Potential' node. Set it to a sensible value, e.g. 1.

(3) Create a 'Hamiltonian' node and connect the 'Potential'.

(4) Create an 'Energy Plot' node and connect the 'Hamiltonian' and 'Potential'. You may have to tick some of the option boxes in the right of the node to display the states and energies. This is a great way of visualizing the eigensolutions of the system.

(5) To get numerical values for the energies, create a 'Spectrum' node and connect the 'Hamiltonian'. Create 5 'Get Eigenvalue' nodes and attach each of them to the output of the 'Spectrum', each with a different value of 'n' specified inside them.

(6) Compare the analytical results stated above to the numerical values found in Composer. Do they agree? Try adjusting the parameters in your simulation, e.g. x_{min}, x_{max}.

(b) Do the same as in (a), but for $H = T + V_{well}$. You can re-use/copy the scene for the harmonic oscillator and change the potential expression to 'infinite(-a/2,+a/2)'. You will probably experience less accurate results than in (a) – why do you think that is? (*Hint*: You can zoom in on the plots by scrolling the mouse wheel, try looking at the wave function near the boundaries of the wall)

(c) Consider now the potential $V_{quartic} = ax^4$. This potential does not have exact analytical solutions, but we can still calculate it numerically. How does the energies roughly scale with n? That is, $E_n \sim ?$. Is the scaling linear, sub-linear, super-linear, or something else?

(d) Do the same as in (c), but for the potential $V = a \cdot abs(x)$, where $abs(x) = |x|$.

(e) Briefly comment qualitatively on the relative energy scaling behaviour of the 4 different potentials by looking at their shapes. Can you now better understand the scaling behaviour of the potentials in question (c), (d)?

Question 4 : Time evolution of an initially displaced oscillator ground state

Consider a harmonic oscillator ground state that has been displaced to x_c:

$$\phi_0(x; x_c) = A \cdot e^{-\frac{\omega(x-x_c)^2}{2}}$$

where A is a normalization constant. We will take this as our initial state $\psi(x, t = 0) = \phi_0(x; x_c)$ and see how it evolves in time in the harmonic potential $V(x) = 0.5\omega^2 x^2$.

(a) Setup a scene with 'Spatial Dimension', 'Potential' (which is harmonic centered on 0), 'Scalar' (for the frequency), 'Hamiltonian', and connect them.

(b) Now we create $\phi_0(x; x_c)$, either analytically or by numerical diagonalization:

- **Analytically**: Create an 'Analytic wave function' and enter the expression given for $\phi_0(x; x_c)$ above. Parametrize x_c by a 'Scalar' node, similar to what we did for the frequency. If you tick off the 'Normalize output' box, the wave function is automatically normalized.
- **Numerically:** Create a new harmonic potential centered on x_c, that is $V(x; x_c) = 0.5\omega(x - x_c)^2$ – the ground state of this potential is exactly $\phi_0(x; x_c)$. We now have 2 potentials; 1 we use for time evolution, and one we use to create the initial state. Create a new 'Hamiltonian', 'Spectrum', and 'Linear combination'. Connect them using the displaced 'Potential'. The default behaviour of 'Linear Combination' is to output the ground state of the input, which in this case is $\phi_0(x; x_c)$.

Ideally you should check that both of these approaches give the same wave function. You can compare them by looking at their overlap, $o = \langle \phi_0^{\text{num}}(x; x_c) | \phi_0^{\text{ana}}(x; x_c) \rangle$, or their fidelity $F = |o|^2$, and verify it is 1. (Fidelity is nicer to work with since it is a real number, while o is complex)

(c) Now we are ready for time evolution. The 'Time Evolution' node takes a single step in time of length Δt, but we want to take many such steps in succession. To do this, create a 'For Loop' Scope (you can find it under the Misc category). Put 'Time Evolution' inside the 'For Loop', and create boundary nodes of the 'Hamiltonian, the initial wave function 'ψ', and the 'Potential' – see my general comment in my scenes on boundary nodes and scopes.

(d) Create three 'Scalar' nodes and attach them to the special 'For Loop' boundary node. These three numbers defines the loop conditions (from, to, increment). Also create a seperate boundary node of the 'Scalar' node representing the increment. You can rename this boundary node to 'dt', if you like.

(e) Connect all necessary parts to the 'Time Evolution'.

(f) Create a 'Position Plot', and attach to it the potential and the output of the 'Time Evolution'. Now you can press the Play button (green arrow in top left corner), and loop will start running! Note: you cannot modify the scene when running the loops; you must reset it by clicking the Reset button (red circle next to Play button).

(g) Describe qualitatively the motion of the wave function.

(h) Create a 'Fidelity' node and attach the output of the 'Time Evolution' and the initial state to it. This quantity is also the norm square of the *correlation-amplitude* (see Sakurai). Create a 'Scalar Time Trace Plot'. Attach the output of the 'For Loop', called 'i', and the output of the fidelity. This will show you the fidelity as a function of time. You should see a periodic structure in time – argue why this happens.