PHY 303, I-Semester 2023/24, Assignment 4 solution

(1) Anharmonic oscillator [8pts]:

(a) The Hamiltonian for an oscillator of mass m with an anharmonic potential is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2 + \kappa x^4, \tag{1}$$

for $\kappa > 0$. Write this Hamiltonian in terms of the same ladder operators that we defined for the harmonic oscillator [4pts].

Solution: In this assignment solution we will use the alternate (and very common) notation for the ladder operators as $\hat{a}^+ = \hat{a}^\dagger$ and $\hat{a}^- = \hat{a}$,(respectively also called creation and annihilation operators in second quantization.... If confused just replace the ladder operators you are familiar with beneath). The $\hat{x}, \hat{p}$ can be written in the form of ladder operators as

$$\hat{x} = \bar{\sigma}(\hat{a} + \hat{a}^\dagger) \text{ where } \bar{\sigma} = \sqrt{\frac{\hbar}{2m\omega}} \tag{2}$$

$$\hat{p} = -i\frac{\hbar}{\bar{\sigma}}(\hat{a} - \hat{a}^\dagger) \tag{3}$$

Notes:

- This uses a re-definition of ladder operators in the lecture notes that happened on 9.9.23, please redownload. The previous ones only differ by a complex phase, but in Eq. (3) this is important.
- To save some writing we defined $\bar{\sigma} = \sigma/\sqrt{2}$, where $\sigma = \sqrt{\frac{\hbar}{m\omega}}$ is the usual ground-state width of the oscillator.

Thus, the terms in the Hamiltonian can be expanded by substituting the above expressions.

$$\hat{x}^4 = \bar{\sigma}^4[(\hat{a} + \hat{a}^\dagger)] \tag{4}$$

$$\begin{aligned}\hat{x}^4 = \bar{\sigma}^4 \Big[&\left(a^4 + a^3a^\dagger + a^2a^\dagger a + a^2a^{\dagger 2}\right) \\ &+ aa^\dagger\left(a^2 + a^\dagger a + aa^\dagger + a^{\dagger 2}\right) \\ &+ \left(a^\dagger a^3 + a^\dagger a^2 a^\dagger + a^\dagger a a^\dagger a + a^\dagger a a^{\dagger 2}\right) \\ &+ a^{\dagger 2}\left(a^2 + a^\dagger a + aa^\dagger + a^{\dagger 2}\right)\Big]\end{aligned} \tag{5}$$

Now, using the commutator $[\hat{a}, \hat{a}^\dagger] = 1$

$$\hat{x}^4 = \bar{\sigma}^4\left[\hat{a}^4 + \hat{a}^{\dagger 4} + 4\hat{a}^{\dagger 3}\hat{a} + 4\hat{a}^\dagger\hat{a}^3 + 6\hat{a}^{\dagger 2}\hat{a}^2 + 6(\hat{a}^2 + \hat{a}^{\dagger 2}) + 12\hat{a}^\dagger\hat{a} + 3\right] \tag{6}$$

Similarly,

$$\hat{x}^2 = \bar{\sigma}^2\left[\hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^{\dagger 2}\right] = \bar{\sigma}^2\left[\hat{a}^2 + 2\hat{a}\hat{a}^\dagger + 1 + \hat{a}^{\dagger 2}\right] \tag{7}$$

$$\hat{p}^2 = -\frac{\hbar^2}{\bar{\sigma}^2}\left[\hat{a}^2 - \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} + \hat{a}^{\dagger 2}\right] = -\frac{\hbar^2}{\bar{\sigma}^2}\left[\hat{a}^2 - 2\hat{a}\hat{a}^\dagger - 1 + \hat{a}^{\dagger 2}\right] \tag{8}$$

Thus the Hamiltonian can now be expressed in terms of the ladder operators (the first two terms were already provided in the lecture notes):

$$\hat{H} = \hbar\omega \left[\hat{a}^\dagger \hat{a} + \frac{1}{2}\right] + \kappa\bar{\sigma}^4 \left[\hat{a}^4 + \hat{a}^{\dagger 4} + 4\hat{a}^{\dagger 3}\hat{a} + 4\hat{a}^\dagger \hat{a}^3 + 6\hat{a}^{\dagger 2}\hat{a}^2 + 6(\hat{a}^2 + \hat{a}^{\dagger 2}) + 12\hat{a}^\dagger \hat{a} + 3\right]. \tag{9}$$

(b) Suppose the state of the particle in the anharmonic oscillator Eq. (1) is described by the wavefunction

$$\Psi(x) = \frac{1}{(\pi\sigma^2)^{1/4}} e^{-\frac{x^2}{2\sigma^2}}, \tag{10}$$

where $\sigma = \sqrt{\hbar/(m\omega)}$. Evaluate the expectation value of energy $\langle \hat{H} \rangle$ in state (10) for Hamiltonian (1) using two different methods: (i) Writing the corresponding integration over x and finding the result of the integral. (ii) Using your result of (a), writing $\Psi(x)$ and all functions appearing in an integral abstractly in terms of harmonic oscillator eigenstates $\phi_n(x)$ [from Eq. (2.65) of the lecture, but you do not need these details] [4pts].

Solution: (i) We know that the wavefunction given, $\psi(x) = \phi_0(x)$, is the zeroth eigenstate for the harmonic oscillator. (See lecture notes) We can use that to write:

$$\langle \hat{H} \rangle = \int_{-\infty}^{\infty} \psi(x)^\dagger \hat{H} \psi(x) dx \tag{11}$$

$$\langle \hat{H} \rangle = \int_{-\infty}^{\infty} \psi(x)^\dagger (\hat{H}_{harmonic} + \kappa \hat{x}^4) \psi(x) dx \tag{12}$$

$$\langle \hat{H} \rangle = \frac{\hbar\omega}{2} + \kappa \int_{-\infty}^{\infty} \frac{1}{(\pi\sigma^2)^{1/2}} x^4 \exp(-\frac{x^2}{\sigma^2}) dx \tag{13}$$

$$\langle \hat{H} \rangle = \frac{\hbar\omega}{2} + \kappa \frac{3\sigma^2}{4} \tag{14}$$

$$\langle \hat{H} \rangle = \frac{\hbar\omega}{2} + \frac{3\kappa\hbar}{4m\omega} \tag{15}$$

(ii) We can use again that the given state is an eigenstate of the Harmonic oscillator Hamiltonian, which allows us to use the relations in Eq. (2.55) of the lecture notes, and $\hat{a}\phi_0 = 0$. These help us to comfortably evaluate the second term of the

Hamiltonian:

$$\langle \hat{H} \rangle = \int dx \phi_0^*(x) \hat{H} \phi_0(x) dx \tag{16}$$

$$\begin{aligned}\langle \hat{H} \rangle &= \int dx \phi_0^* \hbar\omega (\hat{a}^\dagger \hat{a} + \frac{1}{2}) \phi_0 \\ &+ \kappa \frac{\hbar}{4m\omega} \int dx \phi_0^* \left(\hat{a}^4 + \hat{a}^{\dagger 4} + 4\hat{a}^{\dagger 3}\hat{a} + 4\hat{a}^\dagger \hat{a}^3 + 6\hat{a}^{\dagger 2}\hat{a}^2 + 6(\hat{a}^2 + \hat{a}^{\dagger 2}) + 12\hat{a}^\dagger \hat{a} + 3 \right) \phi_0\end{aligned} \tag{17}$$

$$= \frac{\hbar\omega}{2} + \kappa \frac{\hbar}{4m\omega} \int dx \phi_0^* \left(0 + c_1\phi_4 + 0 + 0 + 6 \times 0 + 6(0 + c_2\phi_2) + 12 \times 0 + 3\phi_0\right) \tag{18}$$

$$\langle \hat{H} \rangle = \frac{\hbar\omega}{2} + \frac{3\hbar\kappa}{4m\omega}. \tag{19}$$

Above c_k are numerical constants coming from the $\sqrt{n(+1)}$ prefactors in Eq. (2.65) which are not important since they drop out in the last line, where we use that oscillator eigenfunctions of different n are orthogonal.

Important Point: Beware of the potential confusion that the ϕ_n used throughout are eigenstates of the harmonic oscillator, not the anharmonic one for which the Hamiltonian is Eq. (1). Doing that can sometimes be useful, due to the nice properties of harmonic oscillator eigenstates and ladder operators. Note that we have not actually found the actual eigenstates or eigenenergies of the Hamiltonian (1).

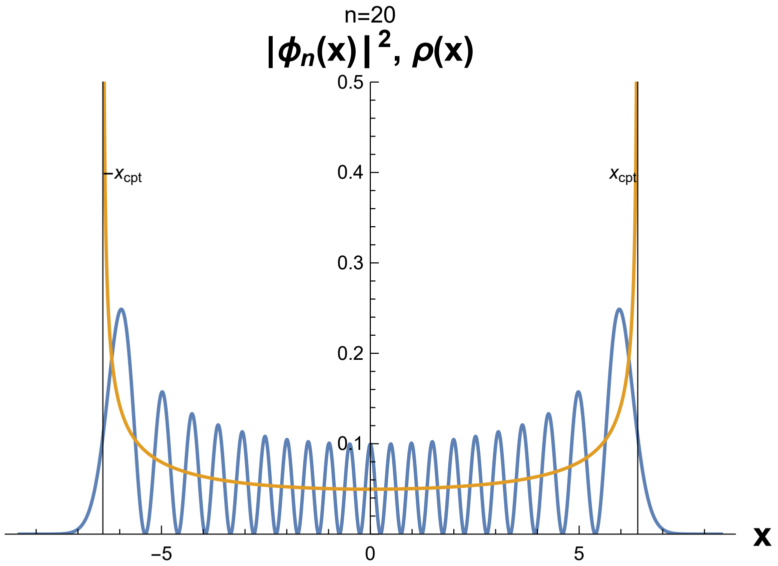

Figure 1: Position probability density in a high lying SHO state ($n = 20$) and the classical probability distribution. We see that the average amplitude of the quantum state precisely follows $\rho(x)$.

(2) Correspondence principle [10pts]:

(a) Make your own exact figure for the drawing in example 15 in mathematica. In particular find x_{ctp} in term of the oscillator energy, then choose an energy E corresponding to a high lying harmonic oscillator state (say e.g. $n_0 = 20$) and plot $\rho(x)$ on top of $|\phi_{n_0}(x)|^2$ [5 pts].

Solution: The main part is finding out x_{ctp} defined in lecture notes and noticing that it is equal to the oscillation amplitude. So we have $\frac{1}{2}m\omega^2 x_{ctp}^2 = E$. Using this and the definition of $\rho(x) = \frac{1}{\pi\omega\sqrt{x_{ctp}^2 - x^2}}$ we could find the classical probability distribution. The Mathematica file `Assignment4_program_solution_v2.nb` *contains the solution; by running it for $n = 20$, we reproduce the plot given in example 15 shown in figure 1.*

(b) Now take the average of the probability density over a few states in the vicinity of E (say $n \pm 2$) thus calculating $\bar{\rho}(x) = \sum_{n;|n-n_0|\leq 2} |\phi_n(x)|^2$ and compare again. Discuss what you find. Where does it agree, where does it not agree? How does agreement change when n_0 is varied? [5 pts].

Solution: See `Assignment4_program_solution_v2.nb` *for the solution, also shown in Fig. 2. We see that they both agree quite well in the central range, and as n_0 is increased the agreement in the centre range increases even further. However close to the classical turning point x_{ctp} deviations remain For $|x| < |x_{ctp}|$ these might disappear if we average over a larger range of oscillator states, for $|x| > |x_{ctp}|$ the two distributions can never agree, since the classical particle cannot reach there.*

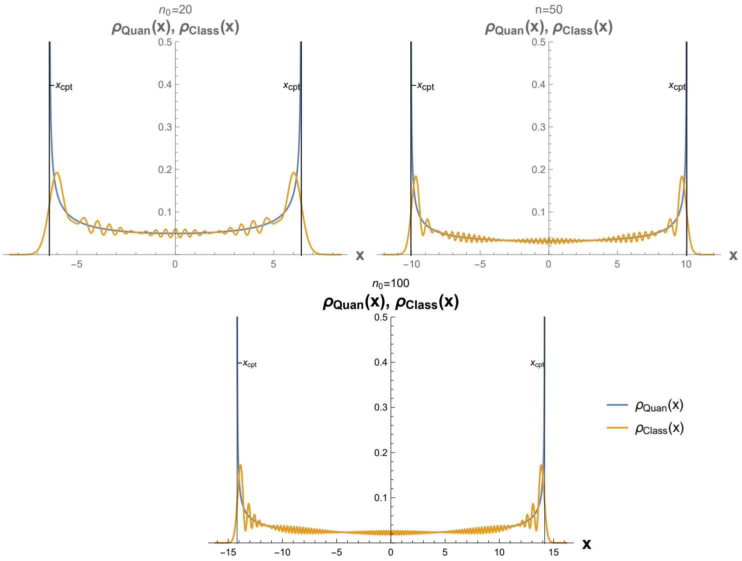

Figure 2: The classical and quantum probability distribution, when averaging the latter over 5 adjacent oscillator quantum numbers, $[n_0-2, n_0-1, n_0, n_0+1, n_0+2]$. We see that they both agree quite well, and as n_0 is increased the agreement in the centre range increases even further.

(3) Harmonic oscillator [10 pts]

(a) Find the expectation values and uncertainties of $\hat{x}$ and $\hat{p}$ in each of the eigenstates of the Harmonic oscillator, and discuss the product of both uncertainties. [6pts]

Solution:

$$\hat{x} = \bar{\sigma}(\hat{a} + \hat{a}^\dagger) \quad \bar{\sigma} = \sqrt{\frac{\hbar}{2m\omega}} \tag{20}$$

$$\hat{p} = -i\frac{\hbar}{\bar{\sigma}}(\hat{a} - \hat{a}^\dagger) \tag{21}$$

$$\langle \hat{x} \rangle = \int \sigma \phi_n^* (\hat{a} + \hat{a}^\dagger) \phi_n dx \tag{22}$$

$$\langle \hat{x} \rangle = \bar{\sigma}(\sqrt{n}\delta_{n,n-1} + \sqrt{n+1}\delta_{n,n+1}) = 0 \tag{23}$$

$$\langle \hat{x}^2 \rangle = \bar{\sigma}^2 \int \phi_n^* (\hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + \hat{a}^{\dagger 2}) \phi_n dx \tag{24}$$

$$\langle \hat{x}^2 \rangle = \bar{\sigma}^2 (n + 1 + n)\delta_{n,n} = \frac{\hbar}{m\omega}(n + \frac{1}{2}) \tag{25}$$

$$\sigma_x = \sqrt{\frac{\hbar}{m\omega}(n + \frac{1}{2})} \tag{26}$$

$$\langle \hat{p} \rangle = -i\frac{\hbar}{\bar{\sigma}} \int \phi_n^* (\hat{a} - \hat{a}^\dagger) \phi_n = -i\frac{\hbar}{\bar{\sigma}}(\sqrt{n}\delta_{n,n-1} - \sqrt{n+1}\delta_{n,n+1}) = 0 \tag{27}$$

$$\langle \hat{p}^2 \rangle = \frac{-\hbar^2}{\bar{\sigma}^2} \int \phi_n^* (\hat{a}^2 - \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} + \hat{a}^{\dagger 2}) \phi_n \tag{28}$$

$$\langle \hat{p}^2 \rangle = \frac{-\hbar^2}{\bar{\sigma}^2}(-(n+1)-n) = \hbar m\omega(n+\frac{1}{2}) \tag{29}$$

$$\sigma_p = \sqrt{\hbar m\omega(n+\frac{1}{2})} \tag{30}$$

The uncertainty product is thus:

$$\sigma_x\sigma_p = \hbar(n+\frac{1}{2}). \tag{31}$$

We see that it takes the minimal value allowed by Heisenberg's uncertainty principle only at $n = 0$, while for all the higher n it exceeds the limit, linearly increasing in n.

(b) From that show the virial theorem $\langle \hat{T} \rangle = \langle \hat{V} \rangle$ relating the expectation values of kinetic and potential energies. [3pts]
Solution:

$$\langle \hat{T} \rangle = \frac{1}{2m}\langle \hat{p}^2 \rangle = \frac{\hbar\omega}{2}(n+\frac{1}{2}) \tag{32}$$

$$\langle \hat{V} \rangle = \frac{m\omega^2}{2}\langle \hat{x}^2 \rangle = \frac{\hbar\omega}{2}(n+\frac{1}{2}) \tag{33}$$

$$\therefore \langle \hat{T} \rangle = \langle \hat{V} \rangle \tag{34}$$

(c) Now find the expectation value of the position in the superposition state $\Psi(x) = (\phi_0(x)+\phi_1(x))/\sqrt{2}$ at all times $t > 0$. [3pts] With which frequency does it oscillate?
Solution: Using the time evolution of the superposition state $\psi(x,t) = e^{-iE_0t/\hbar}\phi_0(x)/\sqrt{2} + e^{-iE_1t/\hbar}\phi_1(x)/\sqrt{2}$

$$\langle \hat{x} \rangle = \int \psi^*(x,t)\bar{\sigma}(\hat{a}+\hat{a}^\dagger)\psi(x,t) \tag{35}$$

$$\langle \hat{x} \rangle = \frac{\bar{\sigma}}{2}\int (e^{iE_0t/\hbar}\phi_0 + e^{iE_1t/\hbar}\phi_1)(\hat{a}+\hat{a}^\dagger)(e^{-iE_0t/\hbar}\phi_0(x) + e^{-iE_1t/\hbar}\phi_1(x)) \tag{36}$$

$$\langle \hat{x} \rangle = \frac{\bar{\sigma}}{2}(e^{-i(E_1-E_0)t/\hbar} + e^{-i(E_0-E_1)t/\hbar}) = \bar{\sigma}\cos((E_1-E_0)t/\hbar) \tag{37}$$

$$\langle \hat{x} \rangle = \bar{\sigma}cos(\omega t) \tag{38}$$

Thus the mean position oscillates with frequency ω as expected for the Harmonic oscillator.

(4) Quantum dynamics: [10pts] The code `Assignment4_program_draft_v1.nb` is set up to solve the TDSE. You only have to define a potential $V(x)$ and an initial state $\Psi(x, t = 0)$ at the indicated places.

Design your own question from here. I want you to: **(a)** make thorough contact with at least one concept of quantum dynamics encountered in the lecture so far. You can reproduce an example, assignment or tutorial question, analytical result, anything from the selection of week 3-5 problems. The only constraint is to look at genuine dynamics, i.e. something significant should vary in time, do not just look at a stationary state (even though you might want to do that for testing and warm up). **(b)**: Then extend that concept towards the unknown (by adding multiple copies of some feature in the potential, combining two features etc.). For both make many plots, verify whichever analytical results you may know, and extensively analyse your findings.

Please be careful about the following list of pitfalls

- We set $\hbar = m = 1$ to avoid any large unitful numbers. Thus mainly use numbers "of order one (0.1-10)" for definitions of potentials, initial states, spatial ranges and times.
- Numerics does not like infinities, hence if you want to use $V(x) \to \infty$, just make it larger than everything else (e.g. 100).
- Numerics also does not like discontinuities, rather use $(\tanh(x/\xi) + 1)/2$ with finite and visible ξ than $\theta(x)$ (Heaviside step function).
- The calculation will take longer, if you do brutal things to your wavefunction, or you go towards very "classical states" (very small quantum wavelength relative to $L_{\max}$). Best avoid these cases. If the solution has not been calculated after a few minutes, best change parameters. The more brutal dynamics you do, the more points you need (Increase `MinPoints`, `MaxPoints`).
- One way to see if anything goes wrong from the start, is set t_{fin} to a very low value.
- avoid wavefunctions hitting the edge of your domain $-L_{\max}$ or $L_{\max}$. If that happens the calculation ceases to make sense. To avoid it, enlarge $L_{\max}$, add a potential or decrease t_{fin}.
- Any numerical solution can be wrong. To make sure it is converged in terms of discretisation, check it does not change when you increase the number of points (`MinPoints`, `MaxPoints`) or increase the tolerances (`AccuracyGoal`, `PrecisionGoal`). Other good checks are whether energy $\langle \hat{H} \rangle$ or normalisation of the wavefunction stay conserved.

After the assignment, let us know about any additional pitfalls you encountered that were not listed here.

Solution: See ***Assignment4_program_solution_v2.nb*** *for the solution. We have used the program to solve for the wobbling harmonic oscillator, which we have seen previously in tutorial 3 Question 2.*

(5) Schrödinger's equation in momentum space: [6 pts] Suppose a particle of mass m can move in one dimension under the influence of the potential $V(x)$. In Eq. (2.93) of the lecture, we introduced the momentum space representation $\tilde{\phi(k)}$ of the wavefunction.

(a) Find also a momentum space representation of the TISE which a momentum space wavefunction has to fulfill.[1] [3pts]

(b) Discuss the physical meaning of each term. Discuss what happens to the momentum probability distribution for the case $V(x) = 0$, or $V(x) \neq 0$. You may want to consider the change of the momentum space wavefunction during an infinitesimal time element dt [3pts].

Solution: 5(a) We start with the TDSE in position space

$$i\hbar \frac{\partial}{\partial t}\phi(x) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\phi(x). \tag{39}$$

To turn this into an equation for the momentum space wavefunction

$$\tilde{\phi}(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx e^{-i\frac{p}{\hbar}x}\phi(x), \tag{40}$$

we take the Fourier transform of both sides of Eq. (39). Let us do this step by step:

$$\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx e^{-i\frac{p}{\hbar}x}\left[i\hbar\frac{\partial}{\partial t}\phi(x)\right] = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx e^{-i\frac{p}{\hbar}x}\left[\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\phi(x)\right] \tag{41}$$

$$i\hbar\frac{\partial}{\partial t}\underbrace{\left(\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx e^{-i\frac{p}{\hbar}x}\phi(x)\right)}_{=\tilde{\phi}(p)} = -\frac{\hbar^2}{2m}\frac{1}{\sqrt{2\pi\hbar}}\underbrace{\int_{-\infty}^{\infty} dx e^{-i\frac{p}{\hbar}x}\frac{\partial^2}{\partial x^2}\phi(x)}_{\overset{I.b.P.}{=}\int_{-\infty}^{\infty} dx \underbrace{\frac{\partial^2}{\partial x^2}e^{-i\frac{p}{\hbar}x}}_{=(-ip/\hbar)^2 e^{-i\frac{p}{\hbar}x}}\phi(x)} + \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx\, e^{-i\frac{p}{\hbar}x}V(x)\phi(x). \tag{42}$$

To change the first term on the right hand side we used integration by parts twice, not getting any boundary terms since $\phi(x)$ and $\phi'(x)$ must vanish for $x \to \pm\infty$. Finally we use again the definition Eq. (40), and its inverse (Eq. (2.92) of lecture) to reach:

$$i\hbar\frac{\partial}{\partial t}\tilde{\phi}(p) = \frac{p^2}{2m}\tilde{\phi}(p) + \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx\, e^{-i\frac{p}{\hbar}x}V(x)\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dp'\, e^{i\frac{p'}{\hbar}x}\tilde{\phi}(p'). \tag{43}$$

[1]The TISE 1(.62) that we have considered so far is said to be in the "position space representation". Its momentum space variant should only have $i\hbar\frac{\partial}{\partial t}\phi(\tilde{k},t) = \cdots$ as the left hand side.

Note that we had to be careful not to use p as the integration variable for the inverse FT, since it is already used in the rest of the equation. This is why we used p' instead. We finally define the Fourier transformed potential

$$\tilde{V}(p-p') = \frac{1}{\sqrt{2\pi\hbar}} \int dx V(x) e^{-i\frac{(p-p')}{\hbar}x} \tag{44}$$

so that we can write

$$i\hbar\frac{\partial}{\partial t}\tilde{\phi}(p) = \frac{p^2}{2m}\tilde{\phi}(p) + \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp'\, \tilde{V}(p-p')\tilde{\phi}(p'). \tag{45}$$

5(b): The first term represents the contribution from kinetic energy, which we say is "diagonal" in the momentum representation: It just multiplies $\phi(p)$ with p^2, for which we do not need to know $\phi(p')$ for any $p' \neq p$. In contrast for calculating $\frac{\partial^2}{\partial x^2}\phi(x)$ in the position representation, you DO need to know $\phi(x)$ at $x' \neq x$ (to calculate the derivative). The second term, from the potential energy was local in the position representation ($V(x)\phi(x)$), but has now become nonlocal. We need to know $\tilde{\phi}(p')$ at $p' \neq p$. The equation Eq. (45) can guide us to the following interpretation of the Fourier transformed potential $\tilde{V}(p-p')$. Since $\tilde{V}(p-p')$ governs how much $\tilde{\phi}(p)$ changes when $\tilde{\phi}(p')$ is nonzero, it must contain information about how likely the momentum-transfer from p' to p is, due to the potential $V(x)$.