# CHAPTER II

# PATH INTEGRALS AND PROPAGATORS IN QUANTUM AND IN STATISTICAL MECHANICS

## 2.1 INTRODUCTION

We first discuss the general concept of the superposition of probability amplitudes in quantum mechanics. We then show how this conceptual be directly extended to define a probability amplitude for any motion or path (position vs time) in space - time. The ordinary quantum mechanics is show to result from the postulate that this probability amplitude has a phase proportional to the action, computed classically, for this path. This is true when the action is the time integral of a quadratic function of velocity. The relation to matrix and operator algebra is discussed in a way formulation as possible. There is no practical advantage to this, but the formulae are very suggestive if a generalization to a wider class of action functionals is contemplated. Finally, we discuss applications of the formulation.

### 2.1.1 The Superposition of Probability Amplitudes

The formulation to be presented contains as its essential idea the concept of a probability amplitude associated with a completely specified motion as a function of time. It is, therefore, worthwhile to review in detail the quantum-mechanical concept of the superposition of probability amplitudes. We shall examine the essential change in physical outlook required by the transition from classical to quantum physics.

For this purpose, consider an imaginary experiment in which we can make three measurements successive in time: first of a quantity $A$, then of $B$, and then of $C$. There is really no need for these to be of different quantities of three successive position measurements is kept in mind. Suppose that $a$ is one of a number of possible results which could come from measurement $A$, $b$ is $a$ result that could arise from $B$, and $c$ is $a$ result possible from the third measure - ments $C$. We shall assume that the measurements $A$, $B$, and $C$ are the type of measurements that completely specify a state in the quantum - mechanical case. That is, for example, the state for which $B$ has the value $b$ is not degenerate.

It is well known that quantum mechanics deals with probabilities, but naturally this is not the whole picture. In order to exhibit, even more clearly, the reationship between classical and quantum theory, we could suppose that classically we are also dealing with probabilities but that all probabilities either are zero or one. A better alternative is to imagine in the classical case that the probabilities are in the sense of classical statistical mechanics (where, possibly, internal coordinates are not completely specified).

We define $P_{ab}$ as the probability that if measurment $A$ gave the result $a$, then measurement $B$ will give the result $b$. Similarly, $P_{bc}$ is the probability that if measurement $B$ gives the result $b$, then measurement $A$ gives $a$, then $C$ gives $c$. Further, let $P_{ac}$ be the chance that if $A$ gives $a$, then $C$ give $c$. finally, denote by $P_{abc}$ the probability of all three, i.e., if $A$ gives $a$, then $B$ gives $b$, and $C$ gives $c$. If the events between $a$ and $b$ are independent of those between $b$ and $c$,

$$P_{abc} = P_{ab} P_{bc}. \tag{2.0.1}$$

This is true according to quantum mechanics when the statement that $B$ is $b$ is $a$ complete specification of the state.

In any event, we expect the relation

$$P_{ac} = \sum_{b} P_{abc}. \tag{2.0.2}$$

This is because, if initially measurement $A$ give $a$ and the system is later found to give the result $c$ to measurement $C$, the quantity $B$ must have had some value at the time intermediate to $A$ and $C$. The probability that it was $b$ is $P_{abc}$ We sum, or integrate, over all the mutually exclusive alternatives for $b$ (symbolizes by $\sum_b$).

Now, the essential difference between classical and quantum physics in eq. (2.0.2). In classical mechanics it is always true. In quantum mechanics it is often false. We shall denote the quantum - mechanical probability that a measurement of $C$ results in $c$ when it follows a measurement of $A$ giving $a$ by $P_{ac}$ . Equation (2.0.2) is replaced in quantum mechanics by this remarkable law: There exist complex numbers $\psi_{ab}, \psi_{bc}, \psi_{ac}$ such that

$$P_{ab} = |\psi_{ab}|^2, P_{bc} = |\psi_{bc}|^2, \text{ and } P_{ac} = |\psi_{ac}|^2, \tag{2.0.3}$$

The classical law, obtained by combining and,

$$P_{ac} = \sum_{b} P_{ab} P_{bc} \tag{2.0.4}$$

is replaced by

$$\psi_{ac} = \sum_{b} \psi_{ab} \psi_{bc} \qquad (2.0.5)$$

However, it seems worth while to emphasize the fact that they are all simply direct consequences of eq. (2.0.5), for it is essentially eq. (2.0.5) that is fundamental in the formulation of quantum mechanics.

The generalization of eqs. (2.0.4) and (2.0.5) to alarge number of measurements, say $A, B, C, D, \ldots, K$, is, of course, that the probability of the sequence $a, b, c, d, \ldots, k$ is

$$P_{abcd\ldots k} = |\psi_{abcd\ldots k}|^2 .$$

The probability of the result $a, c, k$, for example, if $b, d, \ldots$ are measured, is the classical formula:

$$P_{abcd\ldots k} = \sum_{b} \sum_{d} \ldots P_{abcd\ldots k} \qquad (2.0.6)$$

while the probability of the same sequence $a, c, k$ if no measurements are made between $A$ and $C$ and between $C$ and $K$ is

$$P_{ack} = | \sum_{b} \sum_{d} \ldots \psi_{abcd\ldots k} |^2 . \qquad (2.0.7)$$

The quantity $\psi_{abcd\ldots k}$ we can call the probability amplitude for the condition $A = a, B = b, C = c, D = d, \ldots, K = k$. (It is, of course, expressible as a product $\psi_{ab}, \psi_{bc}, \psi_{ac} \cdots \psi_{jk}$.)

### 2.1.2 Measurement of Probability Amplitudes Via Young - slits Experiment.

In his lectures on quantum mechanics, Feynman (1965) introduces a basic concept of the subject, that of *probability amplitudes*, by considering a Young - slits interference experiment performed with electrons. In this experiment, electrons emitted by a source A arrive at a (variable) target point B on a screen $S'$, having first passed through another screen S pierced by two slits (1) and (2). To the two possible trajectories there correspond respectively two probability amplitudes $a_1$ and $a_2$, given by the following rules (in a selfexphanatory notation: see Fig 2.1):[4]

$$a_1 = a_{B1}a_{1A};\, a_2 = a_{B2}a_{2A}$$

The probability amplitude a for observing an electron at B is the sum of $a_1$ and $a_2$

$$a = a_1 + a_2 = \sum_{j=1}^{2} a_{Bj}a_{jA}$$

Let us now complicate the experiment somewhat by introducing several intermediate screen J, K, L, each pierced by several slits numbered j, k, and l. Then the probability amplitude a reads

$$a = \sum_{j,k,l} a_{Bl}a_{lK}a_{Kj}a_{jA}$$

It is a sum over all paths leading from A to B: in Fig. 2.2 for instance we have drawn the path $A \rightarrow J(1) \rightarrow K(2) \rightarrow L(1) \rightarrow B$.

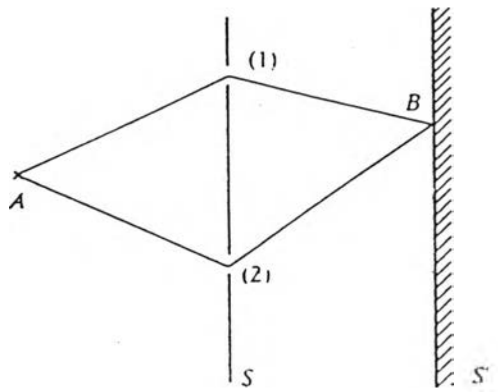



**Fig. 2.1** The young's slits experiment

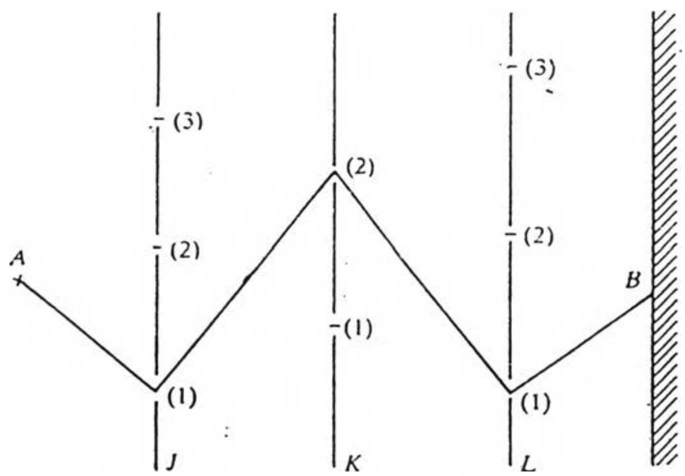



**Fig. 2.2** A complicated variant of the Young's slits experiment

One can now replace the screens by a potential in which the electrons move, and associate with every path [c] leading from A to B a probability amplitude $a$ [c], the total amplitude $a$ being the sum (see Fig. 2.3)

$$a = \sum_{[c]} a[c]. \tag{2.1.1}$$

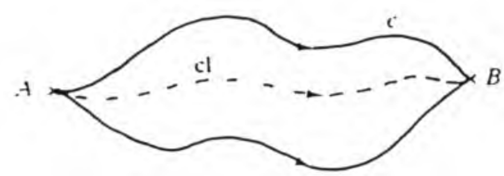



**Fig. 2.3** Paths from A to B

It remains of course to give a prescription for $a$ [c], and for summing over the paths. This will be done in Section 2.2; there, starting from the properties of the evolution operator exp *(-iHt)*, we shall show that the statistical weight of each path, namely $a$ [c], is given by

$$a[c] \sim \exp\left(\frac{i}{\hbar} S(B,A)\right), \tag{2.1.2}$$

where ~ simply denotes proportionality, and where S(B, A) is the classical action evaluated along the path leading from A to B in a given time. Conversely, one can adopt (2.1.1) and (2.1.2) as fundamental postulates, and derive all the results of quantum mechanics from them: in other words one can adopt, as one's quantization postulate, equation (2.1.2) instead of the canonical commutation rule (CCR) $[\hat{q}, \hat{p}] = i\hbar$

In quantum mechanics, an important role is often played by the classical path from A to B, i.e. by the path which makes the action stationary. In the corresponding problem of classical statistical mechanics, the configuration analogous to the classical path is the 'Landau configuration', namely that configuration for which the Hamiltonian is stationary. To the quantum fluctuations around the classical path there correspond the statistical fluctuations around the Landau configuration. Such fluctuations are stadied by means of perturbation theory, and it is not surprising that one should meet the same techniques in both types of problem.

In Section 2.2 we establish the dictionary for traslating the Schroediger equation into the language of the path integrals, by giving a precise meaning to the sum in (2..1.1).

## 2.2 PARTICLE IN POTENTIAL

Envisage now a quantum system slightly more complicated than a spin $\frac{1}{2}$, namely a (nonrelativistic) particle of mass moving on a straight line in a potential V(q). We denote the operatore for position and momentum by $\hat{q}$ and $\hat{p}$ respectively, and their eigenstates in the Schroedinger picture by $|q\rangle$ and $|p\rangle$. We choose the normalization $\langle p|p'\rangle = \delta(p-p'), \langle q|q'\rangle = \delta(q-q'),$ and $\langle p|q\rangle = (2\pi)^{-1/2}$ exp$(iq.p)$. $\hat{q}(t)$ and $|q,t\rangle$ stand for the position operator and for its eigenvectors in the Heisenberg picture.

$$\hat{q}(t) = e^{iHt/\hbar}\hat{q}e^{-iHt/\hbar}$$
$$|q,t\rangle = e^{iHt/\hbar}|q\rangle. \tag{2.2.1}$$

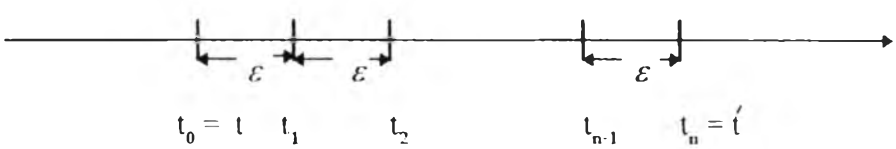
### 2.2.1 The representation of probability amplitudes by path integrals

Let $K(q',t';q,t)$ be the probability amplitude that a particle initially at q time t be found at $q'$ at time $t'$ (so that the boundary condition are $q(t) = q, q(t') = q'$:

$$K(q',t';q,t) = \langle\, q',t'|q,t\,\rangle = \langle\, q'|\; e^{\frac{-iH}{\hbar}(t'-t)}|q\rangle \tag{2.2.2}$$

Drivide the interval $[t,t']$ into (n) subintervals each of length

$\varepsilon = (t'-t)/(n), with\ \varepsilon \to 0$:



and let us write

$$\exp(-\frac{iH}{\hbar}(t'-t)) = \left(\exp\left[-\frac{i\varepsilon}{\hbar}\left(\frac{p^2}{2m}+V(\hat{q})\right)\right]\right)^n$$

We now use Trotter's (or the Lie product) theorem

$$\lim_{n\to\infty}\left(e^{A/n}e^{B/n}\right)^n = e^{A+B} \tag{2.2.3}$$

One can find in the two references just quoted heuristic and rigorous proofs of this formula, as well as the necessary conditions on the operators A and B. It is an instructive (and elementary) exercise to carry through the proof when [A ,B] is a c-number; it is also easy to prove (2.2.3) if A and B are bounded operators (see the references just quoted). Let us now insert at times $t_1, \ldots, t_n$ complete sets of eigenstates of the position operator $\hat{q}$,

$$K(q',t':q,t) = \int_{-\infty}^{\infty}\prod_{L=1}^{n-1}dq_L\prod_{L=1}^{n}\left\langle q_L\left|\exp\left(\frac{i\varepsilon}{\hbar}\frac{\hat{p}^2}{2m}\right)\exp\left(\frac{-i\varepsilon V}{\hbar}(\hat{q})\right)\right|q_{L-1}\right\rangle.$$

and evaluate the matrix element

$$\left\langle q_L\left|\exp\left(\frac{i\varepsilon}{\hbar}\frac{\hat{p}^2}{2m}\right)\exp\left(\frac{-i\varepsilon V}{\hbar}(\hat{q})\right)\right|q_{L-1}\right\rangle$$

$$=\exp\left(\frac{-i\varepsilon}{\hbar}V(q_{L-1})\right)\left\langle q_L\left|\exp\left(\frac{i\varepsilon}{\hbar}\frac{\hat{p}^2}{2m}\right)\right|q_{L-1}\right\rangle.$$

In order to compute the last matrix element we use

$$\left\langle q_L \middle| \hat{p}^2 \middle| q_{L-1} \right\rangle = \int_{-\infty}^{\infty} dp_L \langle q_{L-1} | \hat{p}^2 | p_L \rangle \langle p_L | q_{L-1} \rangle$$

$$= \int_{-\infty}^{\infty} \frac{dp_L}{2\pi\hbar} p_L{}^2 e^{ip_L(q_L - q_{L-1})/\hbar}$$

These results allow us to write K $(q',t';q,t)$ in the form of a path integral:

$$K(q',t':q,t) =$$

$$\lim_{\varepsilon\to 0} \int_{-\infty}^{\infty} \prod_{L=1}^{n-1} dq_L \prod_{L=1}^{n} \left\{ \int_{-\infty}^{\infty} \frac{dp_L}{2\pi\hbar} \exp\left( \frac{ip_L}{\hbar} (q_L - q_{L-1}) \right) \times \exp\left( \frac{-i\varepsilon}{\hbar} \left( \frac{p_L^2}{2m} + V\left( \frac{q_L + q_{L-1}}{2} \right) \right) \right) \right\}$$

(2.2.4)

It is important to notice that in equation (2.2.4) $q_L$ and $q_{L-1}$ and classical variables as was the variable S in the previous section. We have taken as the argument of V for purely aesthetic reasons, since q or would also be correct. However, for reasons to be discussed below, it is important to choose $\frac{1}{2}(q_L + q_{L-1})$ as the argument of the vector potential if one wants to write path integrals for propagation in a magnetic field. As V is a function only of q, it is possible to perform the p-integral in (2.2.4).

$$\int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \exp\left( \frac{ipq}{\hbar} - \frac{i\varepsilon}{\hbar} \frac{p^2}{2m} \right) = \left( \frac{m}{2i\pi\varepsilon\hbar} \right)^{1/2} \exp\left( \frac{imq^2}{2\varepsilon\hbar} \right), \qquad (2.2.5)$$

and equation (2.2.4) becomes

$$K(q',t';q,t) = \lim_{\varepsilon\to 0}\left(\frac{m}{2i\pi\varepsilon\hbar}\right)^{1/2} \int\prod_{L=1}^{n-1}\left[\left(\frac{m}{2i\pi\varepsilon\hbar}\right)^{\frac{1}{2}} dq_L\right]$$

$$\times\exp\left[i\sum_{L=1}^{n}\frac{m(q_{L-1}-q_L)^2}{2\varepsilon\hbar} - \frac{i\varepsilon}{\hbar}\sum_{i=1}^{n}V\left(\frac{q_L+q_{L-1}}{2}\right)\right]$$

(2.2.6)

Here we introduce the compact symbol Dq for integration over the q , and note that

$$\frac{\varepsilon}{\hbar}\sum_{L=1}^{n}V\left(\frac{q_L+q_{L-1}}{2}\right)\to\int_t^{t'}V(q(t''))dt'',$$

$$\frac{\varepsilon}{\hbar}\sum_{L=1}^{n}\frac{m(q_{L-1}-q_L)^2}{2\varepsilon^2\hbar}\to\int_t^{t'}m\left(\frac{dq}{dt''}\right)^2 dt'';$$

then as the final form of the path integral one finds

$$K(q',t';q,t) = \int Dq\exp\left(\frac{i}{\hbar}\int_t^{t'} mq^{\bullet 2} - V(q)\right)dt''\Bigg)$$

$$= \int Dq\exp\left(\frac{i}{\hbar}S\right),$$

(2.2.7)

subject to the boundary conditions $q(t) = q, q(t') = q'$.

In equation (2.2.7) we have reinstated Planck's constant $\hbar$ and set q = dp/dt ;

$$L(q,\dot{q}) = \frac{1}{2}m\dot{q}^2 - V(q) \tag{2.2.8}$$

is the Lagrangean of the particle: and S is the corresponding **action**

$$S = \int_t^{t'} L(q,\dot{q})dt''. \tag{2.2.9}$$

In quantum mechanics, it is diffcult to go further into the mathematical discussion of the paths, since it has not been possible to give a satisfactory mathemati-cal meaning to the measure $\exp(iS)\,Dq$.

Using the totations of (2.2.7) one can transform (2.2.4) and obtain the Humiltonian form of the path integral, namely

$$K(q',t';q,t) = \int DpDq \exp\left(\frac{i}{\hbar}\int_t^{t'} \left[p\dot{q} - H(p,q)\right]dt''\right). \tag{2.2.10}$$

This equation must be used when the Hamiltonian is not quadratic in p; however. it must be handled with care. Contrary to its appearance. it is not invariant under canonical transformations.

Consider eq. (2.2.7) the path from A: (q, t) to B: $(q',t')$; to it there correspond a certain action S. Equation (2.2.7) can be interpreted as assigning to each path a statistical weight $\exp(iS/\hbar)$, and asserting that the probability amplitude is obtained by summing over all such paths. In the procedure we have followed, the sum over paths has been defined thus. The paths are zigzags whose straight portions join the positions $q, q_1 \ldots, q'$ of the particle at times $t, t_1 \ldots t'$ respectively (Fig. 2.4). Summing over the paths consists of integrating, with fixed q and $q'$, over all the $q_L$ corresponding to intermediate times t , with the integration measure

$$\left(\frac{m}{2i\pi\varepsilon\hbar}\right)^{1/2} \prod_{L=1}^{n-1}\left(\frac{m}{2i\pi\varepsilon\hbar}\right)^{1/2} dq_L \rightarrow Dq.$$

Here, as already emphasized, the symbol Dq means nothing more than is implied by (2.2.6).

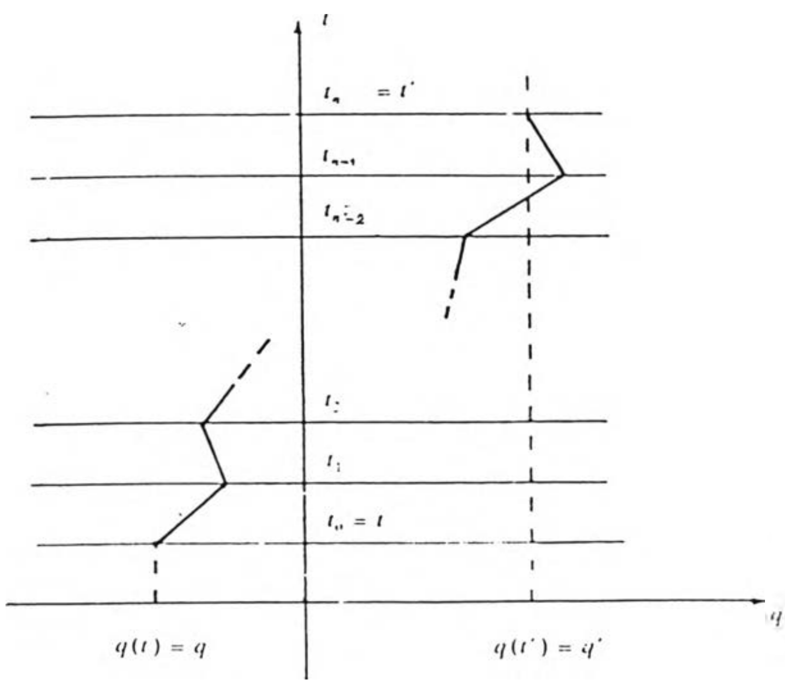



**Fig.** 2.4 Trajectories used in evaluating (2.2.6)