QUANTUM PHYSICS III

Solutions to Problem Set 4

1. Free particle amplitude

Recall that

$$K = \langle X|U(T,0)|0\rangle = \left(\frac{2\pi i\hbar T}{m}\right)^{-1/2} \exp\left(\frac{imX^2}{2\hbar T}\right).$$
(1)

1. Straightforward calculation yields

$$\frac{\partial^2 K}{\partial X^2} = \sqrt{\frac{m}{2\pi i\hbar T}} \exp\left(\frac{imX^2}{2\hbar T}\right) \left(\frac{im}{\hbar T} - \frac{m^2 X)^2}{\hbar^2 T^2}\right),$$

$$\frac{\partial K}{\partial T} = \sqrt{\frac{m}{2\pi i\hbar T}} \exp\left(\frac{imX^2}{2\hbar T}\right) \left(-\frac{imX^2}{2\hbar T^2} - \frac{1}{2T}\right),$$
(2)

and we observe that

$$-\frac{\hbar}{i}\frac{\partial K}{\partial t_f} = -\frac{\hbar^2}{2m}\frac{\partial^2 K}{\partial x_f^2} \,. \tag{3}$$

2. To study the properties of the amplitude, it is convenient to select the real part of the exponent in (1),

$$\operatorname{Re}(\sqrt{i}K) = \sqrt{\frac{m}{2\pi\hbar T}} \cos\left(\frac{mX^2}{2\hbar T}\right).$$
(4)

Let T = const, λ is the period of oscillations of $\text{Re}(\sqrt{i}K)$ as a function of X. Then, for $X \gg \lambda$

$$2\pi = \frac{m(X+\lambda)^2}{2\hbar T} - \frac{mX^2}{2\hbar T} \approx \frac{mX\lambda}{\hbar T} , \qquad (5)$$

and

$$\lambda \approx \frac{2\pi\hbar}{m(X/T)} . \tag{6}$$

In this formula, X/T = V is the classical velocity of the particle, and mX/T is its classical momentum. Hence,

$$\lambda \approx \frac{2\pi\hbar}{p} \tag{7}$$

is the de Broglie wave length of the particle.

3. Let X = const and τ is the period of oscillations of $\text{Re}(\sqrt{i}K)$ as a function of *T*. For large *T*, neglecting the change of the amplitude of oscillations, we have

$$2\pi = \frac{mX^2}{2\hbar T} - \frac{mX^2}{2\hbar (T+\tau)} = \frac{mX^2}{2\hbar T^2} \left(\frac{\tau}{1+\tau/T}\right) \,. \tag{8}$$

Hence

$$\tau \approx \frac{4\pi\hbar}{mV^2} \ . \tag{9}$$

The frequency of oscillations is $\omega = 2\pi/\tau \approx mV^2/2\hbar$. On the other hand, $E = mV^2/2$ is the classical kinetic energy of the particle. We obtain the well-known relation

$$E = \hbar \omega . \tag{10}$$



FIGURE 1 – The real part of the amplitude $\sqrt{i}K$ as a function of X (the left panel), or T (the right panel).

2. Free particle amplitude in momentum representation

The coordinate and the momentum representations are related via Fourier transform,

$$\tilde{\psi}(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int dx \,\psi(x,t) e^{\frac{i}{\hbar}px} \,. \tag{11}$$

1. Applying the Fourier transform to the both sides of the equation

$$\psi(x, t_f) = \int dx' \, K(x, t_f, x', t_i) \, \psi(x', t_i) \,, \tag{12}$$

we have

$$\tilde{\psi}(p,t_f) = \frac{1}{\sqrt{2\pi\hbar}} \int dx \int dx' \, e^{\frac{i}{\hbar}px} K(x,t_f,x',t_i) \, \psi(x',t_i) \,. \tag{13}$$

Applying the inverse Fourier transform to $\psi(x', t_i)$ gives

$$\tilde{\psi}(p,t_f) = \frac{1}{2\pi\hbar} \int dp' \int dx \int dx' \, e^{\frac{i}{\hbar}px} K(x,t_f,x',t_i) \, e^{-\frac{i}{\hbar}p'x'} \psi(p',t_i) \,. \tag{14}$$

Comparing this with

$$\tilde{\psi}(p,t_f) = \int dp' \,\tilde{K}(p,t_f,p',t_i) \,\tilde{\psi}(p',t_i) \,, \tag{15}$$

we conclude that

$$\tilde{K}(p,t_f,p',t_i) = \frac{1}{2\pi\hbar} \int dx \int dx' \, e^{\frac{i}{\hbar}px} K(x,t_f,x',t_i) \, e^{-\frac{i}{\hbar}p'x'} \,. \tag{16}$$

To obtain the inverse relation, we multiply eq. (16) by $e^{\frac{i}{\hbar}p'x''}$ and $e^{-\frac{i}{\hbar}px'''}$, and integrate over p and p'. This gives

$$\int dp \int dp' \, e^{-\frac{i}{\hbar}px'''} \tilde{K}(p, t_f, p', t_i) e^{\frac{i}{\hbar}p'x''} = 2\pi\hbar \int dx \int dx' \, \delta(x' - x'') \delta(x - x''') K(x, t_f, x', t_i) = 2\pi\hbar \, K(x''', t_f, x'', t_i) \,.$$
(17)

Hence,

$$K(x, t_f, x', t_i) = \frac{1}{2\pi\hbar} \int dp \int dp' \, e^{-\frac{i}{\hbar}px} \tilde{K}(p, t_f, p', t_i) e^{\frac{i}{\hbar}p'x'} \,. \tag{18}$$

2. Substituting the amplitude (1) into eq. (16), we have

$$\begin{split} \tilde{K}(p,t_{f},p',t_{i}) &= \frac{1}{2\pi\hbar} \sqrt{\frac{m}{2\pi i\hbar(t_{f}-t_{i})}} \int dx \int dx' \ e^{\frac{i}{\hbar}px} e^{\frac{im(x'-x)^{2}}{2\hbar(t_{f}-t_{i})}} e^{-\frac{i}{\hbar}p'x'} \\ &= \frac{1}{2\pi\hbar} \sqrt{\frac{m}{2\pi i\hbar(t_{f}-t_{i})}} \int dx \int dx' \ e^{\frac{im}{2\hbar(t_{f}-t_{i})}x'^{2}-\frac{i}{\hbar} \left(\frac{mx}{\hbar(t_{f}-t_{i})}+p'\right)x'} e^{\frac{i}{\hbar}px} e^{\frac{imx^{2}}{2\hbar(t_{f}-t_{i})}} \\ &= \frac{1}{2\pi\hbar} \int dx \ e^{\frac{i}{\hbar}(p-p')x} e^{-\frac{i(t_{f}-t_{i})p'^{2}}{2m\hbar}} \\ &= \delta(p-p')e^{-\frac{i(t_{f}-t_{i})p^{2}}{2m\hbar}} \ . \end{split}$$
(19)

Note that this again has a gaussian form as expected for the free particle. Note also that the amplitude is zero unless the initial and the final momenta coincide, p = p'. This is nothing but manifestation of the momentum conservation law.

3. By the means of eqs. (18) and (19), the free particle amplitude can be written in the integral form,

$$\langle x|U(t_f,t_i)|x'\rangle = \frac{1}{2\pi\hbar} \int dp \; e^{\frac{i}{\hbar}p(x'-x)} e^{-\frac{i(t_f-t_i)p^2}{2m\hbar}} \;.$$
(20)

Recall that the evolution operator $U(t_f, t_i)$ is expressed through the free particle Hamiltonian *H* as follows,

$$U(t_f, t_i) = e^{-\frac{i}{\hbar}H(t_f - t_i)} .$$
(21)

Let $\{|\psi_p\rangle, p \in \mathbb{R}\}$ be the complete set of eigenstates of *H*. Then,

$$\langle x|U(t_f, t_i)|x'\rangle = \int dp \, \langle x|e^{-\frac{i}{\hbar}H(t_f - t_i)}|\psi_p\rangle \langle \psi_p|x'\rangle$$

$$= \int dp \, \psi_p(x)\psi_p^*(x')e^{-\frac{i}{\hbar}E_p(t_f - t_i)},$$
(22)

where by E_p we denote the corresponding eigenvalues of *H*. Comparing this with the r.h.s. of eq. (20), we can read off directly the explicit form of $\psi_p(x)$ and E_p ,

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}px}, \quad E_p = \frac{p^2}{2m},$$
(23)

in which we recognize the familiar expressions for the plane waves and the kinetic energy of the particle.

3. Diffraction through a slit

1. Using the transitiveness of the amplitude, we have

$$K(X + x', T + t', 0, 0) = \int_{-b}^{b} dy \, K(X + x', T + t', X + y, T) K(X + y, T, 0, 0)$$

= $\frac{m}{2\pi i\hbar} \sqrt{\frac{1}{t'T}} \int_{-b}^{b} dy \, \exp\left(\frac{im(x' - y)^{2}}{2\hbar t'}\right) \exp\left(\frac{im(X + y)^{2}}{2\hbar T}\right).$ (24)

2. The integral (24) is not Gaussian and cannot be computed in elementary functions. To get some explicit result, one can use the following trick. Introduce the "transparency function" G(y) of the slit. If

$$G(y) = \begin{cases} 1, & -b < y < b, \\ 0, & \text{otherwise}, \end{cases}$$
(25)

the formula (24) can be rewritten as

$$K(X + x', T + t', 0, 0) = \frac{m}{2\pi i\hbar} \sqrt{\frac{1}{t'T}} \int_{-\infty}^{\infty} dy \, G(y) \, \exp\left(\frac{im}{2\hbar} \left(\frac{(x' - y)^2}{t'} + \frac{(X + y)^2}{T}\right)\right).$$
(26)

Now we replace G(y) by a Gaussian function whose full width at half maximum approximately equals the size of the slit (see figure 2), ¹

$$\tilde{G}(y) = \exp\left(-y^2/2b^2\right) \,. \tag{27}$$

With this replacement, the expression (26) turns into

$$K(X + x', T + t', 0, 0) = \frac{m}{2\pi i\hbar} \sqrt{\frac{1}{t'T}} \int_{-\infty}^{\infty} dy \exp\left[\frac{im}{2\hbar} \left[\frac{x'^2}{t'} + \frac{X^2}{T}\right] + \frac{im}{\hbar} \left[\frac{-x'}{t'} + \frac{X}{T}\right] y + \left[\frac{im}{2\hbar} \left(\frac{1}{t'} + \frac{1}{T}\right) - \frac{1}{2b^2}\right] y^2\right].$$
(28)

3. This is a Gaussian integral ! Straightforward computation gives the following result,

$$K(X + x', T + t', 0, 0) = \frac{m}{2\pi i\hbar} \sqrt{\frac{1}{t'T}} \sqrt{\frac{-\pi}{\frac{im}{2\hbar}(1/t' + 1/T) - \frac{1}{2b^2}}} \exp\left[\frac{im}{2\hbar} \left(\frac{x'^2}{t'} + \frac{X^2}{T}\right) + \frac{\frac{m^2}{4\hbar^2} \left(-x'/t' + X/T\right)^2}{\frac{im}{2\hbar}(1/t' + 1/T) - \frac{1}{2b^2}}\right],$$
(29)

or, using the notation V = X/T,

$$K(X + x', T + t', 0, 0) = \sqrt{\frac{m}{2\pi i\hbar}} \left(T + t' + \frac{it'T\hbar}{mb^2}\right)^{-1/2} \exp\left[\frac{im}{2\hbar} \left(x'^2/t'^2 + V^2T\right) + \frac{\frac{m^2}{2\hbar^2 t'^2} (x' - Vt')^2}{\frac{im}{\hbar} (1/t' + 1/T) - 1/b^2}\right].$$
(30)

^{1.} For the discussion of the accuracy of this approximation, see Appendix B.



FIGURE 2 – Modified transparency function $\tilde{G}(y)$ compared to the initial slit. The full width at half maximum of $\tilde{G}(y)$ equals $2\sqrt{2\log 2b} \approx 2.35b$ which is close to the size of the slit 2b.

4. The probability distribution is obtained by taking square of the modulus of the expression above. The answer is

$$P(x') = \frac{m}{2\pi\hbar} \frac{b}{T\Delta X} \exp\left(-\frac{(x' - Vt')^2}{(\Delta X)^2}\right),$$
(31)

where we introduced

$$(\Delta X)^2 = b^2 (1 + t'/T)^2 + \frac{\hbar^2 t'^2}{m^2 b^2} .$$
(32)

We observe that P(x') is a Gaussian distribution centred around the point x' - Vt'. Note that V = X/T is the classical average velocity of the particle between the first and the second measurements. Hence, the quantum wave packet representing the particle is peaked at the point corresponding to particle's averaged classical position.

There are two lessons to learn from eq. (31). First, we check that the group velocity of a Schrödinger wave packet corresponds to the velocity of the particle in the classical limit. Second, the expression for the dispersion (32) exemplifies a nice interplay between classical and quantum probability. It tells us that the total dispersion of the wave packet contains two contributions. The first one is independent of \hbar and represents a purely classical uncertainty in the position of the particle due to inaccuracy of the second measurement. The second contribution is of quantum nature and associated with the wave packet spreading as it moves along the *x*-axis.