Chapter 7

General functional transition amplitudes

The amplitude for transition from a state $\psi(x)$ at t_1 to $\chi(x)$ at t_2 can be written with the help of the propagator $K(x_2, t_2; x_1, t_1)$ as follows

$$<\chi|1|\psi> = \int\int \chi^*(x_2)\, K(x_2, t_2; x_1, t_1)\, \psi(x_1)\, dx_2 dx_1\,. \tag{7.1}$$

One can write it also as follows

$$<\chi|1|\psi>_S = \int\int \chi^*(x_2) \int [\mathcal{D}x(t)]\, e^{\frac{i}{\hbar}S[x(t)]}\, \psi(x_1)\, dx_2 dx_1\,. \tag{7.2}$$

We spell out the content of this formula as follows: This is the matrix element between two states ψ and χ of a functional taken as unity, weighted with $e^{\frac{i}{\hbar}S}$, and summed over trajectories .

This takes us to the general definition in which we replace in (7.2) 1 by $F[x(t)]$ and write

$$<\chi|F|\psi>_S = \int\int \chi^*(x_2) \int [\mathcal{D}x(t)]\, e^{\frac{i}{\hbar}S[x(t)]}\, F[x(t)]\, \psi(x_1)\, dx_2 dx_1 \tag{7.3}$$

where $F[x(t)]$ should not depend on the end points x_2 and x_1, and be well defined in this region. So, $F[x(t)]$ can be many things, starting from some "global" functional which describe complex interactions and ending with some "local" functionals like e.g. $F[x(t)] = x_k$ which ascribes to each trajectory its value at time t_k.

The functional transition amplitude defined in ((7.3) leads to an *important differential relation for* $F[x(t)]$. To see it we first simplify the notation dropping the wave functions because the relations we are going to discuss are valid for any ψ and χ:

$$\langle\, F\, \rangle_S \;= \int [\mathcal{D}x(t)]\, F[x(t)]\, e^{\frac{i}{\hbar}S[x(t)]}\,. \tag{7.4}$$

Now we shift all trajectories by a *fixed*, infinitely small, amount $\eta(t)$

$$x(t) \;\to\; x(t) + \eta(t)\,. \tag{7.5}$$

Since η is fixed, we have

$$[\mathcal{D}(x(t)+\eta(t))] = [\mathcal{D}x(t)]\,, \tag{7.6}$$

and $\langle\, F\,\rangle_S$ does not change when $x \to x+\eta$. Therefore, to lowest order in η we have

$$\begin{aligned}\langle\, F\,\rangle_S \;&= \int F[x(t)+\eta(t)]\, e^{\frac{i}{\hbar}S[x(t)+\eta(t)]}\,[\mathcal{D}(x(t)+\eta(t))] \\ &= \int F[x(t)]\, e^{\frac{i}{\hbar}S[x(t)]}\,[\mathcal{D}x(t)] \;+\; \int \left(\int \frac{\delta F}{\delta x(s)}\eta(s)ds\right)\, e^{\frac{i}{\hbar}S[x(t)]}\,[\mathcal{D}x(t)] \\ &+ \frac{i}{\hbar}\int F[x(t)] \left(\int \frac{\delta S}{\delta x(s)}\eta(s)ds\right) e^{\frac{i}{\hbar}S[x(t)]}\,[\mathcal{D}x(t)] \;+\; ... \end{aligned} \tag{7.7}$$

where we have used the functional derivatives defined as follows

$$F[x(t)+\eta(t)] - F[x(t)] \;=\; \int ds\, \frac{\delta F}{\delta x(s)}\,\eta(s)\,. \tag{7.8}$$

Since $\langle\, F\,\rangle_S$ and the first term in the second line of (7.7) are equal, and η is arbitrary (though fixed), we obtain the following functional equation

$$\left\langle \frac{\delta F}{\delta x(s)} \right\rangle_S \;=\; -\frac{i}{\hbar}\left\langle F \frac{\delta S}{\delta x(s)} \right\rangle_S, \tag{7.9}$$

or in a more compact notation

$$\langle\, \delta F\,\rangle_S \;=\; -\frac{i}{\hbar}\,\langle\, F\delta S\,\rangle_S \;. \tag{7.10}$$

This differential relation for a very large class of transition amplitudes is very remarkable; *it contains virtually all quantum mechanical relations like equations of motion and also commutation relations.* Arbitrariness of the functional $F[x(t)]$ leads to a potentially very rich physical content of (7.9).

Very often it is very convenient to employ the discretized form of (7.9). Then the functionals become functions of many variables and the sum over trajectories becomes a multi-dimensional integral. Since

$$\frac{\partial}{\partial x_k}\left[F(...,x_k,...)\, e^{\frac{i}{\hbar}S(...,x_k,...)}\right] \;=\; \frac{\partial F}{\partial x_k}\, e^{\frac{i}{\hbar}S} \;+\; F\frac{i}{\hbar}\frac{\partial S}{\partial x_k}\, e^{\frac{i}{\hbar}S}\,,$$

we get, after integrating both sides of the above equation, and neglecting the surface contributions

$$\int \frac{\partial F}{\partial x_k}\,\frac{i}{\hbar}S...\frac{dx_k}{\mathcal{N}}... \;=\; -\frac{i}{\hbar}\int F\frac{\partial S}{\partial x_k}\, e^{\frac{i}{\hbar}S}...\frac{dx_k}{\mathcal{N}}...\,, \tag{7.11}$$

or

$$\left\langle \frac{\partial F}{\partial x_k} \right\rangle_S = -\frac{i}{\hbar}\left\langle F\frac{\partial S}{\partial x_k} \right\rangle_S, \tag{7.12}$$

where $\mathcal{N} = \sqrt{2\pi i\hbar\epsilon/m}$.

Let us look at a few applications for the simple action

$$S = \int_{t_1}^{t_2} dt \left[m\dot{x}^2 - V(x(t))\right] . \tag{7.13}$$

First, let us take $F = 1$, hence $\delta F = 0$. We obtain from (7.10)

$$-\frac{i}{\hbar}\left\langle \int \left[m\frac{d^2x}{dt^2} + V'(x)\right] \delta x(t) dt \right\rangle_S = 0 \,. \tag{7.14}$$

Since $\delta x(t)$ is arbitrary we have

$$\left\langle m\frac{d^2x}{dt^2} \right\rangle_S = -\left\langle V'(x)\right\rangle_S . \tag{7.15}$$

This is a quantum mechanical analogue of the Newton law.

Let us take now the discretized form (7.12). We obtain

$$\left\langle \frac{\partial F}{\partial x_k} \right\rangle_S = \frac{i\epsilon}{\hbar}\left\langle F\left[m\frac{x_{k+1} - 2x_k + x_{k-1}}{\epsilon^2} + V'(x_k)\right]\right\rangle_S . \tag{7.16}$$

Note that taking $F = 1$ in (7.16) we obtain again (7.15) but in the discretized form. Let us take $F = x_k$. To leading order ($\epsilon \to 0$) we can neglect the term $\epsilon x_k V'(x_k)$ and obtain from (7.16)

$$-i\hbar \left\langle 1 \right\rangle_S = \left\langle m\frac{x_{k+1} - x_k}{\epsilon} x_k \right\rangle_S - \left\langle x_k m\frac{x_k - x_{k-1}}{\epsilon} \right\rangle_S . \tag{7.17}$$

Clearly this is to be compared with the commutation relation

$$-i\hbar = [p, x] \,. \tag{7.18}$$

Indeed we shall argue that the physical content of (7.17) is the same as the physical content of the commutation relation (7.18). Before doing it let us discuss yet another consequence of (7.17). We compare two terms

$$\left\langle x_k m\frac{x_k - x_{k-1}}{\epsilon} \right\rangle_S \quad \text{and} \quad \left\langle x_{k+1} m\frac{x_{k+1} - x_k}{\epsilon} \right\rangle_S . \tag{7.19}$$

The difference of these two terms is of order ϵ because they represent the same quantity evaluated at the neighboring moments differing by ϵ. So, when we replace the second term on the r.h.s. of (7.17) by the second term of (7.19) we obtain to leading order

$$\left\langle m\frac{x_{k+1} - x_k}{\epsilon} x_k \right\rangle_S - \left\langle x_{k+1} m\frac{x_{k+1} - x_k}{\epsilon} \right\rangle_S = \frac{\hbar}{i} \left\langle 1 \right\rangle_S , \tag{7.20}$$

which we can write in the following form

$$\left\langle \frac{(x_{k+1} - x_k)^2}{\epsilon^2} \right\rangle_S = i\frac{\hbar}{m\epsilon} \left\langle 1 \right\rangle_S \tag{7.21}$$

or

$$\left\langle \frac{(x_{k+1}-x_k)^2}{\epsilon} \right\rangle_S = i\frac{\hbar}{m}\langle 1 \rangle_S \,. \tag{7.22}$$

This last relation is nothing else than the relation characterizing Brownian motion in imaginary time. Indeed, *something to be expected!*. On the other hand, (7.21) tells us that quantal trajectories do not have derivatives, i.e. velocities are undefined, again just as in the case of Brownian trajectories.

Note

In three dimensions we have the following generalizations of (7.21)

$$\begin{aligned}
\langle (x_{k+1}-x_k)^2 \rangle_S &= \langle (y_{k+1}-y_k)^2 \rangle_S = \langle (z_{k+1}-z_k)^2 \rangle_S = i\frac{\epsilon\hbar}{m}\,, \\
\langle (x_{k+1}-x_k)(y_{k+1}-y_k) \rangle_S &= \langle (x_{k+1}-x_k)(z_{k+1}-z_k) \rangle_S \\
&= \langle (y_{k+1}-y_k)(z_{k+1}-z_k) \rangle_S = 0\,.
\end{aligned} \tag{7.23}$$

End of Note

Thus a question arises what expression we may identify with the square of velocity? One can convince oneself through several different reasonings that the following "time splitting" expression is the right choice for the kinetic energy

$$\tfrac{1}{2}m\left\langle \frac{x_{k+1}-x_k}{\epsilon}\frac{x_k-x_{k-1}}{\epsilon} \right\rangle_S = \left\langle \tfrac{1}{2}m\left(\frac{x_{k+1}-x_k}{\epsilon}\right)^2 + \frac{\hbar}{2i\epsilon} \right\rangle_S . \tag{7.24}$$

For example: take $F = x_{k+1} - x_k$ in (7.13). We have $\partial F/\partial x_k = -1$. Neglecting $\epsilon V'(x_k)$ we obtain

$$\frac{\hbar}{2i\epsilon}\langle 1 \rangle_S = -\frac{1}{2\epsilon^2}\langle m(x_{k+1}-x_k)(x_{k+1}-2x_k+x_{k-1}) \rangle_S \,. \tag{7.25}$$

Indeed, inserting this into the r.h.s. of (7.24) we obtain the l.h.s.:

$$\left\langle \tfrac{1}{2}m\left(\frac{x_{k+1}-x_k}{\epsilon}\right)^2 + \frac{\hbar}{2i\epsilon} \right\rangle_S = \tfrac{1}{2}m\left\langle \frac{x_{k+1}-x_k}{\epsilon}\frac{x_k-x_{k-1}}{\epsilon} \right\rangle_S \tag{7.26}$$

Note that when the kinetic energy is integrated over time (hence multiplied by ϵ) one can use

$$\tfrac{1}{2}m\left(\frac{x_{k+1}-x_k}{\epsilon}\right)^2$$

as the kinetic energy. However as a "local object" one must employ (7.24). Note also that according to (7.21), the r.h.s. of (7.24) vanishes but only to order $O(\frac{1}{\epsilon})$. To order $O(1)$ it is finite and, as (7.24) tells us, represents the kinetic energy.

In order to support the statement that (7.17) is equivalent to the commutation relation (7.18) let us check that the functional

$$F = \frac{m}{\epsilon}(x_{k+1} - x_k)$$

indeed acts as the operator of momentum. We write the matrix element of F in a discretized form

$$<\chi|\frac{m}{\epsilon}(x_{k+1} - x_k)|\psi>_S \; = \; \frac{m}{\epsilon}\big(\langle\chi|x_{k+1}|\psi\rangle_S - \langle\chi|x_k|\psi\rangle_S\big) \tag{7.27}$$

where

$$<\chi|x_k|\psi>_S \; = \; \frac{1}{\mathcal{N}}\int \chi^*(x_N)\, x_k\, e^{\frac{i}{\hbar}S(\ldots x_{k+1},x_k,x_{k-1}\ldots)}\,\psi(x_1)\ldots\frac{dx_k}{\mathcal{N}}\ldots dx_N dx_1 \tag{7.28}$$

where $\mathcal{N} = \sqrt{2\pi i\hbar\epsilon/m}$, and

$$\begin{aligned} S(\ldots x_{k+1}, x_k, x_{k-1}, \ldots) \; &= \; \sum_{k=1}^{N-1} S[x_{k+1}, t_{k+1}; x_k, t_k] \\ &= \; \sum_{k=1}^{N-1} \epsilon L\Big(\frac{x_{k+1} - x_k}{\epsilon}, \frac{x_{k+1} + x_k}{2}, \frac{t_{k+1} + t_k}{2}\Big)\,. \end{aligned} \tag{7.29}$$

The propagator

$$K(x_{k+1}, x_k) \; = \; \frac{1}{\mathcal{N}}\, e^{\frac{i}{\hbar}\epsilon L(\frac{x_{k+1}-x_k}{\epsilon}, \frac{x_{k+1}+x_k}{2}, \frac{t_{k+1}+t_k}{2})} \tag{7.30}$$

shifts the wave functions one step, either forward

$$\psi(x_{k+1}) \; = \int K(x_{k+1}, x_k)\,\psi(x_k)\,dx_k \tag{7.31}$$

or backward in time

$$\chi^*(x_k) \; = \int \chi^*(x_{k+1})\,K(x_{k+1}, x_k)\,dx_{k+1}\,. \tag{7.32}$$

(Show that $K^*(x_{k+1}, x_k)$ propagates *backward in time*!). Thus

$$\begin{aligned} &<\chi|\frac{m}{\epsilon}(x_{k+1} - x_k)|\psi>_S \; = \\ &\qquad = \; \frac{m}{\epsilon}\Big[\int \chi^*(x, t+\epsilon)\, x\, \psi(x, t+\epsilon)\, dx \; - \; \int \chi^*(x,t)\, x\, \psi(x,t)\, dx\Big]\,. \end{aligned} \tag{7.33}$$

Since

$$\psi(x, t+\epsilon) \; = \; \psi(x,t) \; - \; \frac{i\epsilon}{\hbar}\, H\psi(x,t)$$

$$\chi^*(x, t+\epsilon) \; = \; \chi^*(x,t) \; + \; \frac{i\epsilon}{\hbar}\,(H\chi(x,t))^*\,,$$

we obtain from (7.33)

$$\lim_{\epsilon\to o} <\chi|\frac{m}{\epsilon}(x_{k+1}-x_k)|\psi>_S \;=\; -\frac{i}{\hbar}m\int \chi^*(x)\,(xH-Hx)\,\psi(x)\,dx\,. \qquad (7.34)$$

Since

$$Hx - xH \;=\; -\frac{\hbar^2}{m}\frac{\partial}{\partial x}\,,$$

we finally obtain

$$\lim_{\epsilon\to o} <\chi|\frac{m}{\epsilon}(x_{k+1}-x_k)|\psi>_S = \int \chi^*(x)\,\frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x)\,dx\,. \qquad (7.35)$$

`====>  Example added`

Example

In this example we shall show that the proper way of discretizing the commutation relation for the momentum operator (7.35) consists in writing a *path ordered* product

$$\frac{m}{\epsilon}\,\langle\chi\,|x_{k+1}(x_{k+1}-x_k)-(x_{k+1}-x_k)x_k|\,\psi\rangle \stackrel{?}{=} i\hbar\,\langle\chi|\psi\rangle \qquad (7.36)$$

which can be conveniently rewritten as

$$\left\langle\chi\left|x_{k+1}^2+x_k^2-2x_{k+1}x_k\right|\psi\right\rangle \stackrel{?}{=} \frac{i\hbar\epsilon}{m}\,\langle\chi|\psi\rangle\,. \qquad (7.37)$$

For further calculations let us denote

$$t_{k+1}=t,\; t_k=t-\epsilon,\; x_{k+1}=x,\; x_k=y=x+\eta. \qquad (7.38)$$

(which is more convenient here than previously used $t_k = t$). Therefore

$$\begin{aligned}\left\langle\chi\left|x_k^2\right|\psi\right\rangle &= \int dy\,\chi^*(y,t-\epsilon)y^2\psi(y,t-\epsilon)\\ \left\langle\chi\left|x_{k+1}^2\right|\psi\right\rangle &= \int dx\,\chi^*(x,t)x^2\psi(x,t). \end{aligned}\qquad (7.39)$$

Although for the purpose of this example it is enough to work up to linear order in ϵ, we shall shortly need expression (7.37) up to ϵ^2. In the first integral the dummy integration variable y can be renamed as x and the remainder has to be expanded in ϵ:

$$\begin{aligned}\left\langle\chi\left|x_k^2\right|\psi\right\rangle &= \int dx\,\chi^*(x,t-\epsilon)x^2\psi(x,t-\epsilon)\\ &= \int dx\,\left[\chi^*x^2\psi-\epsilon\left(\chi^*x^2\frac{d\psi}{dt}+\frac{d\chi^*}{dt}x^2\psi\right)\right.\\ &\qquad\left.+\frac{\epsilon^2}{2}\left(\chi^*x^2\frac{d^2\psi}{dt^2}+2\frac{d\chi^*}{dt}x^2\frac{d\psi}{dt}+\frac{d^2\chi^*}{dt^2}x^2\psi\right)\right] \end{aligned}\qquad (7.40)$$

where we omit arguments of the wave functions if they refer to the point (x,t). We shall make use of the Schrödinger equation

$$\begin{aligned} \frac{d\psi}{dt} &= -\frac{i}{\hbar}H\psi, \quad \frac{d\chi^*}{dt} = \frac{i}{\hbar}\chi^* H, \\ \frac{d^2\psi}{dt^2} &= -\frac{1}{\hbar^2}H^2\psi, \quad \frac{d\chi^*}{dt} = -\frac{1}{\hbar^2}\chi^* H^2 \end{aligned}$$

which leads to

$$\begin{aligned} \langle\chi\,|x_k^2|\,\psi\rangle = \int dx\,\chi^* x^2\psi \quad &- \quad \frac{i\epsilon}{\hbar}\int dx\chi^*\left[H,x^2\right]\psi \\ &- \quad \frac{\epsilon^2}{2\hbar^2}\int dx\chi^*[H,[H,x^2]]\psi. \end{aligned} \tag{7.41}$$

In order to check (7.37) we shall work with accuracy $\mathcal{O}(\epsilon)$. Evaluating the commutator

$$\left[H,x^2\right] = -\frac{\hbar^2}{2m}\left[\frac{d^2}{dx^2},x^2\right] = -\frac{\hbar^2}{m}\left\{1+2x\frac{d}{dx}\right\}. \tag{7.42}$$

gives

$$\langle\chi\,|x_{k+1}^2+x_k^2|\,\psi\rangle = 2\int dx\,\chi^* x^2\psi + \frac{i\epsilon\hbar}{m}\int dx\chi^*\left\{1+2x\frac{d}{dx}\right\}\psi. \tag{7.43}$$

Now let us consider

$$\langle\chi\,|x_{k+1}x_k|\,\psi\rangle = \int dx\,dy\,\frac{1}{A}e^{-\beta(x-y)^2}\chi^*(x,t)\,yx\,e^{-\frac{i\epsilon}{\hbar}U}\psi(y,t-\epsilon) \tag{7.44}$$

Expanding in η we get (see exercise on the Schrödinger equation, eq.(**??**))

$$\begin{aligned} \langle\chi\,|x_{k+1}x_k|\,\psi\rangle &= \int dx\,\chi^* x^2\left(\psi+\epsilon\frac{d\psi}{dt}+\frac{\epsilon^2}{2}\frac{d^2\psi}{dt^2}\right)\Bigg|_{t=t-\epsilon} \\ &+ \int dx\,\chi^* x\int\frac{d\eta}{A}e^{-\beta\eta^2} \\ &\quad \left(\eta^2\psi'+\frac{1}{6}\eta^4\psi'''-\frac{i\epsilon}{\hbar}\eta^2\left(\frac{1}{2}V'\psi+V\psi'\right)\right)\Bigg|_{t=t-\epsilon}. \end{aligned}$$

Note that the argument of function ψ is here $\psi(x,t-\epsilon)$. The first line above equals ψ by virtue of the Schrödinger equation. Indeed

$$\begin{aligned} \left(\psi+\epsilon\frac{d\psi}{dt}+\frac{\epsilon^2}{2}\frac{d^2\psi}{dt^2}\right)\Bigg|_{t=t-\epsilon} &= \psi-\epsilon\frac{d\psi}{dt}+\frac{\epsilon^2}{2}\frac{d^2\psi}{dt^2} \\ &+ \epsilon\frac{d\psi}{dt}-\epsilon^2\frac{d^2\psi}{dt^2}+\frac{\epsilon^2}{2}\frac{d^2\psi}{dt^2} \\ &= \psi. \end{aligned} \tag{7.45}$$

Integrating the second line over η gives

$$\begin{aligned} \langle\chi\,|x_{k+1}x_k|\,\psi\rangle &= \int dx\chi^* x^2\psi \\ &+ \int dx\,\chi^* x\left(\frac{i\hbar\epsilon}{m}\psi'-\frac{\hbar^2\epsilon^2}{2m^2}\psi'''+\frac{\epsilon^2}{m}\left(\frac{1}{2}V'\psi+V\psi'\right)\right)\Bigg|_{t=t-\epsilon} \end{aligned} \tag{7.46}$$

To calculate (7.37) we need (7.47) with accuracy linear in ϵ:

$$\langle\chi\left|x_{k+1}x_k\right|\psi\rangle = \int dx\chi^* x^2\psi + \frac{i\hbar\epsilon}{m}\int dx\chi^* x\frac{d\psi}{dx}. \tag{7.47}$$

So finally

$$\begin{aligned}\left\langle\chi\left|x_{k+1}^2 + x_k^2 - 2x_{k+1}x_k\right|\psi\right\rangle &= 2\int dx\,\chi^* x^2\psi + \frac{i\hbar\epsilon}{m}\int dx\chi^*\left\{1 + 2x\frac{d}{dx}\right\}\psi \\ &\quad -2\int dx\chi^* x^2\psi - 2\frac{i\hbar\epsilon}{m}\int dx\chi^* x\frac{d\psi}{dx} \\ &= \frac{i\hbar\epsilon}{m}\left\langle\chi|\psi\right\rangle. \end{aligned} \tag{7.48}$$

in agreement with the commutation rule $[x,p] = i\hbar$.

End of Example

The exercise above boils down to the equalities:

$$<\chi|m\frac{x_{k+1}-x_k}{\epsilon}x_k|\psi>_S = \int \chi^*(x,t)\,\frac{\hbar}{i}\frac{\partial}{\partial x}x\psi(x,t)\,dx \tag{7.49}$$

and

$$<\chi|x_{k+1}m\frac{x_{k+1}-x_k}{\epsilon}|\psi>_S = \int \chi^*(x,t)\,x\frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x,t)\,dx\,, \tag{7.50}$$

thus, indeed, the content of (7.17) is equivalent to the commutation relation (7.18).

`====>  Example added below`

Example

In this example we shall show explicitly that the properly defined discrete kinetic energy reads

$$T = \frac{m}{2}\left\langle\chi\left|\left(\frac{x_{k+1}-x_k}{\epsilon}\right)^2 - \frac{i\hbar}{m\epsilon}\right|\psi\right\rangle. \tag{7.51}$$

Since, the $\mathcal{O}(1/\epsilon)$ term is equal 0 (once we have subtracted $\frac{i\hbar}{m\epsilon}$) by virtue of the commutation relation (7.36), we have to extend calculation from the previous example to the second order in ϵ. Consider first (see eqs.(7.47,7.41))

$$\begin{aligned}\left.\left\langle\chi\left|x_{k+1}^2\right|\psi\right\rangle\right|_{\epsilon^2} &= 0 \\ \left.\left\langle\chi\left|x_k^2\right|\psi\right\rangle\right|_{\epsilon^2} &= -\frac{\epsilon^2}{2\hbar^2}\int dx\chi^*[H,[H,x^2]]\psi. \end{aligned} \tag{7.52}$$

The double commutator can be written as:

$$[H,[H,x^2]] = 2\frac{\hbar^2}{m}\left(\frac{\hbar^2}{m}\frac{d^2}{dx^2} + x\,V'\right) \tag{7.53}$$

and we get

$$\langle \chi \left| x_k^2 \right| \psi \rangle \big|_{\epsilon^2} = \frac{1}{m^2} \int dx\, \chi^* p^2 \psi - \frac{1}{m} \int dx\, \chi^* x V'\, \psi. \tag{7.54}$$

Similarly, from the next term we have to retain only pieces proportional to ϵ^2:

$$\langle \chi \left| x_{k+1} x_k \right| \psi \rangle|_{\epsilon^2} = \frac{1}{m} \int dx\, \chi^* x \left(-i\hbar \frac{d\psi'}{dt} - \frac{\hbar^2}{2m} \psi''' + \left(\frac{1}{2} V' \psi + V \psi' \right) \right). \tag{7.55}$$

Since

$$-i\hbar \frac{d\psi'}{dt} = -i\hbar \frac{d}{dx} \frac{d\psi}{dt} = -\frac{d}{dx} (H\psi). \tag{7.56}$$

The last term reads

$$\begin{aligned} -\frac{d}{dx}(H\psi) &= -\frac{d}{dx} \left(-\frac{\hbar^2}{2m} \psi'' + V\psi \right). \\ &= \frac{\hbar^2}{2m} \psi''' - V'\psi - V\psi'. \end{aligned} \tag{7.57}$$

Hence the round bracket in eq. (7.55) reads

$$(\ldots) = \frac{\hbar^2}{2m} \psi''' - V'\psi - V\psi' - \frac{\hbar^2}{2m} \psi''' + \frac{1}{2} V'\psi + V\psi' = -\frac{1}{2} V'\psi$$

and

$$\langle \chi \left| x_{k+1} x_k \right| \psi \rangle|_{\epsilon^2} = -\frac{1}{2m} \int dx\, \chi^* x V' \psi \tag{7.58}$$

which cancels the V' term in eq.(7.54). Summarizing, we get

$$T = \frac{m}{2} \langle \chi | \frac{1}{\epsilon^2} \left(x_{k+1}^2 - 2 x_{k+1} x_k + x_k^2 \right)^2 - \frac{i\hbar}{m\epsilon} | \psi \rangle = \frac{1}{2m} \langle \chi | \, p^2 \, | \psi \rangle \tag{7.59}$$

where $p = -i\hbar\, d/dx$. Hence we have shown explicitly that (7.51) is the proper expression for a discretized kinetic energy operator.

End of Example

To close this part let us discuss some useful formulae for Gaussian amplitudes. Now S is a quadratic form and we can evaluate the transition amplitudes for the functional

$$F = e^{\frac{i}{\hbar} \int f(t) x(t) dt}, \tag{7.60}$$

where $f(t)$ is an arbitrary function of time. We have

$$\left\langle e^{\frac{i}{\hbar} \int f(t) x(t) dt} \right\rangle_S = \int\limits_{x(t_a)=a, x(t_b)=b} e^{\frac{i}{\hbar} [S + \int f(t) x(t) dt]} \, [\mathcal{D}x(t)] \, . \tag{7.61}$$

When S is Gaussian, so is $S' = S + \int f(t) x(t) dt$, and we know how to calculate (7.61). We have a factor $\exp(i\hbar S'_{\rm cl}/\hbar)$, where $S'_{\rm cl}$ is evaluated for a classical trajectory, and the remaining factor is the sum over trajectories $y(t)$, which run from $y(t_a) = 0$ to $y(t_b) = 0$. Denoting the quadratic part of S' by S'_2 (the quadratic part of $S = S_2 = S'_2$), we have

$$\left\langle e^{\frac{i}{\hbar}\int f(t)x(t)dt} \right\rangle_S = e^{\frac{i}{\hbar}S'_{\rm cl}}\,\Phi \tag{7.62}$$

where

$$\Phi = \int [\mathcal{D}y(t)]\, e^{\frac{i}{\hbar}S'_2[y(t)]}\,. \tag{7.63}$$

On the other hand

$$\langle 1 \rangle_S = \int [\mathcal{D}x(t)]\, e^{\frac{i}{\hbar}S[x(t)]} = e^{\frac{i}{\hbar}S_{\rm cl}}\,\Phi\,, \tag{7.64}$$

because $S'_2 = S_2$. Thus

$$\Phi = \langle 1 \rangle_S \; e^{-\frac{i}{\hbar}S_{\rm cl}}\,. \tag{7.65}$$

Inserting it into (7.62) we obtain

$$L = \left\langle e^{[\frac{i}{\hbar}\int f(t)x(t)dt]} \right\rangle_S = \langle 1 \rangle_S \; e^{\frac{i}{\hbar}(S'_{\rm cl} - S_{\rm cl})} = R\,. \tag{7.66}$$

From (7.66) we get some useful relations. For instance,

$$\left.\frac{\delta L}{\delta f(t)}\right|_{f(t)=0} = \left.\frac{\delta R}{\delta f(t)}\right|_{f(t)=0} \tag{7.67}$$

gives an average

$$\langle x(t) \rangle_S = \left.\frac{\delta S'_{\rm cl}}{\delta f(t)}\right|_{f(t)=0} \langle 1 \rangle_S\;, \tag{7.68}$$

whereas a double functional differentiation gives a correlation function:

$$\begin{aligned}\langle x(t)x(s) \rangle_S &= \left(\frac{\hbar}{i}\right)^2 \frac{\delta^2}{\delta f(t)\delta f(s)}\, e^{\frac{i}{\hbar}(S'_{\rm cl} - S_{\rm cl})}\bigg|_{f=0} \langle 1 \rangle_S \\ &= \langle 1 \rangle_S \left(\frac{\hbar}{i}\frac{\delta^2 S'_{\rm cl}}{\delta f(t)\delta f(s)} + \frac{\delta S'_{\rm cl}}{\delta f(t)}\frac{\delta S'_{\rm cl}}{\delta f(s)} \right)\bigg|_{f=0}\,. \end{aligned} \tag{7.69}$$

Since $S'_{\rm cl}$ is a quadratic function of $f(t)$, a correlation function of an arbitrary number of x's is expressible through the first and the second functional derivatives,

$$\frac{\delta S'_{\rm cl}}{\delta f(t)} \qquad \text{and} \qquad \frac{\delta^2 S'_{\rm cl}}{\delta f(t)\delta f(s)}\,,$$

only!