Physics 731 Lecture Notes 4

Summary: Time Evolution

This is a summary of the lectures on time evolution in quantum mechanics, including the propagator for time-independent Hamiltonians, and one-dimensional scattering theory. Much of this material is in Chapter 2 of Sakurai's text (all editions). For more information regarding the wavepacket treatment of scattering in one dimension, see Shankar 5.4, and Norsen at al., arXiv:0808.3566 [quant-ph].

Time evolution operator. In the Schrödinger picture, the state vector $|\alpha, t_0\rangle$ specified at some initial time t_0 evolves with time. This time evolution can be expressed as

$$|\alpha, t_0; t\rangle = U(t, t_0)|\alpha, t_0\rangle, \tag{1}$$

in which $U(t, t_0)$ is the time evolution operator. To preserve the norm of the state, $U(t, t_0)$ must be unitary:

$$U(t, t_0)^\dagger U(t, t_0) = \mathbb{1}. \tag{2}$$

$U(t, t_0)$ must also satisfy the composition property that for $t_2 > t_1 > t_0$,

$$U(t_2, t_0) = U(t_2, t_1)U(t_1, t_0). \tag{3}$$

In addition,

$$U(t_0, t_0) = \mathbb{1}. \tag{4}$$

Given these properties, we can see by examining infinitesimal time translations that the time evolution operator $U(t, t_0)$ satisfies the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}U(t, t_0) = HU(t, t_0), \tag{5}$$

in which H is the Hamiltonian. When the operator relation Eq. (5) acts on a state $|\alpha, t_0\rangle$, we obtain the more familiar version of the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\alpha, t_0; t\rangle = H|\alpha, t_0; t\rangle. \tag{6}$$

The operator $U(t, t_0)$ is a Green's function, and is also known as the propagator.

Given the form of the Hamiltonian H, there are three possible general forms for $U(t, t_0)$:

1. H is *time-independent*. The solution to Eq. (5) is

$$U(t, t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}. \tag{7}$$

2. H is *time-dependent*, but *commutes with itself at later times*. In this case, the solution to Eq. (5) is

$$U(t, t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t} H(t')dt'}. \tag{8}$$

3. H is *time-dependent*, and it *does not commute with itself at later times*. In this case, operator ordering is of critical importance. The formal solution is the Dyson series:

$$U(t, t_0) = \mathbb{1} + \sum_{n=1}^{\infty}\left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_{n-1}} dt_n H(t_1)H(t_2)\ldots H(t_n). \tag{9}$$

For now, we will focus on case 1 (time-independent H). Let us also, for simplicity, set $t_0 = 0$. It is convenient to write $U(t,0)$ in terms of the basis of eigenstates of H:

$$U(t,0) = e^{-iHt/\hbar} = \sum_n e^{-iE_n t/\hbar} |n\rangle\langle n|. \tag{10}$$

Here the expression involves a sum if the spectrum of H is discrete, and an integral if the spectrum of H is continuous. With this result, given the initial state $|\alpha, t_0 = 0\rangle = |\alpha(0)\rangle$,

$$|\alpha(0)\rangle = \sum_n |n\rangle\langle n|\alpha, 0\rangle = \sum_n c_n(0)|n\rangle, \tag{11}$$

the time-evolved state $|\alpha, t_0 = 0; t\rangle = |\alpha(t)\rangle$ is

$$|\alpha(t)\rangle = \sum_n c_n(0) e^{-iE_n t/\hbar}|n\rangle = \sum_n c_n(t)|n\rangle. \tag{12}$$

Hence, if the initial state is one of the eigenstates of H, time evolution results in an (unobservable) global phase. However, for a superposition of eigenstates of H, time evolution results in nontrivial relative phases. If we now do measurements of an operator A on any state, we have the following two cases to consider:

- $[A, H] = 0$. The eigenstates of A are then also the eigenstates $|n\rangle$ of H, with $A|n\rangle = a_n|n\rangle$. Hence, for an arbitrary initial state $\langle A\rangle$ is constant:

$$\langle\alpha(t)|A|\alpha(t)\rangle = \sum a_n |c_n(t)|^2 = \sum a_n |c_n(0)|^2 = \langle\alpha(0)|A|\alpha(0)\rangle. \tag{13}$$

- $[A, H] \neq 0$. Here generically $\langle A\rangle$ will have a complicated t dependence for an arbitrary initial state.

A useful example (covered in your text) is spin precession, *i.e.*, a spin $1/2$ particle in a uniform B field.

Propagator. Let us now look at the time evolution operator in position space. We will consider the Hamiltonian $H = \mathbf{p}^2/(2m) + V(\mathbf{x})$. Projecting Eq. (1) into the position eigenstate basis, we have the condition

$$\psi(\mathbf{x}, t) = \langle\mathbf{x}|\alpha, t\rangle = \sum_n e^{-iE_n(t-t_0)/\hbar}\langle\mathbf{x}|n\rangle\langle n|\alpha, t_0\rangle. \tag{14}$$

Inserting a complete set of $|\mathbf{x}'\rangle$ states, we obtain

$$\begin{aligned}
\psi(\mathbf{x}, t) &= \sum_n e^{-iE_n(t-t_0)/\hbar}\langle\mathbf{x}|n\rangle \int d^3x' \langle n|\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha, t_0\rangle \\
&= \int d^3x' \sum_n e^{-iE_n(t-t_0)/\hbar}\psi_n(\mathbf{x})\psi_n^*(\mathbf{x}')\psi(\mathbf{x}', t_0) \\
&= \int d^3x' K(\mathbf{x}, t; \mathbf{x}', t_0)\psi(\mathbf{x}', t_0),
\end{aligned} \tag{15}$$

in which

$$K(\mathbf{x}, t; \mathbf{x}', t_0) = \langle\mathbf{x}|U(t,0)|\mathbf{x}'\rangle = \sum_n e^{-iE_n(t-t_0)/\hbar}\psi_n(\mathbf{x})\psi_n^*(\mathbf{x}'). \tag{16}$$

$K(\mathbf{x}, t; \mathbf{x}', t_0)$ is the amplitude for a particle localized at $\mathbf{x}'$ at time t_0 to be found at position $\mathbf{x}$ at a later time t. It is the Green's function of the Schrödinger operator in 4 dimensions (3 space, 1 time):

$$\left(-\frac{\hbar^2}{2m}\nabla_{\mathbf{x}}^2 + V(\mathbf{x}) - i\hbar\frac{\partial}{\partial t}\right) K(\mathbf{x}, t; \mathbf{x}', t_0)\theta(t - t_0) = -i\hbar\delta^{(3)}(\mathbf{x} - \mathbf{x}')\delta(t - t_0). \tag{17}$$

Example 1: Free Particle. For the free particle ($V(\mathbf{x}) = 0$). The eigenstates of the Hamiltonian are the momentum states $|\mathbf{p}\rangle$, and hence

$$U(t,0) = \int d^3p |\mathbf{p}\rangle\langle\mathbf{p}| e^{-ip^2t/(2m\hbar)}. \tag{18}$$

The propagator $K(\mathbf{x},t;\mathbf{x}',0)$ is

$$K(\mathbf{x},t;\mathbf{x}',0) = \int d^3p \langle\mathbf{x}|\mathbf{p}\rangle\langle\mathbf{p}|\mathbf{x}'\rangle e^{-ip^2t/(2m\hbar)} = \frac{1}{(2\pi\hbar)^3}\int d^3p e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')/\hbar} e^{-ip^2t/(2m\hbar)}. \tag{19}$$

This is a Gaussian integral, which evaluates to

$$K(\mathbf{x},t;\mathbf{x}',0) = \left(\frac{m}{2\pi i\hbar t}\right)^{3/2} e^{im(\mathbf{x}-\mathbf{x}')^2/(2\hbar t)}. \tag{20}$$

Now, let's apply it, first using a simple (unrealistic) example of a delta function initial state: $\psi(\mathbf{x}',0) = \delta^{(3)}(\mathbf{x}'-\mathbf{x}_0)$. Then we have

$$\psi(\mathbf{x},t) = \left(\frac{m}{2\pi i\hbar t}\right)^{3/2} e^{im(\mathbf{x}-\mathbf{x}_0)^2/(2\hbar t)}. \tag{21}$$

Note that it spreads rapidly; this is the "fate" of the δ-function. A more realistic but mathematically harder example is to start with a Gaussian wavepacket, which we will consider in one dimension for simplicity. The initial state is given by

$$\psi(x,0) = \frac{1}{\pi^{1/4}\sqrt{d}} e^{ik_0x - x^2/(2d^2)}. \tag{22}$$

Note that for this state, $\langle x\rangle_0 = 0$, $\langle x^2\rangle_0 = d^2/2$, $\langle p\rangle_0 = \hbar k_0$, and $\langle p^2\rangle_0 = \hbar^2k_0^2 + \hbar^2/(2d^2)$. The propagator in one dimension is

$$K(x,t;x',0) = \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} e^{im(x-x')^2/(2\hbar t)}. \tag{23}$$

The wave function at future times is

$$\psi(x,t) = \frac{1}{\pi^{1/4}\sqrt{d}}\left(\frac{m}{2\pi i\hbar t}\right)^{1/2}\int_{-\infty}^{\infty} dx' e^{im(x-x')^2/(2\hbar t)} e^{ik_0x' - x'^2/(2d^2)}, \tag{24}$$

which evaluates to

$$\psi(x,t) = \frac{1}{\pi^{1/4}\left(d + \frac{i\hbar t}{md}\right)^{1/2}} e^{ik_0(x-p_0t/(2m))} \exp\left[-\frac{(x-p_0t/m)^2}{2d^2\left(1+\frac{i\hbar t}{md^2}\right)}\right]. \tag{25}$$

This is a wavepacket with center at the correct classical position,

$$\langle x\rangle_t = \frac{p_0t}{m} = \frac{\langle p\rangle t}{m}. \tag{26}$$

but with a different width:

$$\langle(\Delta x)^2\rangle = \frac{d^2}{2}\left[1 + \frac{\hbar^2t^2}{m^2d^4}\right] \equiv \frac{d^2(t)}{2}, \tag{27}$$

in which $d(t)$ is an effective width. For large times,

$$d(t) \approx \frac{\hbar t}{md}, \tag{28}$$

which shows that it is governed by quantum effects. Finally, note that all momentum expectation values (and expectation values of functions of momentum) are constant, since the momentum operator commutes with the Hamiltonian. Therefore,

$$\langle p\rangle_t = \hbar k_0 = \langle p\rangle_0, \quad \langle p^2\rangle_t = \hbar^2 k_0^2 + \frac{\hbar^2}{2d^2} = \langle p^2\rangle_0. \tag{29}$$

Example 2: Simple Harmonic Oscillator. This is another example in which the propagator can be evaluated in closed form. Again, we will work in one dimension for simplicity. We have

$$U(t,0) = \sum_{n=0}^{\infty} |n\rangle\langle n| e^{-iE_n t/\hbar}, \tag{30}$$

with $E_n = (n+1/2)\hbar\omega$. The position space propagator is then

$$K(x,t;x',0) = \sum_{n=0}^{\infty} \psi_n(x)\psi_n(x') e^{-i(n+1/2)\omega t}, \tag{31}$$

recalling that the $\psi_n(x)$ are real. The sum in Eq. (31) can be explicitly evaluated in closed form:

$$K(x,t;x',0) = \left[\frac{m\omega}{2\pi i\hbar \sin\omega t}\right]^{1/2} \exp\left[\frac{im\omega((x^2+x'^2)\cos\omega t - 2xx')}{2\hbar\sin\omega t}\right]. \tag{32}$$

This can now be applied an initial state. As an example, consider a Gaussian wavepacket with $k_0 = 0$ which is localized at $x = a$. In this case, we obtain the expression

$$\psi(x,t) = \frac{1}{\pi^{1/4}\sqrt{d}}\left[\frac{m\omega}{2\pi i\hbar\sin\omega t}\right]^{1/2} \int dx' e^{\left[\frac{im\omega((x^2+x'^2)\cos\omega t - 2xx')}{2\hbar\sin\omega t}\right]} e^{-(x'-a)^2/(2d^2)}. \tag{33}$$

This is also a (messy) Gaussian integral. Evaluating this integral and calculating $|\psi(x,t)|^2$ shows that the probability density is that of a wavepacket with center at $x = a\cos\omega t$ (as expected classically). Furthermore, it can be shown that for the special case of $d^2 = \hbar/(m\omega)$, the wavepacket is a perfect Gaussian packet, of the form

$$|\psi(x,t)|^2 = \frac{1}{\sqrt{\pi}d} e^{-(x-a\cos\omega t)^2/d^2}. \tag{34}$$

However, for any other d, the wavepacket will spread.

Probability current. Recall in classical electrodynamics, the continuity equation involving the charge density $\rho_{\rm E}(\mathbf{x},t)$ and current density $\mathbf{j}_{\rm E}(\mathbf{x},t)$:

$$\frac{\partial\rho_{\rm E}(\mathbf{x},t)}{\partial t} = -\nabla\cdot\mathbf{j}_{\rm E}(\mathbf{x},t), \tag{35}$$

which is an expression of the conservation of charge. In quantum mechanics, we'll develop a similar idea for the conservation of probability. The quantity analogous to charge density is the probability density $\rho(\mathbf{x},t) = |\psi(\mathbf{x},t)|^2$. The probability current can be determined by considering the difference between

$$\psi^*\left(i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi\right) \tag{36}$$

and its complex conjugate:

$$\psi\left(-i\hbar\frac{\partial\psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V^*\psi^*\right). \tag{37}$$

The result is

$$\frac{\partial \rho(\mathbf{x},t)}{\partial t} = -\nabla \cdot \mathbf{j}(\mathbf{x},t) + \frac{2}{\hbar}\psi^* \mathrm{Im}(V)\psi, \tag{38}$$

in which

$$\mathbf{j}(\mathbf{x},t) = \frac{\hbar}{2mi}(\psi^* \nabla\psi - \psi\nabla\psi^*). \tag{39}$$

Taking $V = V^*$ (required for a Hermitian Hamiltonian) results in the continuity equation. The probability current $\mathbf{j}(\mathbf{x},t)$ is to be interpreted as the rate of flow of probability density. Note that $\mathbf{j}(\mathbf{x},t) = 0$ for a real wavefunction ψ. Note also that for an energy eigenstate, $\nabla \cdot \mathbf{j}(\mathbf{x},t) = 0$.

Scattering in 1d: wavepacket treatment. To describe scattering of a quantum mechanical state from a fixed source of potential, we should start with a normalizable propagating state (a wavepacket). For a sufficiently localized wavepacket in momentum space (and to some extent, also in position space), the full wavepacket treatment of the scattering problem can be replaced by the usual plane wave treatment. Here we provide a brief overview of the logic and assumptions involved in this procedure.

Given an incident wavepacket that is sufficiently localized in both position and momentum at some initial time t_0 (which we will set to zero), scattering from a potential in the large t limit leads to a wavefunction with two contributions: the reflected wave $\psi_R(x,t)$, which travels in the opposite direction to the incident wave, and the transmitted wave $\psi_T(x,t)$), with

$$R = \int |\psi_R|^2 dx, \quad T = \int |\psi_T|^2 dx, \quad R + T = 1. \tag{40}$$

In the above, R is the reflection probability and T is the transmission probability; the condition $R + T = 1$ demonstrates that there is negligible overlap between the reflected and transmitted waves.

Let us work this out with an example. Consider an initial Gaussian wavepacket of the form

$$\psi_I(x,0) = \frac{1}{\pi^{1/4}\sqrt{d}} e^{ik_0(x+a)} e^{-(x+a)^2/(2d^2)}, \tag{41}$$

i.e., a Gaussian wavepacket of width d and mean momentum $p_0 = \hbar k_0$ localized initially at $x = -a$. We will work in the limit that $a >> d$, *i.e.*, the width is much smaller than the initial value of $\langle x \rangle$. Suppose this wave is incident from the left onto a step function potential:

$$V(x) = V_0 \theta(x). \tag{42}$$

Classically, if the energy $E = \hbar^2 k_0^2/(2m)$ is greater than V_0, the probability of transmission is 100%, while if $E < V_0$, the probability of reflection is 100%.

Quantum mechanically, it is found that if $\langle E \rangle > V_0$, there are nonvanishing reflection and transmission probabilities, while if $\langle E \rangle \ll V_0$, the probability of reflection approaches 100%. Here, we will also assume that $p_0^2/2m > V_0$, and also that $p_0 - \sqrt{2mV_0} \gg \Delta p$, such that all momentum components have enough energy classically to go over the barrier.

The general procedure to solve the scattering problem is as follows:

1. Find the normalized eigenfunctions of the Hamiltonian, $\psi_E(x)$.
2. Project the initial wavepacket $\psi_I(x,0)$ onto the basis of $\psi_E(x)$ states.
3. Find $\psi(x,t)$ by letting each component evolve in time, picking up the phase factor $e^{-iEt/\hbar}$.
4. In the large t limit, identify $\psi_R(x,t)$ and $\psi_T(x,t)$.

Let us now work out these steps in turn.
1. For the step function, there are no bound states, only positive energy states and therefore a continuum of solutions. The (delta-function) normalized eigenfunctions can be labeled by $k_1 = \sqrt{2mE_1}/\hbar$. The solutions can be categorized according to whether $E > V_0$ or $E < V_0$; furthermore, for the $E > V_0$ states, it is useful to categorize the solutions further into whether the incoming wave is incident from the left or from the right. For our problem at hand, the most important set of eigenstates are the $E > V_0$ states with the incoming wave incident from the left, for these are the ones that will overlap most strongly with our initial wavepacket. This set of eigenfunctions is given as follows:

$$\psi_{k_1}(x) = \frac{1}{\sqrt{2\pi}}\left[\left[e^{ik_1x} + \frac{B}{A}e^{-ik_1x}\right]\theta(-x) + \frac{C}{A}e^{ik_2x}\theta(x)\right], \tag{43}$$

in which $k_2 = \sqrt{2m(E-V_0)}/\hbar = \sqrt{k_1^2 - 2mV_0/\hbar^2}$, and

$$\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2}, \quad \frac{C}{A} = \frac{2k_1}{k_1 + k_2}. \tag{44}$$

2. Projecting $\psi_I(x,0)$ onto the basis of $\psi_{k_1}(x)$ states leads to the expression:

$$|\psi_I\rangle = \int dk_1 |k_1\rangle\langle k_1|\psi_I\rangle = \int dk_1 a(k_1)|k_1\rangle, \tag{45}$$

in which

$$a(k_1) = \int_{-\infty}^{\infty} \psi_{k_1}^*(x)\psi_I(x,0)dx. \tag{46}$$

Here we will only insert the eigenstates given in Eq. (43), as neglecting the others gives errors of the order $O(e^{-((p_0-\sqrt{2mV_0})/\Delta p)^2})$. Doing so, we find the following expression:

$$a(k_1) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{0}\left[e^{-ik_1x} + \frac{B^*}{A^*}e^{ik_1x}\right]\psi_I(x,0)\,dx + \frac{1}{\sqrt{2\pi}}\int_0^{\infty}\frac{C^*}{A^*}e^{-ik_2x}\psi_I(x,0)\,dx. \tag{47}$$

Note that since $\psi_I(x,0)$ has no support for positive values of x, the third term is exponentially suppressed and can be taken to zero (corrections are of order $e^{-(a/d)^2}$). The first term,

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{0} dx \frac{1}{(\pi d^2)^{1/4}} e^{-ik_1x}e^{ik_0(x+a)}e^{-(x+a)^2/(2d^2)}, \tag{48}$$

is a Gaussian integral which can be evaluated easily under the approximation that we extend the upper limit of the integral to positive infinity (again, this introduces errors of order $e^{-(a/d)^2}$). The result is

$$\left(\frac{d^2}{\pi}\right)^{1/4} e^{-(k_1-k_0)^2d^2/2}e^{ik_1a}. \tag{49}$$

Note that the second term is of identical form with the replacement $k_1 \to -k_1$ in the exponent. Hence, the result from this term is of the order $e^{-(k_1+k_0)^2d^2/2}$, which is highly suppressed since $k_1 + k_0$ is never negative. Therefore, we drop this term, and get the final result

$$a(k_1) = \left(\frac{d^2}{\pi}\right)^{1/4} e^{-(k_1-k_0)^2d^2/2}e^{ik_1a}. \tag{50}$$

3. We now determine $\psi(x,t)$ as follows:

$$\psi(x,t) = \int dk_1 \psi_{k_1}(x)a(k_1)e^{-i\hbar k_1^2 t/(2m)}. \tag{51}$$

4. We now need to examine $\psi(x,t)$ in the large t limit. Once again, we have an expression with three terms; let's take them one at a time. The first term is

$$\left(\frac{d^2}{4\pi^3}\right)^{1/4}\int dk_1 e^{-i\hbar k_1^2 t/(2m)}e^{-(k_1-k_0)^2d^2/2}e^{ik_1a}e^{ik_1x}\theta(-x). \tag{52}$$

The result of this integral is a Gaussian wavepacket traveling to the right centered at $x=-a+p_0t/m$, multiplied by $\theta(-x)$. It takes the form

$$\theta(-x)\frac{1}{\pi^{1/4}\left(d+\frac{i\hbar t}{md}\right)^{1/2}}\exp\left[-\frac{\left(x+a-\frac{\hbar k_0 t}{m}\right)^2}{2d^2\left(1+\frac{i\hbar t}{md^2}\right)}\right]e^{ik_0(x+a-\hbar k_0 t/(2m))}. \tag{53}$$

This means that in the large t limit, the Gaussian is centered at $x>0$ and the theta function kills the expression. Therefore, the incident wave has vanished, and in its place are the reflected and transmitted waves. Considering now the second term, we have

$$\left(\frac{d^2}{4\pi^3}\right)^{1/4}\int dk_1 \frac{B}{A}e^{-i\hbar k_1^2 t/(2m)}e^{-(k_1-k_0)^2d^2/2}e^{ik_1a}e^{-ik_1x}\theta(-x). \tag{54}$$

In Shankar's approach, since the integrand is strongly peaked at $k_1\sim k_0$, we can replace B/A with its value at $k_1=k_0$ (the corrections here are power law corrections in the quantity $\Delta p/(p_0-\sqrt{2mV_0})$). In this limit, the integral is then a Gaussian wavepacket centered at $x=+a$ and traveling to the left with mean momentum $-\hbar k_0$, multiplied by $\theta(-x)$ and $(B/A)_{k_1=k_0}$. Therefore, in the large t limit, this is the reflected wave $\psi_R(x,t)$. Since the Gaussian wavepacket is normalized, the reflection coefficient is then

$$R=\int|\psi_R(x,t)|^2dx=\left|\left(\frac{B}{A}\right)_{k_1=k_0}\right|^2, \tag{55}$$

in which B/A is evaluated at $k_1=k_0$. For the third term, we have

$$\left(\frac{d^2}{4\pi^3}\right)^{1/4}\int dk_1 \frac{C}{A}e^{-i\hbar k_1^2 t/(2m)}e^{-(k_1-k_0)^2d^2/2}e^{ik_1a}e^{i\sqrt{k_1^2-2mV_0/\hbar^2}x}\theta(x). \tag{56}$$

Again, we can replace C/A with its value at $k_1=k_0$. The expectation is that this is the transmitted wave, which is a packet traveling to the right with mean momentum $\hbar\sqrt{k_0^2-2mV_0/\hbar^2}$. Evaluating the integral requires a careful treatment of the branch cut arising from the $\sqrt{k_1^2-2mV_0/\hbar^2}$ factor in the exponential. An approach that allows for a straightforward determination of the power-law corrections (following Norsen et al. 2008) is to note that the reflected wave and the transmitted wave can be expressed as follows:

$$\psi_R(x,t)=\frac{1}{\sqrt{2\pi}}\int e^{ik_1x}\phi_R(k_1,t)dk_1,\qquad \psi_T(x,t)=\frac{1}{\sqrt{2\pi}}\int e^{ik_1x}\phi_T(k_1,t)dk_1, \tag{57}$$

which yields

$$\phi_R(k_1,t)=\left(\frac{d^2}{\pi}\right)^{1/4}e^{-i\hbar k_1^2t/(2m)}e^{-(k_1+k_0)^2d^2/2}e^{-ik_1a}\left(\frac{k_1+k_2}{k_1-k_2}\right) \tag{58}$$

$$\phi_T(k_1,t)=\left(\frac{d^2}{\pi}\right)^{1/4}e^{-i\hbar(k_1^2+2mV_0/\hbar^2)t/(2m)}e^{-\sqrt{k_1^2+2mV_0/\hbar^2}-k_0)^2d^2/2}e^{ik_1a}\mathcal{N}(k_1), \tag{59}$$

in which $\mathcal{N}(k_1)$ is given by

$$\mathcal{N}(k_1) = \left(\frac{2\sqrt{k_1^2 + 2mV_0/\hbar^2}}{k_1 + \sqrt{k_1^2 + 2mV_0/\hbar^2}}\right)\left(\frac{k_1}{\sqrt{k_1^2 + 2mV_0/\hbar^2}}\right). \tag{60}$$

(To obtain these results, there has been a change of variables of $k_1 \to -k_1$ for the reflected wave, and $k_1 \to k_2$ for the transmitted wave.) The reflection and transmission coefficients take the following form:

$$\begin{aligned} R = \int |\phi_R(k_1,t)|^2 dk_1 &= \left(\frac{d^2}{\pi}\right)^{1/2} \int e^{-(k_1+k_0)^2 d^2} \left(\frac{k_1+k_2}{k_1-k_2}\right)^2 dk_1 \\ &= \left(\frac{d^2}{\pi}\right)^{1/2} \int e^{-(k_1+k_0)^2 d^2} \left|\frac{B}{A}\right|^2 dk_1 \end{aligned} \tag{61}$$

$$\begin{aligned} T = \int |\phi_T(k_1,t)|^2 dk_1 &= \left(\frac{d^2}{\pi}\right)^{1/2} \int e^{-(\sqrt{k_1^2 - 2mV_0/\hbar^2} - k_0)^2 d^2} \mathcal{N}(k_1)^2 dk_1 \\ &= \left(\frac{d^2}{\pi}\right)^{1/2} \int e^{-(k_1-k_0)^2 d^2} \left|\frac{C}{A}\right|^2 \frac{k_2}{k_1} dk_1, \end{aligned} \tag{62}$$

where we note that to obtain the final expressions, there has been another change of variables of $k_1 \to -k_1$ for the reflected wave, and $k_1 \to \sqrt{k_1^2 + 2mV_0/\hbar^2}$ for the transmitted wave.

These expressions can be Taylor expanded about $k_1 = k_0$ to obtain the leading values of R and T, and their power-law corrections. To leading order, the result is exactly as obtained in Shankar's treatment:

$$R = \left|\left(\frac{B}{A}\right)_{k_1=k_0}\right|^2, \qquad T = \left|\left(\frac{C}{A}\right)_{k_1=k_0}\right|^2 \frac{\sqrt{k_0^2 - 2mV_0/\hbar^2}}{k_0}. \tag{63}$$

The leading power-law corrections take the form

$$\pm\left(\frac{k_0 - \sqrt{k_0^2 - 2mV_0/\hbar^2}}{k_0 + \sqrt{k_0^2 - 2mV_0/\hbar^2}}\right)^2 \left(\frac{2k_0}{(k_0^2 - 2mV_0/\hbar^2)^{3/2}} + \frac{8}{k_0^2 - 2mV_0/\hbar^2}\right)\frac{1}{d^2}, \tag{64}$$

where the upper sign gives the correction to R, and the lower sign gives the correction to T. Note that these corrections are negligible in the limit of small width of the packet in momentum space, Δp. It is also worth noting that $R + T = 1$ including these corrections, as it must be.

This complicated calculation has a very simple answer, which suggests that in the limit of sufficiently localized wavepackets, the dynamical scattering problem can be replaced by the steady state problem of plane wave states. Let us write the eigenstate with the label k_0 as

$$\psi_{k_0} = (e^{ik_0 x} + re^{-ik_0 x})\theta(-x) + te^{i\sqrt{k_0^2 - 2mV_0/\hbar^2}\,x}\theta(x), \tag{65}$$

in which we have dropped an irrelevant normalization factor, and the coefficients r and t are given by $r = (B/A)_{k_1=k_0}$, $t = (C/A)_{k_1=k_0}$, as given previously with $k_1 = k_0$. Taking the probability current in pieces for each individual component, the contributions are given by

$$j_I = |\mathbf{j}_I| = \frac{\hbar k_0}{m}, \qquad j_R = |\mathbf{j}_R| = |r|^2 \frac{\hbar k_0}{m}, \qquad j_T = |\mathbf{j}_T| = |t|^2 \frac{\hbar\sqrt{k_0^2 - 2mV_0/\hbar^2}}{m}. \tag{66}$$

The reflection and transmission coefficients can then be determined using the following prescription:

$$R = \left|\frac{j_R}{j_I}\right| = |r|^2, \quad T = \left|\frac{j_T}{j_I}\right| = |t|^2 \frac{\sqrt{k_0^2 - 2mV_0/\hbar^2}}{k_0}. \tag{67}$$

As stated, this much simpler plane wave approximation method requires highly localized wavepackets (the specific requirements can be seen from the approximations given above). However, it is worth noting that if the scattering region has a finite width that is not small compared with the width of the incident packet, the plane wave approximation generally gives results that are qualitatively as well as quantitatively incorrect. Therefore, when using this approximation in the future, it is important always to keep in mind whether the necessary assumptions that have been made here can be justified.

Heisenberg picture. In the Schrödinger picture, state kets evolve with time and observables such as x, p, etc. are fixed in time. In the Heisenberg picture, the story is reversed: state kets are fixed in time and operators evolve in time. This is just another representation of QM; the physics is independent of representation. The Heisenberg state ket is given by

$$|\alpha\rangle_H = \mathcal{U}^\dagger(t)|\alpha\rangle_S = e^{iHt/\hbar}|\alpha\rangle_S, \tag{68}$$

where the last equality holds for the case of time-independent H. Note that the Heisenberg state at time t coincides with the Schrödinger state at some time $t = 0$. Operators in the Heisenberg picture are related to Schrödinger picture operators by

$$A_H = \mathcal{U}^\dagger(t) A_S \mathcal{U}(t) = e^{iHt/\hbar} A_S e^{-iHt/\hbar}. \tag{69}$$

It is clear that the expectation value of A_H with respect to $|\alpha\rangle_H$ is equal to the expectation value of A_S with respect to $|\alpha\rangle$. The equation of motion for Heisenberg operator A_H is given by

$$\frac{dA_H}{dt} = \frac{1}{i\hbar}[A, H] + \frac{\partial A_H}{\partial t}, \tag{70}$$

in which $\partial A_H/\partial t = \mathcal{U}^\dagger(t)(\partial A_S/\partial t)\mathcal{U}(t)$. Note that $\partial A_H/\partial t \neq 0$ only if the corresponding operator in the Schrödinger picture has explicit time dependence. In the case in which the Schrödinger picture operator does not depend on time, Eq. (70) shows that if this operator in the Heisenberg picture commutes with the Hamiltonian, it is a constant of the motion.

The Heisenberg picture lends itself to the classical correspondence with Poisson brackets, and allows for an operator statement of the Ehrenfest theorem (which only holds at the level of expectation values in the Schrödinger or any other picture):

$$m\frac{d^2\mathbf{x}_H}{dt^2} = -\nabla V(\mathbf{x}_H). \tag{71}$$

Since operators evolve in the Heisenberg picture, so too do their eigenstates (eigenvalues, of course, remain fixed). For an operator A_S which satisfies

$$A_S|a_i\rangle_S = a_i|a_i\rangle_S, \tag{72}$$

in the Heisenberg picture we have

$$A_H|a_i\rangle_H = a_i|a_i\rangle_H, \tag{73}$$

in which

$$|a_i\rangle_H = \mathcal{U}^\dagger(t)|a_i\rangle_S. \tag{74}$$

Transition amplitudes are the same in either picture; *i.e.*. the probability that a state $|\alpha\rangle$ has overlap with an eigenstate $|\beta\rangle$ of some given operator is

$$\langle\beta|\mathcal{U}(t)|\alpha\rangle. \tag{75}$$

In the Schrödinger picture, we interpret $\mathcal{U}(t)|\alpha\rangle = |\alpha(t)\rangle$ with $\langle\beta|$ fixed in time, while in the Heisenberg picture, we interpret $\langle\beta|\mathcal{U}(t) = \langle\beta(t)|$, with $|\alpha\rangle$ fixed in time.

Note also that in the case of a time-independent Hamiltonian, since $A_H(t) = e^{iHt/\hbar}A_H(0)e^{-iHt/\hbar}$ (recall $A_H(0) = A_S(0)$), the following general result can be used to determine the time evolution:

$$e^{i\lambda G}Ae^{-i\lambda G} = A + i\lambda[G,A] + \frac{(i\lambda)^2}{2!}[G,[G,A]] + \frac{(i\lambda)^3}{3!}[G,[G,[G,A]]] + \ldots \tag{76}$$

Alternatively, we can solve the Heisenberg equations of motion. A standard example (worked out in class) is the one-dimensional harmonic oscillator.