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PATH INTEGRALS IN
QUANTUM AND STATISTICAL MECHANICS

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PATH INTEGRALS IN QUANTUM AND STATISTICAL MECHANICS

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ABSTRACT

The path integral formalism of Quantum Mechanics is developed from both the Lagrangian and Hamiltonian point of view. Some exact propagators are calculated. Several statistical mechanics problems are discussed via a path integral formulation of the statistical density matrix and an application to second quantized Hamiltonians using coherent states is described. The variational technique is considered with illustrative examples. A review of some selected recent achievements of the technique is presented.

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PROLOGUE

Quantum mechanics began with seemingly two distinct formulations, one due to Schrodinger and other due to Heisenberg. Later on these were show n to be unitarily equivalent.

Approximately two decades later Feynman, in trying to find out the meaning of what he himself describes as some mysterious remarks by Dirac[2] came up with an entirely new formulation which turned out to be equivalent to quantum mechanics. Whereas the Schrodinger formulation is Hamiltonian based, the Feynman formulation is tied to Lagrangian mechanics.

With the above fact in mind nothing new can be expected to come out of the Feynman formulation but there surely is a pleasure in recognizing old things from a new point of view as Feynman puts it. The formalism is worth it for its aesthetic value.

Besides, it is extremely gratifying from a conceptual point of view. By imposing a sensible set of requirements on a physical theory, we are inescably led to a formalism equivalent to the usual quantum mechanics is remarkable in itself. It makes one wonder whether it is at all possible to construct a sensible alternative theory that is equally successful in accounting for microscopic phenomena.

The path integral formulation does not lead to simplifications, in general, but, in a class of problems it does give the full propagator or the transition amplitude with tremendous ease as well as it provides valuable insight into the relation between classical and quantum mechanics.

At the outset it is hard to say where a given approach can find its best applications directly or indirectly. So it has been with the path integral approach. Originally designed to apply to problems in quantum electrodynamics where it commonly goes in the name of Feynman's space time approach, or propagator theory, it has now become a valuable and powerful tool in problems of statistical mechanics and probability theory besides a quantum field theory. Some of these we shall get a flavour of as we go along.[3]

Finally, the relation between Schrodinger mechanics and path integrals is parallel to that between the Newtonian and least action formalism of mechanics. Whereas the former approach is local in time and deals with time evolution over infinitesimal periods, the latter is global and deals directly with propagation over finite times.[4]

The plan of this presentation goes as follows. We begin with a discussion of the time evolution operator in quantum mechanics and then obtain the Feynman path integral following Dirac's hint.[5] We then see how the path integral can directly obtained from the Schrodinger equation.[6] The next chapter is devoted to some simple evaluations and the Bohm-Aharnov effect. We gradually learn that the path integral is closely related to the density matrix in statistical mechanics which then leads to survey statistical mechnics via path integrals. One can also see that path integrals can be used for second quantized Hamiltonians. The variational method with some discussion of the partition function comes next. A small survey at the end discusses the problems which can be handled with the path integral technique but which we could not cover in this limited study. This, incidently, at least demonstrates to us the powerful nature of this technique using functional integrals.[7,8]

CHAPTER ONE

THE TIME EVOLUTION OPERATOR AND ITS PATH INTEGRAL FORMULATION

..1 The Properties of the Time Evolution Operator

We begin by reviewing the properties of the time evolution operator (also known as the propagator) in quantum mechanics.

Let a system at time t_0 be represented by the state vector $|\alpha> \equiv |\alpha, t_0>$. At a later time let the state vector be $|\alpha, t>$. If $t \to t_0$, we expect $|\alpha, t> \to |\alpha>$. $|\alpha, t>$ is related to $|\alpha>$ via the time evolution operator $U(t,t_0)$ i.e., $|\alpha, t> = U(t,t_0)\ |\alpha>$. U is a unitary operator satisfying the following properties:

$$U(t_3,t_2)\ U(t_2,t_1) = U(t_3,t_1),$$

$$U(t_1,t_1) = I,$$

$$U^{+}(t_1,t_2) = U(t_2,t_1)\ . \qquad 1.1.1$$

Further, since $|\alpha, t> = U(t,t_0)|\alpha>$ is a solution of the Schrodinger equation and $|\alpha>$ is arbitrary it follows that

$$i\bar{h}\ \frac{dU}{dt} = HU\ . \qquad 1.1.2$$

If U is known the time evolution of the state is completely specified. Ultimately solving the time dependent

Schrodinger equation boils down to the determination of the propagator. There are three cases to be considered.

1. H is time independent, e.g., the Hamiltonian for a spin magnetic moment interacting with a time independent field. In such a case the above differential equation gives

$$U(t,t_0) = \exp\{\frac{-iH}{\hbar}(t-t_0)\} . \qquad 1.1.3$$

If t differs from t_0 by an infinitesimal amount $\Delta t(\equiv t-t_0)$ we have

$$U(t,t_0) = I - \frac{iH}{\hbar}\Delta t. \qquad 1.1.4$$

Alternatively, we can borrow from classical mechanics the idea that H is the generator of time evolution so that eq. (1.1.4) holds. Using the composition property from eq. (1.1.1) we obtain for a finite time evolution, the operator

$$\lim_{n\to\infty}\{1 - \frac{iH(t-t_0)}{n\hbar}\}^n = \exp\{\frac{-iH}{\hbar}(t-t_0)\} \qquad 1.1.5$$

where we have divided the time interval $t-t_0$ into steps of width $\varepsilon = (t-t_0)/n$ and considered successive time evolutions over each width ε. This is the case of fine partitioning which shall be used in our future discussions as well.

2. H is time dependent but H at different times commute. This would be the case of the spin - field coupling above if the direction of the field remains fixed but its magnitude becomes time dependent. Now we solve eq. (1.1.2) to obtain

$$U(t,t_0) = \exp\{-\frac{i}{\hbar}\int_{t_0}^{t} H(t')dt'\}. \qquad 1.1.6$$

3. The Hamiltonians at different times do not commute. In the above example, the field directions may be changing so that non-commuting combination of spin-operator may be involved. The formal solution in such a case is given by the Dyson series:

$$U(t,t_0) = I + \sum_{n=1}^{\infty} (-\frac{i}{\hbar})^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_{n-1}} dt_n H(t_1)\ldots H(t_n)\,. \qquad 1.1.7$$

1.2 Further on Propagators

We start with

$$|\alpha,t\rangle = \exp\{\frac{-iH}{\hbar}(t-t_0)\}|\alpha\rangle = \sum_j |j\rangle\langle j|\alpha\rangle \exp\{\frac{-iE_j}{\hbar}(t-t_0)\} \qquad 1.2.1$$

where H is time independent and $|j\rangle$ is its eigenket. Taking the inner product with a coordinate state vector $\langle\bar{r}|$ we have

$$\langle\bar{r}|\alpha,t\rangle = \sum_j \langle\bar{r}|j\rangle\langle j|\alpha\rangle \exp\{\frac{-iE_j}{\hbar}(t-t_0)\} \qquad 1.2.2$$

i.e., the wave function of the system at time t is given as

$$\psi(r,t) = \sum_j \psi_j(\bar{r}) c_j(t_0) \exp\{\frac{-iE_j(t-t_0)}{\hbar}\} \qquad 1.2.3$$

where $\psi(\bar{r},t) = \langle\bar{r}|\alpha,t\rangle$, $\psi_j = \langle\bar{r}|j\rangle$ and

$$c_j = \langle j|\alpha\rangle = \int\langle j|\vec{r}\rangle\langle\vec{r}|\alpha\rangle d^3\bar{r}' = \int\psi_j^*(\vec{r})\psi(\vec{r})d^3\bar{r}! \qquad 1.2.4$$

Eqs. (1.2.3) and (1.2.4) suggest an integral operator interpretation:

$$\psi(\bar{r},t) = \int d^3\bar{r}'\ K(\bar{r},t;\bar{r}',t_0)\psi(\bar{r}',t_0) \qquad 1.2.5$$

where the kernel of the integral operator known as the propagator in wave mechanics is given by

$$k(\bar{r},t;\bar{r}',t_0) = \sum_j \psi_j(\bar{r})\psi_j^*(\bar{r}')\exp\{\frac{-iE_j}{\hbar}(t-t_0)\}. \qquad 1.2.6$$

In any given problem the propagator depends only on the potential and is independent of the initial wave function. It can be constructed once the energy eigen functions and eigenvalues are given. The time evolution of the wave function is completely predicted if $K(\bar{r},t;\bar{r}',t_0)$ and the initial wave function are given. Schrodinger wave mechanics is thus a completely causal theory. The time development of a wave function subjected to a potential is as "deterministic" as anything else in classical mechanics provided that the system is left undisturbed.

Eq. (1.2.5) is amenable to an interpretation reminiscent of Huygens construction in wave optics. The streng of the wave amplitude arriving at $(\bar{r},t)$ from $(\bar{r}',t_0)$ will b proportional to the original amplitude $\psi(\bar{r}',t_0)$. If we denote the constant of proportionality by $K(\bar{r},t;\bar{r}',t_0)$, the total wave arriving at $(\bar{r},t)$ will be

$$\psi(\bar{r},t) = \int K(\bar{r},t;\bar{r}',t_0)\psi(\bar{r}',t_0)d^3\bar{r}' \ , \ t > t_0 \ .$$

We note two properties of K:

1. For $t > t_0$, $K(\bar{r},t;\bar{r}',t_0)$ satisfies the time-dependent Schrodinger equation. This follows trivially using either eq.(1.2.5) or eq.(1.2.6).

2. $\lim_{t\to t_0} K(\bar{r},t;\bar{r}',t_0) = \delta^3(\bar{r}-\bar{r}')$ for then the right hand side of eq. (1.2.6) becomes $\langle\bar{r}|\bar{r}'\rangle = \delta^3(\bar{r}-\bar{r}')$.

Because of these two properties the propagator regarded as a function of $\bar{r}$ is simply the wave function of a particle which was located precisely at $\bar{r}'$ at the time t_0. This follows also by noting that

$$K(\bar{r},t;\bar{r}',t_0) = \langle\bar{r}|\exp\{\frac{-iH}{\hbar}(t-t_0)\}|\bar{r}'\rangle \qquad 1.2.7$$

where the time evolution operator acting on $|\bar{r}'\rangle$ is just the state ket at t of a particle that was localized at $\bar{r}'$ at $t_0 < t$. If we wish to solve a more general problem where the initial wave function extends over a finite region of space, all we have to do is to multiply $\psi(\bar{r}',t_0)$ by the propagator $K(\bar{r},t;\bar{r}',t_0)$ and integrate over all $\bar{r}'$ adding thereby the various contributions from different positions $\bar{r}'$. This reminds us of the situation in electrostatics; if we wish to find the electrostatic potential due to a general charge distribution $\rho(\bar{r}')$, we first solve the point charge problem, multiply the solution by the charge distribution and integrate so as to get

$$\psi(\bar{r}) = \int \frac{\rho(\bar{r}')}{|\bar{r}-\bar{r}'|} d^3\bar{r}'.$$

It is easily seen that the propagator is simply the Green's function for the time-dependent wave equation

$$\{ \frac{-h^2}{2m}\nabla^2 + V(\bar{r}) - i\hbar\frac{\partial}{\partial t} \} K(\bar{r},t;\bar{r}',t_0) = -i\hbar\delta^3(\bar{r}-\bar{r}')\delta(t-t_0). \quad 1.2.8$$

proof:

Using the step function $\Theta(t-t_0)$ eq. (1.2.5) is written as

$$\Theta(t-t_0)\psi(\bar{r},t) = \int K(\bar{r},t;\bar{r}',t_0)\psi(\bar{r}',t_0)d^3\bar{r}'.$$

Now,

$$\{i\hbar \frac{\partial}{\partial t} - H(\bar{r},t)\}\Theta(t-t_0)\psi(\bar{r},t) = i\hbar\ (t-t_0)$$

$$= \int\{i\hbar\frac{\partial}{\partial t} - H(\bar{r})\}K\psi(\bar{r}')$$

Which gives

$$\{i\hbar \frac{\partial}{\partial t} - H\}\ K = i\hbar\delta^3(\bar{r}-\bar{r}')\delta(t-t_0)$$

with the boundary condition

$$K(\bar{r},t;\bar{r}',t_0) = 0, \quad t < t_0. \quad 1.2.9$$

The particular form of the propagator depends on the potential. Consider as an example a free particle in one dimension. We can use the momentum eigenfunctions $|p\rangle$, $P|p\rangle = p|p\rangle$ and

$H|p\rangle = (p^2/2m)|p\rangle$ which are plane waves to get

$$K(x,t;x',t_0) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \exp\{\frac{ip(x-x')}{\hbar} - \frac{i}{\hbar}\frac{p^2}{2m}(t-t_0)\}dp. \quad 1.2.10a$$

This integral is easily done by completing the square in the exponent giving

$$K(x,t;x',t') = \sqrt{\frac{m}{2\pi i\hbar T}} \exp\{\frac{im(x-x')^2}{2\hbar T}\} \qquad 1.2.10b$$

where $T = t-t_0$. This expression can be used to see how a Goussian wave packet spreads in time. Later we shall consider the propagator of the simple harmonic oscillator which is more easily derived using the path integral approach.

We note that certain space and time integrals derivable from K are immensely important. We set $t_0=0$ (no loss of generality). Moreover set $\bar{r} = \bar{r}'$ and integrate over all space

$$G(t) = \int K(\bar{r}',t;\bar{r}',0)d^3\bar{r}'$$

$$= \sum_j \int |\langle\bar{r}'|j\rangle|^2 d^3\bar{r}'\, e^{-\frac{iE_j}{\hbar}t}$$

$$\text{or} \quad G(t) = \sum_j e^{-\frac{iE_j}{\hbar}t} . \qquad 1.2.12$$

Not a surprising result. For setting $\bar{r} = \bar{r}'$ and integrating are equivalent to taking the trace of the time evolution operator in the $\bar{r}$ - representation. But trace is basis independent and in the $|j\rangle$ basis it is readily equal to the right hand side of the last equation. Now $\sum_j \exp(\frac{-iE_j}{\hbar}t)$ is just the sum over states reminiscent of the partition function in statistical mechanics. If we analytically continue in t and make t pure imaginary such that $\beta = it/\hbar > 0$, we end up with the partition function itself,

$$Z = \sum_j \exp(-\beta E_j). \qquad 1.2.13$$

The techniques encountered in studying propagators can obviously be useful in statistical mechanics and they indeed are as we shall see.

Next consider the Laplace-Fourier transform of G(t)

$$\bar{G}(E) = \frac{-i}{\hbar} \int G(t) \exp(\frac{iEt}{\hbar}) dt = \frac{1}{\hbar} \sum_j \int_0^\infty \exp i(\frac{E-E_j}{\hbar}) t \, dt. \qquad 1.2.14$$

The integral oscillates indefinitely. We make it meaningful by replacing E by $E+i\varepsilon$ and finally let $\varepsilon \to 0$. We thus obtain

$$\bar{G}(E) = \sum \frac{1}{E-E_j}. \qquad 1.2.15$$

The complete energy spectrum is exhibited as simple poles of $\bar{G}(E)$ in the complex E-plane. To know the energy spectrum of a physical system we only have to study the analytic properties of $\bar{G}(E)$.

1.3 Propagator as a Transition Amplitude

We shall now try to analyze the propagator a bit deeper

Our wave function is the scalar product of bra $\langle\bar{r}'|$ with the moving ket $|\alpha,t\rangle$. We can regard it also as the scalar product of the Heiseberg picture bra $\langle\bar{r}',t_0|$ which "rotates" oppositely with time with the fixed Heisenberg ket $|\alpha\rangle$.

Similarly,

$$K(\bar{r},t;\bar{r}',t_0) = \sum_j \langle\bar{r}|j\rangle \langle j|\bar{r}'\rangle \exp\{\frac{-iE_j}{\hbar}(t-t_0)\}$$

$$= \sum_j \langle\bar{r}|\exp(\frac{-iH}{\hbar}t)|j\rangle\langle j|\exp(\frac{iHt_0}{\hbar})|\bar{r}'\rangle$$

or

$$K(\bar{r},t;\bar{r}',t_0) = \langle\bar{r},t|\bar{r}',t_0\rangle \qquad 1.3.1$$

Where we have an eigenket and eigenbra of the position operator in the Heisenberg picture. Thus $\langle\bar{r},t|\bar{r}',t_0\rangle$ is the probability amplitude for the particle prepared at time t_0 with position eigenvalue $\bar{r}'$, to be found at a later time t at a position $\bar{r}$. Or roughly speaking $\langle\bar{r},t|\bar{r}',t_0\rangle$ is the amplitude for the particle to go from a space time point $(\bar{r}',t_0)$ to another space time point $(\bar{r},t)$. Hence we call it the transition amplitude. We are quite in line with the interpretation we gave to $K(\bar{r},t;\bar{r}',t_0)$ before.

One more useful interpretation is the following: Let the kets $|\bar{r}',t_0\rangle$ and $|\bar{r},t\rangle$ be chosen as base kets in the Heisenberg picture at the times t_0 and t respectively. So we can regard $\langle\bar{r},t|\bar{r}',t_0\rangle$ as the transformation function that connects the two sets of base kets at different times. Thus time evolution in the Heisenberg picture can be viewed as a unitary transformation in the sense of changing bases, that connects one set of base kets to another. This corresponds to classical physics where the time development of a dynamical variable corresponds to the continuous evolution of a canonical transformation generated by the Hamiltonian.

Let us now use t' in place of t_0. We know

$I = \int |\bar{r},t\rangle\langle\bar{r},t| d^3\bar{r}$ whence

$$\langle\bar{r}'',t''|\bar{r}',t'\rangle = \int \langle\bar{r}'',t''|\bar{r},t\rangle\langle\bar{r},t|\bar{r}',t'\rangle d^3\bar{r}', \quad t''>t>t' \qquad 1.3.2$$

This is called the composition property of the transition amplitude. Clearly we can divide the time interval into as many parts as we wish. Thus if we somehow guess the form of $\langle\bar{r}'',t''|\bar{r}',t'\rangle$ for an infinitesimal time interval between t' and $t'' = t' + dt$ we should be able to obtain $\langle\bar{r}'',t''|\bar{r}',t'\rangle$ for a finite time interval via the composition property. This is the underlying reasoning that led Feynman to his independent formulation of quantum mechanics in 1948[1].

1.4 Path Integrals as a Sum Over Paths[2,3]

To illustrate this scheme we now consider a one dimensional problem. The generalization to higher dimensior is trival. We are interested in the transition amplitude for a particle to go from a space time point (x',t') to another point (x'',t''). Divide the independent variable time into steps of width ε. This gives us a set of values t_j spaced a distance ε apart between the values t' and t''.

At each time t_j we select a point x_j. Now a path is constructed by connecting all the points so selected by some type of line.

$$\epsilon = t_j - t_{j-1} = \frac{t''-t'}{n} = \frac{tn-t'}{n}$$

Eq. (1.3.2) implies

$$\langle x_n,t_n|x_1,t_1\rangle = \int dx_{n-1}\ldots\int dx_2 \langle x_n,t_n|x_{n-1},t_{n-1}\rangle\langle x_{n-1},t_{n-1}|x_{n-2},t_{n-2}\rangle$$

$$\ldots\langle x_2,t_2|x_1,t_1\rangle \qquad 1.4.1$$

This can best be visualized with the help of figure 1.4.1 below.

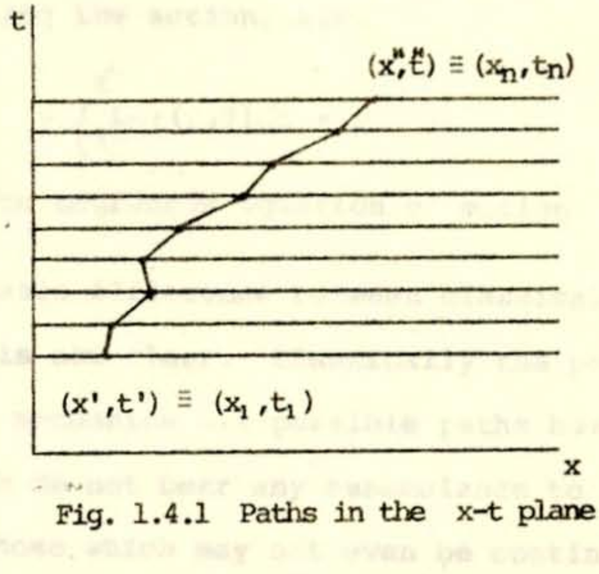

Fig. 1.4.1 Paths in the x-t plane

For each time segment, say between t_{j-1} and t_j we find the transition amplitude to go from (x_{j-1},t_{j-1}) to (x_j,t_j). We then integrate over all intermediate points $x_2,\ldots x_{n-1}$. This means that we must sum over all possible paths in the space time plane with fixed end points. This also means that the points x_{j-1} and x_j may be very far apart inspite of the smalness of the time interval t_j-t_{j-1}. The paths envisaged may, therefore, not be continuous.

Let us pause a bit and see how paths arise in classic mechanics. Considering one dimension let the classical Lagrangian be

$$L_{c\ell} = m\frac{\dot{x}_{c\ell}^2}{2} - V(x_{c\ell}).$$

Given this and th points (x',t') and (x'',t''), we do not consider just any path between these points but the actual motion takes place alo a unique path; for example, given $V(y) = mgy$ for a freely falling body and $(y',t') = (h,0)$, $(y'',t'') = (0,\sqrt{2h/g})$, the classical path is $y(t) = h-\frac{1}{2}gt^2$. This unique path is give by minimizing the action, i.e.

$$\delta \int_{t'}^{t''} L_{c\ell}(y,\dot{y})dt = 0$$

and leads to Lagranges equation of motion.

The basic difference between classical and quantum mechanics is now clear. Classically the path is unique. In quantum mechanics all possible paths have a role includi those which do not bear any resemblance to the classical path and those which may not even be continuous. Yet wha ever theory we write down should lead to classical mechan as $\hbar \to 0$.

1.5 Feynman's Formulation

Feynman tried to attack this problem. He was greatl intrigued by a mysterious remark in Diracs book[4] which in our notation reads

$$\exp \{ \frac{i}{\hbar} \int_{t'}^{t''} L_{c\ell} (x,\dot{x})dt\} \text{ corresponds to } \langle x'',t''|x',t'\rangle.$$

In trying to make sense out of this remark he was led to his celebrated space-time approach to quantum mechanics via path integrals. We now demonstrate how does the above correspondance lead to the path integral. Since the classical action is going to play a vital role we introduce a useful notation

$$S(j,j-1) = \int_{t_{j-1}}^{t_j} L_{c\ell} (x,\dot{x})dt \cdot \qquad 1.5.1$$

Since $L_{c\ell}$ is a function of x and $\dot{x}$, $S(j,j-1)$ is defined only after a definite path has been prescribed along which integration has to be carried out. That a particular path is involved in the above integration is thus implied eventhough this is not explicit in the definition. Consider the segment between (x_{j-1},t_{j-1}) and (x_j,t_j). Dirac says that associate $\exp \{\frac{iS(j,j-1)}{\hbar}\}$ with this segment. Going along the prescribed path we successively multiply expressions of this type to get

$$\prod_{j=2}^{n} \exp \{\frac{iS(j,j-1)}{\hbar}\} = \exp \{ \sum_j \frac{i}{\hbar} S(j,j-1)\} = \exp\{\frac{i}{\hbar}S(n,1)\} \qquad 1.5.2$$

This is the contribution from the chosen path to $\langle x'',t''|x',t'\rangle \equiv \langle x_n,t_n|x_1,t_1\rangle$. Next we have to integrate over $x_2,\ldots x_{n-1}$. Using the composition property from eq.(1.1.1) we let $t_j - t_{j-1}$ to be infinitesimally small. Thus symbolically,

$$\langle x_n, t_n | x_1, t_1 \rangle \simeq \sum_{\text{all paths}} \exp \{\frac{i}{\hbar} S(n,1)\}. \qquad 1.5.3$$

The summation is over an infinite set of paths. Before proceeding further let us examine the limit $\hbar \to 0$. Then the phase of the contribution of a path, $S/\hbar$ is some very large angle. The real (or imaginary) part of the exponential is the cosine (or sine) of this angle which is as likely to be plus as minus. Now if we move the path by a small amount δx, small on the classical scale, the change in S is likewise small on the classical scale but not when measured in the tiny unit $\hbar$. These small changes in path will, generally, make enormous changes in phase, and our cosine or sine will oscillate exceedingly rapidly between plus and minus values. The total contribution will then add to zero; for if one path makes a positive contribution, another infinitesimally close (on a classical scale) makes an equal negative contribution, so that no net contribution arises.

Therefore, no path really needs to be considered if the neighbouring path has a different action; for the paths in the neighbourhood cancel out the contribution. But for the special path $x_{c\ell}$, for which S is an extremum, a small change in the path produces in the first order at least, no change in S. All the contributions from the paths in this region are nearly in phase i.e., paths near the classical path contribute coherently and we have constructive interference. Finally in the case $\hbar = 0$, the classical path gets singled out.

We now go back to $\langle x_j, t_j | x_{j-1}, t_{j-1} \rangle$ with $t_j - t_{j-1} = \varepsilon$,

$$\langle x_j, t_j | x_{j-1}, t_{j-1} \rangle = \frac{1}{\omega(\varepsilon)} \exp\{\frac{iS(j,j-1)}{\hbar}\}. \qquad 1.5.4$$

We have inserted a weighting factor which depends on $t_j - t_{j-1}$ but not on $V(x)$. The need for such a factor arises purely on dimensional grounds since the left hand side must have the dimension of $(\text{length})^{-1}$. Now let us evaluate $S(j,j-1)$ for $\varepsilon \to 0$. Given this we can make a straightline approximation to the path joining (x_{j-1}, t_{j-1}) and (x_j, t_j) as follows:

$$S(j,j-1) = \int_{t_{j-1}}^{t_j} (\frac{m}{2}\dot{x}^2 - V(x))dt$$

$$= \varepsilon \{ \frac{m}{2} (\frac{x_j - x_{j-1}}{\varepsilon})^2 - V(\frac{x_j + x_{j-1}}{2}) \}. \qquad 1.5.5$$

Notice that for $V = 0$, the exponent is precisely the same as for the free particle propagator discussed earlier. Since the weighting factor is independent of V we can as well evaluate it for the free particle case. We use the orthonormality of the Heisenberg picture eigenkets at equal times, namely,

$$\langle x_j, t_j | x_{j-1}, t_{j-1} \rangle \Big|_{\varepsilon \to 0} = \delta (x_j - x_{j-1}).$$

Further, $\lim_{\varepsilon \to 0} \sqrt{\frac{m}{2\pi i\hbar\varepsilon}} \exp \frac{im(x_j - x_{j-1})^2}{2\hbar\varepsilon}$

$$= \delta(x_j - x_{j-1});$$

using these two relations together with eq. (1.5.4) we get

$$\frac{1}{\omega(\varepsilon)} = \sqrt{\frac{m}{2\pi i h\varepsilon}} \qquad 1.5.6$$

It then follows

$$<x_n, t_n | x_1, t_1> = \lim_{n \to \infty} \left(\frac{m}{2\pi i h\varepsilon}\right)^{\frac{n-1}{2}} \int dx_{n-1} \cdots$$

$$\int dx_2 \prod_{j=1}^{n} \exp\left\{\frac{iS(j,j-1)}{\hbar}\right\} \qquad 1.5.7$$

where the limit $n \to \infty$ is taken with x_n and x_1 fixed. We define a new kind of infinite dimensional integral operator

$$\int_{x_1}^{x_n} Dx(t) = \lim_{n \to \infty} \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{\frac{n-1}{2}} \int dx_{n-1} \cdots \int dx_2 \qquad 1.5.8$$

so that

$$<x_n, t_n | x_1, t_1> = \int_{x_1}^{x_n} Dx(t) \exp\left\{\frac{i}{\hbar} \int_{t_1}^{t_n} L_{cl}(x, \dot{x})\, dt\right\}. \qquad 1.5.9$$

This is Feynman's path integral. Its meaning as the sum over paths is explicit in eq. (1.5.7).

We have here a new formulation of quantum mechanics based on the concept of paths, which, Feynman motivated by Dirac's remarks arrived at. The only ideas borrowed from conventional quantum mechanics are:

1. Superposition principle used in summing the contributions from various paths.

2. The composition property of the transition amplitude.

3. The classical correspondence.

Let us summarize our results. The Feynman method tells us how to calculate the propagator directly. To find $K(x'',t'';x',t')$ (one dimensional case) do the following:

1. Draw all paths in the x-t plane connecting (x',t') and (x'',t'').

2. Find the action $S\{x(t)\}$ for each path $x(t)$.

3. $$K = A^n \sum_{\text{all paths}} \exp\left(\frac{i\, S\{x(t)\}}{\hbar}\right).$$

That means all paths are given the same weight but each path contributes with a different phase and contributions essentially cancel out until we come near the classical path. Near it the contributions add constructively and produce a large sum. Away from the classical path destructive interference sets in. Thus kis dominated by paths near the classical path. The classical path is important not because it contributes a lot but because paths in its vicinity contribute coherently. We ask how far should we deviate from $x_{c\ell}$ before destructive intereference sets in. One may say crudely that coherence is lost once the phase differs from the stationary value $S\{x_{c\ell}(t)\}/\hbar$ by about π. Thus the action from coherent paths should be approximately $\pi\hbar$ of

$S_{c\ell}$. For a macroscopic particle this means a very tight constraint but for an electron it allows a lot of latitude. That is why the assumption that the electron follows the well defined classical path leads to a conflict with experiment.

Now we would like to show the equivalence of the Feynman formulation to conventional quantum mechanics. We can do this in two ways. Either we can show that we can obtain Schrodinger equation directly from the present formulation or the converse i.e., starting from the Schrodinger equation we should obtain the Feynman path integral. We shall do both, leaving the second proof (the methodology of which we shall exploit in the section on statistical mechanics) to Appendix A_1.

1.6 Schrodinger's Equation from the Path Integral

Let us start with

$$<x_n t_n|x_1,t_1> = \int <x_n,t_n|x_{n-1},t_{n-1}><x_{n-1},t_{n-1}|x_1,t_1>dx_{n-1}$$

$$= \sqrt{\frac{m}{2\pi i\hbar\varepsilon}} \int \exp\{\frac{im(x_n - x_{n-1})^2}{2\hbar\varepsilon} - \frac{iV\varepsilon}{\hbar}\}<x_{n-1},t_{n-1}|x_1,t_1> dx_{n-1}.$$

1.6.1

Introducing $\xi = x_n - x_{n-1}$ and using x in place of x_n

and t in place of t_n we obtain

$$<x,t+\varepsilon|x_1,t_1> = \sqrt{\frac{m}{2\pi i\hbar\varepsilon}} \int_{-\infty}^{\infty} \exp\{\frac{im\xi^2}{2\hbar\varepsilon} - \frac{iV\varepsilon}{\hbar}\}$$

$$<x-\xi,t|x_1,t_1>d\xi. \qquad 1.6.2$$

As $\varepsilon \to 0$, the main contribution to the integral comes from $\xi \approx 0$. It is legitmate to expand $<x-\xi,t|x_1,t_1>$ in powers of ξ. We also expand $<x,t+\varepsilon|x_1,t_1>$ and exp $(-\frac{iV\varepsilon}{\hbar})$ in powers of ε whence

$$<x,t|x_1,t_1> + \varepsilon \frac{\partial}{\partial t} <x,t|x_1,t_1>$$

$$= \sqrt{\frac{m}{2\pi i\hbar\varepsilon}} \int_{-\infty}^{\infty} \exp(\frac{im\xi^2}{2h\varepsilon})\{1-\frac{i\varepsilon V}{\hbar}\}$$

$$(<x,t|x_1,t_1> + \frac{\xi^2}{2}\frac{\partial^2}{\partial x^2} <x,t|x_1,t_1>)d\xi \qquad 1.6.3$$

Since we are working to order ε (or order ξ^2). The linear term in ξ in the last bracket does not contribute to the integral and that is why it is omitted. We finally get

$$i\hbar \frac{\partial}{\partial t} <x,t|x_1,t_1> = \frac{-\hbar^2}{2m}\frac{\partial}{\partial x^2} <x,t|x_1,t_1>$$

$$+ V<x,t|x_1,t_1> \qquad 1.6.4$$

This completes the demonstration of the equivalence. In the next chapter we move on to some explicit evaluations of path integrals.

CHAPTER TWO

EVALUATION OF SOME PATH INTEGRALS AND THE BOHM-AHARONOV EFFECT

2.1 Potentials of the Form $V = a + bx + cx^2 + d\dot{x} + ex\dot{x}$

Having laid down the formalism in chapter one we now come to some illustrative examples. For the present case the Lagrangian is given by

$$L = \tfrac{1}{2}m\dot{x}^2 - a - bx - cx^2 - d\dot{x} - ex\dot{x} \cdot \qquad 2.1.1$$

We wish to evaluate the path integral

$$K(x_b, t_b; x_a t_a) = \int_{x_a}^{x_b} \{\exp(\frac{iS\{x(t)\}}{\hbar})\} \, Dx(t) \qquad 2.1.2$$

Where we have considered a one dimensional problem in which a particle moves from an initial space-time point (x_a, t_a) to reach a final space-time point (x_b, t_b) under the influence of the potential V given above.

Let us write every path as

$$x(t) = x_{c\ell}(t) + y(t) \qquad 2.1.3a$$

Where Y gives the displacement of any of the paths from the classical path. Differentiating this equation with respect to time one has

$$\dot{x}(t) = \dot{x}_{c\ell}(t) + \dot{y}(t). \qquad 2.1.3b$$

since all paths have the same end points $y(t_a) = y(t_b) = 0$.

If we slice up the time interval $t_b - t_a$ into n parts, we have for the intermediate integration variables

$$x_j = x(t_j) = x_{c\ell}(t_j) + y(t_j) \equiv x_{c\ell}(t_j) + y_j .$$

Since $x_{c\ell}(t_j)$ is some constant at $t_j, dx_j = dy_j$ and

$$\int_{x_a}^{x_b} Dx(t) = \int_0^0 Dy(t) \cdot \qquad 2.1.4$$

Now eq. (2.1.2) becomes

$$K(x_b,t_b;x_a,t_a) = \int_0^0 \exp\{\frac{i}{\hbar} S\{x_{c\ell}(t)+y(t)\}\}Dy(t) \cdot \qquad 2.1.5$$

Next we expand the functional S into Taylor's series

$$S\{x_{c\ell}+ y\} = \int_{t_a}^{t_b} L(x_{c\ell}+ y, \dot{x}_{c\ell}+ \dot{y})dt$$

$$= \int_{t_a}^{t_b} \{L(x_{c\ell},\dot{x}_{c\ell})+(\frac{\partial L}{\partial x})_{x_{c\ell}} y+(\frac{\partial L}{\partial \dot{x}})_{x_{c\ell}} \dot{y} + \frac{1}{2}\left[(\frac{\partial^2 L}{\partial x^2})_{x_{c\ell}} y^2 + (2\frac{\partial^2 L}{\partial x \partial \dot{x}})_{x_{c\ell}} y\dot{y} + (\frac{\partial^2 L}{\partial \dot{x}^2})_{x_{c\ell}} \dot{y}^2\right]\} dt \cdot \qquad 2.1.6$$

The series terminates here since L is a quadratic polynomial. The first term $L(x_{c\ell},\dot{x}_{c\ell})$ integrates to give $S\{x_{c\ell}\} \equiv S_{c\ell}$. The second term, linear in y and $\dot{y}$, vanishes upon integration due to the classical equation of motion. Making use of eq. (2.1.1) we obtain

$$\frac{1}{2} \frac{\partial^2 L}{\partial x^2} = - c, \quad \frac{\partial^2 L}{\partial x \partial \dot{x}} = - e , \quad \frac{\partial^2 L}{\partial \dot{x}^2} = m \cdot \qquad 2.1.7$$

So now using eqs. (2.1.5),(2.1.6) and (2.1.7) we finally obtain $K(x_b,t_b;x_a,t_a)$

$$= \exp(\frac{iS_{c\ell}}{\hbar}) \int_0^0 \exp\{\frac{i}{\hbar} \int_{t_a}^{t_b} (\frac{1}{2}m\dot{y}^2 - cy^2 - ey\dot{y})dt\}Dy(t) \cdot \qquad 2.1.8$$

Since the path integral has no memory of $x_{c\ell}$, it can only depend on the time interval $t_b - t_a$. So

$$K(x_b,t_b;x_a,t_a) = A(t_b-t_a) \exp(\frac{iS_{c\ell}}{\hbar}) \qquad 2.1.9$$

where $A(t_b - t_a)$ represents the path integral and is some unknown function of $t_b - t_a = T$. For the free path particle problem we set $c = e = 0$ and from chapter one we have

$$A(T) = \left(\frac{m}{2\pi i\hbar T}\right)^{\frac{1}{2}}. \qquad 2.1.10$$

In eq. (2.1.8), the coefficient b does not appear so that the same expression A(T) holds for linear potential $V = a + bx$ too.

2.2 The Harmonic Oscillator

For the harmonic oscillator we take $c = \frac{1}{2}m\omega^2$ and $e = 0$ in eq. (2.1.8). Further for $t_a = 0$ i.e., $t_b = T$ we have

$$A(T) = \int_0^0 \exp\left\{\frac{im}{2\hbar}\int_0^T(\dot{y}^2 - \omega^2 y^2)dt\right\}Dy(t)\,. \qquad 2.2.1$$

To evaluate this integral we consider the isomeric partition of the time interval T into steps of width $\varepsilon = t_j - t_{j-1} = T/n$ (n divisions).

$$A_n(T) = \frac{1}{B}\int\exp\left(\frac{im}{2\hbar\varepsilon}\left[\sum_{j=1}^{n-1}\{(y_{j+1}-y_j)^2 - \omega^2\varepsilon^2(\frac{y_j+y_{j+1}}{2})^2\}\right]\right)\prod_{j=1}^{n-1}B^{-1}dy_j$$

2.2.2a

where B^{-n} with

$$B = \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{\frac{1}{2}} \qquad 2.2.2b$$

is the normalization factor. We denote

$$\lim_{\substack{n\to\infty \\ (\varepsilon\to 0)}} A_n(T) = A(T)\,. \qquad 2.2.3$$

Assume that y_{j+1} is a small distance away from y_j whence

$$\sum_{j=1}^{n-1}\left[(y_{j+1}-y_j)^2-\omega^2\varepsilon^2\left(\frac{y_j+y_{j+1}}{2}\right)\right]=\sum_{j=1}^{n-1}(2-\omega^2\varepsilon^2)y_j^2-2\sum_{j=1}^{n-2}y_j\,y_{j+1}. \qquad 2.2.4$$

We thus write

$$A_n(T) = \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{-\frac{n}{2}}\int\exp\frac{im}{2\hbar\varepsilon}\left[\sum_{j=1}^{n-1}(2-\omega^2\varepsilon^2)y_j^2 - 2\sum_{j=1}^{n-2}y_j\,y_{j+1}\right]\prod_{j=1}^{n-1}dy_j\,. \qquad 2.2.5a$$

This expression can be written in a simpler form as follows:

$$A_n(T) = \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{-\frac{n}{2}}\int\exp\frac{im}{2h\varepsilon}\left\{\sum_{j=1}^{n-1}a_j(y_j-Q_jy_{j+1})^2\right\}\prod_{j=1}^{n-1}dy_j \qquad 2.2.5b$$

where

$$\begin{aligned} a_1 &= 2-\omega^2\varepsilon^2 \\ a_{j+1}+a_jQ_j^2 &= 2-\omega^2\varepsilon^2 \;\}\; j=1,\dots n-2 \\ a_jQ_j &= 1\,. \end{aligned} \qquad 2.2.5c$$

We elliminate Q_j and obtain

$$a_{j+1} = a_j^{-1} + 2 - \omega^2\varepsilon^2\,. \qquad 2.2.6$$

Let us pass over to a variable η_j where

$$\eta_j = y_j - Q_jy_{j+1}\,. \qquad 2.2.7$$

The jacobian of the transformation is 1.

So now the path integral which has been reduced to a multiple integral becomes

$$A_n(T) = \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{-\frac{n}{2}}\int\exp\left(\frac{im}{2\hbar\varepsilon}\sum_{j=1}^{n-1}a_j\,\eta_j^2\right)\prod_{j=1}^{n-1}d\eta_j\,. \qquad 2.2.8$$

performing the integration we obtain

$$A_n(T) = \{\frac{m}{2\pi i\hbar\, D_n(T)}\}^{\frac{1}{2}} \qquad 2.2.9a$$

where

$$D_n(T) = \varepsilon\, a_1 a_2 \ldots a_{n-1}\,. \qquad 2.2.9b$$

Next we determine the value of D_n in the limit $n\to\infty$ i.e., $\varepsilon\to 0$ to obtain $A(T)$. The above equation implies

$$D_{k+1}(T+\varepsilon) = \varepsilon\, a_1 a_2 \ldots a_k = D_k a_k \qquad 2.2.10a$$

$$D_{k-1}(T-\varepsilon) = \varepsilon\, a_1 a_2 \ldots a_{k-2} = D_k\, a_{k-1}^{-1}\,. \qquad 2.2.10b$$

Using these two expressions together with eq. (2.2.6)

$$\frac{1}{\varepsilon^2}\{D_{k+1}(T+\varepsilon) - 2\omega_k(T) + D_{k-1}(T-\varepsilon)\} = -\omega^2 D_k(T)\cdot \qquad 2.2.11a$$

This is a difference equation of second order. But we are interested in the limit $k\to\infty$ (or $\varepsilon\to 0$). Now using Taylor's expansion we get the differential equation

$$\ddot{D} = -\omega^2 D \qquad 2.2.11b$$

which in view of the initial conditions $D(0) = 0$, $\dot{D}(0) = 1$ gives

$$D(T) = \frac{\sin \omega T}{\omega}\,. \qquad 2.2.12$$

There is another way of obtaining this same result[3]. We know every path $y(t)$ starts from a point $(0,0)$ and goes to another point $(0,T)$ i.e., the motion is periodic. We then write such a path as a Fourier sine series with period T or $y(t) = \sum_n a_n \sin(n\pi t/T)$. The details are worked out in Appendix A_2. Finally using eq. 2.2.9a we obtain

$$A(T) = (\frac{m\omega}{2\pi i\hbar\, \sin\omega T})^{\frac{1}{2}} \qquad 2.2.13$$

which in view of eq. (2.1.9) gives

$$K(x_b,t_b;x_a,0) = \left(\frac{m\omega}{2\pi i\hbar \sin\omega T}\right)^{\frac{1}{2}} \exp\left(\frac{iS_{c\ell}}{\hbar}\right) \cdot \qquad 2.2.14a$$

The classical action as derived in Appendix A_3 is

$$S_{c\ell} = \frac{m\omega}{2\sin\omega T}\{(x_b^2 + x_a^2)\cos\omega T - 2x_b x_a\}$$

so that the full propagator is given by

$$K(x_b,t_b;x_a,0) = \left(\frac{m\omega}{2\pi i\hbar \sin\omega T}\right)^{\frac{1}{2}*}$$

$$\exp\{\frac{im\omega}{2\hbar\sin\omega T})\{(x_b^2+x_a^2)\cos\omega T - 2x_a x_b\}\} \cdot \qquad 2.2.14b$$

As an extension of the above problem we consider the harmonic oscillator driven by an external force $f(t)$. For every path of the oscillator between the points (x_a,t_a) and (x_b,t_b) we write

$$x(t) = x_{c\ell}(t) + y(t) \cdot \qquad 2.2.15$$

The Lagrangian of the oscillator is

$$\begin{aligned} L = \; & \{\frac{m}{2}(\dot{x}_{c\ell}^2 - \omega^2 x_{c\ell}^2) + f(t)x_{c\ell}\} \\ & + \{m(\dot{x}_{c\ell}\dot{y} - \omega^2 x_{c\ell} y) + f(t)y\} \\ & + \{\frac{m}{2}(\dot{y}^2 - \omega^2 y^2)\} \cdot \qquad 2.2.16 \end{aligned}$$

The integral of the first term from t_a to t_b gives $S_{c\ell}$, the

---

* The normalization factor $A(T)$ can be written in the form $K(0,T;0,0)$ which is amenable to a physical interpretation. It is seen that $A(T)$ represents the propagator of the harmonic oscillator with cyclic return to the origin.

second term vanishes due to the equation of motion and the last term as in the previous case gives

$$A(T) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega T}} \qquad 2.2.17a$$

whence

$$K(x_b,t_b;x_a,t_a) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega T}} \exp\left(\frac{iS_{c\ell}}{\hbar}\right) . \qquad 2.2.17b$$

$X_{c\ell}$ is the solution of Lagrange's equation i.e., the equation of motion:

$$\ddot{x}_{c\ell} + \omega^2 x_{c\ell} = \frac{f(t)}{m} . \qquad 2.2.18$$

The solution to this equation is the sum of the solution to the homogeneous differential equation and the particular solution.

$$x_{c\ell} = x_{c\ell,H} + x_{c\ell,P}$$

From Appendix A_3

$$x_{c\ell,H}(t) = \frac{x_b \sin\omega(t-t_a) + x_a \sin\omega(t_b-t)}{\sin\omega T} \qquad 2.2.19a$$

By using the variational method for finding the particular solution of the differential equation (2.2.18)

$$x_{c\ell,P}(t) = \frac{1}{m\omega \sin\omega T}\{\sin\omega(t-t_a)\int_{t_a}^{t} f(S)\sin\omega(t_b-s)ds$$

$$- \sin\omega(t_b-t)\int_{t_a}^{t} f(s)\sin\omega(S-t_a)ds\}$$

$$= \frac{1}{m\omega}\int_{t_a}^{t} f(s)\sin\omega(t-s)ds . \qquad 2.2.19b$$

Eqs. (2.2.19a) and (2.2.19b) give

$$x_{c\ell}(t) = \frac{x_b \sin\omega(t-t_a) + x_a \sin\omega(t_b-t)}{\sin\omega T}$$

$$+ \frac{1}{m\omega\sin\omega T}\{\sin\omega(t-t_a)\int_t^{t} f(s)\sin\omega(t_b-s)ds$$

$$- \sin\ (t_b-t)\int_{t_a}^{t} f(s)\sin\omega(s-t_a)ds\} . \qquad 2.2.19$$

Now,

$$L = \{\frac{m}{2}(\dot{x}^2_{c\ell,H} - \omega^2 x^2_{c\ell,H}) + f(t)\,x_{c\ell,H}\}$$

$$+ \{m(\dot{x}_{c\ell,H}\,\dot{x}_{c\ell,P} - \omega^2 x_{c\ell,H}\,x_{c\ell,P})\}$$

$$+ \{\frac{m}{2}(\dot{x}^2_{c\ell,P} - \omega^2 x^2_{c\ell,P}) + (f(t)\,x_{c\ell,P}\} . \qquad 2.2.20$$

Integration of the first term gives

$$I_1 = \frac{m\omega}{2\sin\omega T}\{(x_b^2 + x_a^2)\cos\omega T - 2x_a x_b\}$$

$$+ \frac{1}{\sin\omega T}\{x_a\int_{t_a}^{t_b} f(s)\sin\omega(t_b-s)ds$$

$$+ x_b\int_{t_a}^{t_b} f(s)\sin\omega(s-t_a)ds\} . \qquad 2.2.21a$$

The first term here is the one calculated in Appendix A_3 whereas the remining part is straight forward. Consider the last two terms in eq. (2.2.20). They are written as

$$\frac{m}{2}\{\dot{x}_{c\ell,P}(\dot{x}_{c\ell,P} + 2\dot{x}_{c\ell,H}) - \omega^2 x_{c\ell,P}(x_{c\ell,P} + 2x_{c\ell,H}\} + f(t)\,x_{c\ell,P}$$

Let $I_2 = \int_{t_a}^{t_b} \frac{m}{2}\{\dot{x}_{c\ell,P}(\dot{x}_{c\ell,P} + 2\dot{x}_{c\ell,H}) - \omega^2 x_{c\ell,P}(x_{c\ell,P} + 2x_{c\ell,H})\}$

$$+ f(t)\,x_{c\ell,P}\}dt$$

This can be integrated by parts to give

$$I_2 = \frac{m}{2} \int_{t_a}^{t_b} \frac{d}{dt} \{ x_{c\ell,p}(\dot{x}_{c\ell,p} + 2\dot{x}_{c\ell,H}) \} dt$$

$$- \frac{m}{2} \int_{t_a}^{t_b} \{ x_{c\ell,p}(\ddot{x}_{c\ell,p} + \omega^2 x_{c\ell,p} - \frac{f(t)}{m}) .$$

$$+ 2x_{c\ell,p} (\ddot{x}_{c\ell,H} + \omega^2 x_{c\ell,H}) - \frac{f(t)}{m} x_{c\ell,p} \} dt$$

In the second integral the only nonvanishing term is the last one; others vanish due to the equation of motion. Thus we have

$$I_2 = \frac{m}{2} \int_{t_a}^{t_b} \frac{d}{dt} \{ x_{c\ell,p} (\dot{x}_{c\ell,p} + 2\dot{x}_{c\ell,H}) dt$$

$$+ \tfrac{1}{2} \int_{t_a}^{t_b} f(t) \, x_{c\ell,p} \, dt$$

$$= \frac{m}{2} \, x_{c\ell,p}(\dot{x}_{c\ell,p} + 2\dot{x}_{c\ell,H})\} \Big|_{t_a}^{t_b}$$

$$+ \tfrac{1}{2} \int_{t_a}^{t_b} f(t) \, x_{c\ell,p} \, dt$$

Then using the expression for $x_{c\ell,H}$ and $x_{c\ell,p}$ from eqs. (2.2.19a) and (2.2.19b) respectively and simplifing we finally get

$$I_2 = - \frac{1}{m\omega \sin \omega T} \int_{t_a}^{t_b} \int_{t_a}^{\gamma} f(\gamma) \, f(s) \sin \omega (t_b - \gamma)$$

$$. \sin \omega (s - t_a) \, ds \, d\gamma \qquad 2.2.21$$

Using eqs. (2.2.21a) and (2.2.21b) we obtain

$$S_{c\ell} = \frac{m\omega}{2\sin\omega T}\{[(x_b^2 + x_a^2)\cos\omega T - 2x_a x_b]$$

$$+ \frac{2x_a}{m\omega}\int_{t_a}^{t_b} f(s)\sin\omega(t_b - s)\,ds$$

$$+ \frac{2x_b}{m\omega}\int_{t_a}^{t_b} f(s)\sin\omega(s - t_a)\,ds$$

$$- \frac{2}{m^2\omega^2}\int_{t_a}^{t_b}\int_{t_a}^{\gamma} f(\gamma)f(s)\sin\omega(t_b - \gamma)\sin\omega(s - t_a)\,ds\,d\gamma\}. \qquad 2.2.21c$$

Finally, this result together with eq. (2.2.17b) yields

$$K(x_b, t_b; x_a, t_a) = \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}}\exp\{\frac{im\omega}{2\hbar\sin\omega T}\{(x_b^2 + x_a^2)\cos\omega T - 2x_a x_b$$

$$+ \frac{2x_a}{m\omega}\int_{t_a}^{t_b} f(s)\sin\omega(t_b - s)\,ds + \frac{2x_b}{m\omega}\int_{t_a}^{t_b} f(s)\sin\omega(s - t_a)\,ds$$

$$- \frac{2}{m^2\omega^2}\int_{t_a}^{t_b}\int_{t_a}^{\gamma} f(\gamma)f(s)\sin\omega(t_b - \gamma)\sin\omega(s - t_a)\,ds\,d\gamma\}\}.$$

2.2.22

Next we briefly indicate the way how the energy levels and eigenfunctions of the simple harmonic oscillator can be deduced from the path integral approach. In eq. (1.2.6) we wrote the propagator in terms of the energy levels and eigenfunctions of a system whose eigenvalue problem we can solve. So now using that expression together with eq. (2.2.14b) we have

$$\sum_{j=0}^{\infty} \psi_j(x)\psi^*_j(x')\exp\{-\frac{iE_j}{h}T\}$$

$$= \sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega T}} \exp\{\frac{im\omega}{2\hbar \sin \omega T}\left[(x^2+x'^2)\cos\omega T - 2x'x\right]\} \qquad 2.2.23a$$

where now the initial and final points are taken to be (x',t') and (x,t) respectively,

$$i \sin \omega T = \frac{e^{i\omega T}}{2}(1-e^{-2i\omega T}), \cos \omega T = \frac{e^{i\omega T}}{2}(1+e^{-2i\omega T}) \cdot \qquad 2.2.23b$$

The right hand side of eq. (2.2.23a) becomes

$$(\frac{m\omega}{\pi h})^{\frac{1}{2}} e^{-\frac{i\omega T}{2}} (1-e^{-2i\omega T})^{-\frac{1}{2}}$$

$$x \exp\left\{-\frac{m\omega}{2\hbar}\{(x^2+x'^2)(\frac{1+e^{-2i\omega T}}{1-e^{-2i\omega T}}) - \frac{4x'x e^{-i\omega T}}{1-e^{-2i\omega T}}\}\right\} .$$

Expanding this last expression in successive powers of $e^{-i\omega T}$ we obtain a series exactly identical to the left hand side of eq.(2.2.23a). Because we have a factor $e^{-i\omega T/2}$, all the terms in the expansion will be of the form $e^{-i\omega T/2}e^{-ij\omega T}$ for $j = 0,1,2,\ldots$. This maens the energy levels are given by

$$E_j = (j+\tfrac{1}{2})h\omega \cdot \qquad 2.2.24$$

The wave functions are obtained by making the expansion completely and are identical to the familiar results obtained by solving the Schrodinger equation.

2.3 The Bohm-Aharonov Effect[5, 10]

Consider a hollow cylind rical shell as shown below

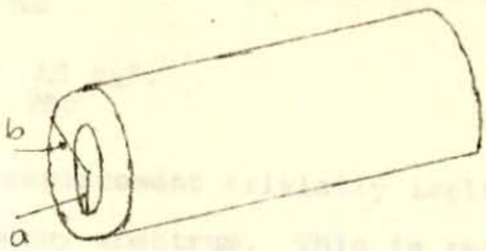

Fig. 2.3.1 A hollow cylind rical shell. The ends of the shell are closed so that a particle inside does not have a way to move out of the shell.

A particle of charge e is confined in the cylind rical region between $\rho = a$ and $\rho = b$ with rigid walls. The wave function is required to vanish on the inner and outer walls as well as at the bottom and top of the walls. It is a simple boundary value problem.

Now let us fit a solenoid in the region $0 < \rho < a$ so that no field leaks into the region $\rho \geq a$. The boundary conditions for the particle are still the same. Intuitively we may conjecture that the energy spectrum is unchanged. Quantum mechanics disagrees! The field vanishes in the space available to the particle but the vector potential does not. Assume the field is oriented along the axis of the cylinder (taken to be the Z-axis). Noting that $\bar{B} = \nabla \times \bar{A}$ and applying Stokes theorem one finds

$$\bar{A} = \frac{Ba^2}{2\rho}\bar{e}_\varphi \qquad 2.3.1$$

where $\bar{e}_\varphi$ is a unit vector in the direction of increasing φ. The momentum operator in the presence of the field becomes $\nabla - \frac{ie}{\hbar c}\bar{A}$ which in cylind rical coordinate means that $\partial/\partial\varphi \to \partial/\partial\varphi - \frac{ie}{2\hbar c} Ba^2$.

This replacement trivially implies an observable change in the energy spectrum. This is remarkable for the particle never reaches the magnetic field. There is no Lorentz-force acting on the particle yet the energy depends on the field in the hole where the particle never can be. This problem is a bound state version of the so called Bohm-Aharonov effect. Let us discuss the original form of the problem. Consider a particle of charge e going above or below a very long impenetrable cylinder which is very thin and inside which is a magnetic field parallel to the cylinder axis.

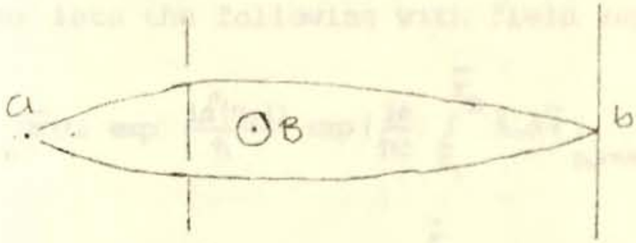

Fig. 2.3.2 A particle moves either above or below an impenetrable cylinder

We would like to see how the probability of finding the particle in the interference region b depends on the magnetic flux. Let $\bar{r}_I$ and $\bar{r}_n$ be typical points in the regions a and b respectively. If $L^0_{c\ell}$ is the Lagrangian for the no field case, the Lagrangian for $B \neq 0$ is

$$L_{c\ell} = L^0_{c\ell} + \frac{e}{c}\frac{d\bar{r}}{dt}\cdot\bar{A} \quad . \qquad 2.3.2$$

The change in action for a definite path segment between

(x_{i-1},t_{i-1}) and (x_i,t_i) is given by

$$s(i,i-1)-s^{\circ}(i,i-1) = \frac{e}{c}\int_{t_{i-1}}^{t_i} \frac{d\bar{r}}{dt}.\bar{A}dt = \frac{e}{c}\int_{\bar{r}_{i-1}}^{\bar{r}_i} \bar{A}.d\bar{r}$$

where $d\bar{r}$ is a differential line element along the path segment. Thus the net change for the whole path is calculated from

$$\Pi \exp \frac{is^{\circ}(i,i-1)}{\hbar} \rightarrow \{\Pi \exp \frac{is^{\circ}(i,i-1)}{\hbar}\}\{\exp \frac{ie}{\hbar c}\int_{\bar{r}_1}^{\bar{r}_n} \bar{A}.d\bar{r}\} \cdot \quad 2.3.3$$

This is for a particular path. We have to sum over all paths. This is easy for $\int \bar{A}.d\bar{r}$ is path independent as long as the loop formed by a pair of paths does not enclose any magnetic flux. Hence for all paths above the cylinder we have one common phase factor. Now the net no field transition amplitude goes over into the following with field amplitude

$$\int_{above} D\bar{r}(t) \exp \frac{is^{\circ}(n,1)}{\hbar} \exp\{\frac{ie}{\hbar c}\int_{\bar{r}_1}^{\bar{r}_n} \bar{A}.d\bar{r}\}_{above}$$

$$+ \int_{below} D\bar{r}(t) \exp \frac{is^{\circ}(n,1)}{\hbar} \exp \frac{ie}{\hbar c}\int_{\bar{r}_1}^{\bar{r}_n} \bar{A}.d\bar{r}\}_{below} .$$

The probability of finding the particle in the interference region b depends on the modulus squard of the entire transition amplitude and thus on the phase difference between contributions from the paths going above and below the cylinder. This phase difference due to the $\bar{B}$ field alone is just

$$\frac{e}{\hbar c}\int_{\bar{r}_1}^{\bar{r}_n} A.d\ell\Big|_{above} - \frac{e}{\hbar c}\int_{\bar{r}_1}^{\bar{r}_n} A.d\ell\Big|_{below} = \frac{e}{\hbar c}\oint A.d\ell = \frac{e}{\hbar c}\phi_B \quad 2.3.4$$

where Φ_B is the magnetic flux inside the impenetrable cylinder. Thus as $\bar{B}$ is varied, there is a sinusoidal component in the probability of observing the particle in the region b with a period given by a fundamental unit of magnetic flux, namely $2\pi\hbar c/|e|$.

This effect is purely quantum mechanical and gauage independent for the phase depends only on the total flux Φ_B. Classically the motion is specified solely by Newtons law and Lorentz force which is identically zero in the region accessible to the particle. Yet quantum mechanics says that the interference pattern depends crucially on what is inside the impenetrable cylinder. It is tempting indeed to conclude that in quantum mechanics it is $\bar{A}$ rather than $\bar{B}$ which is fundamental. However, one must emphasize that the net effect in both examples discussed here depends only on Φ_B which is directly measurable interms of $\bar{B}$ and vanishes for no $\bar{B}$. Experiments to verify the effect have been performed using a thin magnetized iron filament called a whisker. The above conclusion, we might add, can of course be drawn without using the path integral approach, our approach was meant to illustrate the path integral formulation of the problem.

CHAPTER THREE

SOME APPLICATIONS OF PATH INTEGRALS IN STATISTICAL MECHANICS[3,11]

.1 Path Integral Formulation of the Density Matrix and the Parition Function

In chapter one we indicated that the path integral method can prove useful in statistical mechanics as well. We now build up this connection.

We are interested in a quantum system in thermal equilibrium at temperature T. We know the probability to find such a system in a state of energy E_j is proportional to the Boltzmann factor $e^{-Ej/kT}$ where k is the Boltzmann constant. Hence the probability to find the system in a state of energy Ej is

$$P_j = \frac{1}{Z} e^{-\beta E_j} \qquad 3.1.1$$

where $\beta = 1/kT$ and $Z = \sum_j e^{-\beta E_j}$ is known as the partition function and E_j are assumed to be nondegenerate. Z and the free energy F are realted as $Z = e^{-\beta F}$. Given the partition function or F one can determine the macroscopic parameters of interest. However, the determination of some physical quantities, even for a system in thermal equilibrium needs more than just the partition function. For example, suppose a system is a configuration space having a coordinate x; we ask what is the probability of finding the system at x?

To answer this question we must remember that in statistical mechanics a double averaging process is involved: one is quantum mechanical averaging and the other is statistical averaging (averaging over ensemble). Then if the system is in a single state defined by the wave function $\psi_j(x)$ and E_j is the corresponding eigenvalue, the probability of observing x is $\psi_j(x)\,\psi_j^*(x)$ and averaging over all possible states one finds

$$P(x) = \frac{1}{Z} \sum_j \psi_j(x)\,\psi_j^*(x)\,e^{-\beta E_j} . \qquad 3.1.2$$

For a general quantity A, the average value is given by

$$\bar{A} = \frac{1}{Z} \sum_j A_j e^{-\beta E_j} \qquad 3.1.3a$$

where $A_j = \langle A\rangle\psi_j = \int \psi_j^*(x) A\, \psi_j(x)\,dx$. Thus

$$\bar{A} = \frac{1}{Z} \sum_j \int \psi_j^*(x)\, A\psi_j(x) e^{-\beta E_j}\, dx . \qquad 3.1.3b$$

Now we define a useful quantity

$$\rho(x,x') = \sum_j \psi_j(x)\,\psi_j^*(x') e^{-\beta E_j} \qquad 3.1.4$$

It is called the statistical density matrix for the temperature T.

In eq. (3.1.3b) the operator A acts on $\psi_j(x)$ only. We can form $A\,\rho(x,x')$ and integrate over x setting $x' = x$. We have found the trace of $A\rho$ in the x-basis. (The trace, is, of course, basis independent). Thus

$$\bar{A} = \frac{\mathrm{Tr}A\rho}{Z} \qquad 3.1.5$$

From eq. (3.1.4)

$$Z = \int \rho(x,x)dx = Tr\rho \quad 3.1.6$$

whence

$$\bar{A} = \frac{TrA\rho}{Tr\rho} . \quad 3.1.7$$

It is obvious that the central problem of statistical mechanics is to find $\rho(x,x')$. For conventional thermodynamics variables Z satisfies the need.

Now compare eq. (3.1.4) with eq. (1.2.6) introduced in chapter one for a time independent Hamiltonian i.e.,

$$K(x,t;x',t') = \sum_j \psi_j(x)\ \psi_j^*(x')e^{\frac{-iE_j}{\hbar}(t-t')} . \quad 3.1.8$$

Replace t-t' by $-i\beta\hbar$ and the kernel goes over into the density matrix. Let us write

$$\rho(x,x';u) = \sum_j \psi_j(x)\psi_j^*(x')e^{\frac{-u}{\hbar}E_j} \quad 3.1.9$$

Where $u = \beta\hbar$.

Differentiating eq. (3.1.9) with respect to u one has

$$-\hbar\ \frac{\partial\rho}{\partial u} = H\rho \quad 3.1.10a$$

or

$$-\frac{\partial\rho}{\partial\beta} = H\rho \quad 3.1.10b$$

where H acts on the variable x. Eq. (3.1.10) is similar to the Schrodinger equation for the propagator:

$$-\frac{\hbar}{I}\frac{\partial K}{\partial t} = HK \quad \text{for } t > t' \quad 3.1.11$$

To develop the path integral formulation of ρ we assume u represents "time" interval and divide it into steps of width η i.e., $\eta = u/n$ where n is the number of divisions. Now the particle goes from x' to x through a series of intermediate points $x_1, \dots x_{n-1}$ which define a "path" x(u). Next we follow the procedure used in chapter one where we derived the path integral of the propagator starting from Schrodinger's equation. The result will be

$$\rho(x,x';u) = \int (\exp\{ \sum_{j=0}^{n-1} [\frac{m}{2\hbar\eta}(x_{j+1}-x_j)^2 + \frac{\eta}{\hbar}V(x_j)]\}$$

$$\frac{1}{A} \cdot \prod_{j=1}^{n-1} (\frac{dx_j}{A})\ ^* \qquad 3.1.12$$

where $A = \sqrt{2\pi\hbar\eta/m}$.

If we consider the case $n \to \infty$ (or $\eta \to 0$) and call $\dot{x}$ the derivative dx/du, we have

$$\rho(x,x';U) = \int_{x'}^{x} (\exp\{-\frac{1}{\hbar}\int_0^U [\frac{m}{2}\dot{x}^2(u) + V(x(u))]\,du\})$$

$$Dx(u) \qquad 3.1.13$$

which gives the complete statistical behaviour of a quantum mechanical system as a path integral without the appearance of i anywhere. Although all possible paths are to be considered in eq. (3.1.13), the main contribution comes from a

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* This result is also obtained starting from the path integral of the propagator for the 1 - D motion of a particle. The time interval $t_{j+1} - t_j = \varepsilon$ is replaced by $-i\eta$ here.

limited set of paths for which the integrand is not too small.

The partition function is derived by considering the cases in which the final and initial configurations are the same and summing over all possible initial configurations.

Let us consider the classical limit of high temperature or small $\hbar$ so that $\beta\hbar$ is very small and thus the path of the system does not deviate much from the initial point $x' = x(0)$. In fact, the "paths" cannot ever wander very far from x', because travelling far away and returning again in the short "time" available requires a high "velocity and a large "kinetic energy". This implies that the first approximation in eq. (3.1.13) is to replace $V(x(u))$ by the initial value $V(x')$ and we have

$$\rho(x',x';U) = e^{-\frac{U}{\hbar}V(x')} \int_{x'}^{x'} \{\exp\left[\frac{-m}{2\hbar}\int_0^U \dot{x}^2(u)\,du\right]\} Dx(u) \cdot \qquad 3.1.14a$$

In this last expression the path integral is that of a free particle. So using the result from chapter two we obtain

$$\rho(x',x') = \sqrt{\frac{m}{2\pi\hbar U}}\; e^{-\frac{U}{\hbar}V(x)} = \sqrt{\frac{mKT}{2\pi\hbar^2}}\; e^{-\beta V(x)} \qquad 3.1.14b$$

Since $U = \beta\hbar$.

The partition function is the integral of this expression over all possible initial configurations i.e.,

$$Z = \sqrt{\frac{mKT}{2\pi\hbar^2}} \int_{-\infty}^{\infty} e^{-\beta V(x')}\, dx' \cdot \qquad 3.1.15$$

This is the well known classical result. In the case of a large number of variables (for systems such as solids, liquids and gases) the classical partition function is a product of two factors. The first of these is the path integral which one would get by considering all particles of the system to be free. The second factor is the integral of $e^{-\beta V}$, where V is the potential of the system which depends upon all the coordinates of the particles.

The next step is to improve on this classical approximation so as to take quantum effects into account. Here it is necessary to include changes in the potential function which result from the motion along the "path". We observe that since x' and x are equal, it appears natural to use an average

$$\bar{x} = \frac{1}{U} \int_0^U x(u)\,du \qquad 3.1.16$$

in place of x'. We then expand V(x) about this mean position which is defined for every path. The partition function becomes

$$Z = \int_{-\infty}^{\infty} d\bar{x} \int_{x'}^{x'} \left(\exp\left|-\frac{1}{\hbar}\int_0^U \left\{\frac{m}{2}\dot{x}^2(u)+V(x(u))\right\}\right|\right)Dx(u)\cdot \qquad 3.1.17$$

Using Taylor's series about $\bar{x}$

$$\int_0^U V\{x(u)\}du = UV(\bar{x}) + \frac{1}{2}\int_0^U (x-\bar{x})\ V''(\bar{x})du + \ldots \qquad 3.1.18$$

The first term vanishes in view of eq. (3.1.16).

Thus the first nonzero correction term is of second order and to this order the partition function becomes

$$Z = \int_{-\infty}^{\infty} e^{-\frac{U}{\hbar}V(\bar{x})} d\bar{x} \int_{x'}^{x'} (\exp\{-\frac{1}{2\hbar}\int_0^U [m\dot{x}^2 + (x-\bar{x})^2 V''(\bar{x})]du\})$$

$$. Dx(u). \qquad 3.1.19a$$

The allowed paths x(u) are those constrained by $\int_0^U (x-\bar{x})du = 0$ or if we denote $y = \bar{x}$ the constraint becomes $\int_0^U ydu = 0$. In terms of y, Z becomes

$$Z = \int_{-\infty}^{\infty} e^{-\frac{U}{\hbar}V(\bar{x})} d\bar{x} \int_{x'}^{x'} (\exp\{-\frac{1}{2\hbar}\int_0^U | m\dot{y}^2 + V''(0)y^2 | dU\})Dy(u). \qquad 3.1.19b$$

The integrand of the path integral is the same as that for the harmonic oscillator with frequency $\omega^2 = -V''(0)/m$. To apply the constraint we multiply eq. (3.1.19b) by the delta function $\delta(\int_0^U ydu)$, we can express this delta function by its Fourier transform:

$$\delta(y) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \exp(iky)\, dk$$

so now the partition function becomes

$$Z = \int_{-\infty}^{\infty} e^{-\frac{U}{\hbar}V(\bar{x})} d\bar{x} \int_{x'}^{x'} \frac{dK}{2\pi} \int_{x'-\bar{x}}^{x'-\bar{x}} \exp\{-\frac{1}{\hbar}\int_0^U \{\frac{m}{2}\dot{y}^2 + \frac{V''}{2}y^2 + iky\}du\})$$

$$. Dy(u) \qquad 3.1.20$$

In this form the path integral contains the constraint eq. (3.1.16). It is also seen that the path integral has the same form as the path integral of the forced harmonic oscillator with imaginary m and V". The solution to the path integral is worked out in Appendix A_4 and we have

$$Z = \sqrt{\frac{mKT}{2\pi\hbar^2}} \int_{-\infty}^{\infty} (\exp\{-\beta\{V(\bar{x}) + \frac{\beta\hbar^2}{24m} V''(\bar{x})\}\})dx \qquad 3.1.21$$

In this expression the corrective term $(\beta\hbar^2/24m)V''(\bar{x})$ is clearly quantum mechanical because it contains the plancks constant $\hbar$. For a many particle system moving in three dimensions the correction term will be $(\beta\hbar^2/24\ )\ \Sigma\ \nabla_i^2 V/m_i$. It is therefore seen that the classical formula is applicable provided one replaces $V(x)$ by $V + (\beta\hbar^2/24m)V''$. This suggests that we seek some possibly better potential $U(\bar{x})$ to replace V in the classical result to get a good approximation to the correct quantum mechanical partition function. There exists a way of binding the quantum partition function from below by using an effective classical potential U. We shall come back to this problem after we have laid down the variational technique in the next chapter. We only add that the real challenge in this game lies in finding a good effective classical potential and as yet it remains an open question.

3.2 Many Particle Systems

Such systems can be described by a large number of variables and the results obtained in the previous section are directly extended except in cases where symmetry properties are to be taken into account. Consider a system of N identical particles of mass m that are interacting. The Lagrangian of this system will be

$$L = \sum_j \frac{1}{2} m \dot{r}_j^2 - \frac{1}{2} \sum_{j,k} V(r_{jk}) \qquad 3.2.1$$

where $V(r_{jk})$ is the interaction potential between the j^{th} and k^{th} particles.

The partition function is

$$Z = \int d^N\bar{r}(0) \int_{\bar{r}(0)}^{\bar{r}(U)=r(0)} \left(\exp\left\{-\left[\frac{m}{2\hbar}\sum_j \int_0^U \dot{\bar{r}}_j^2 du + \frac{1}{2\hbar}\int_0^U \sum V(|\bar{r}_j - \bar{r}_k|)\, du\right]\right\}\right) D^N \bar{r}(u) \qquad 3.2.2$$

where $d^N\bar{r} = d^3\bar{r}_1\, d^3\bar{r}_2 \ldots d^3\bar{r}_N$; $D\bar{r}_N = D\bar{r}_1 \ldots D\bar{r}_N$.

But we do not claim eq.(3.2.2) is true in general. The symmetry properties of identical particles must be taken into account. This property actually finds its root in quantum mechanics. The wave function (solution of the Schrodinger equation) must be symmetric (anti symmetric for fermions) though other solutions may exist. Thus we must find a symmetrized expression for the density matrix. If $\psi_j(x)$ is a solution to Schrodinger's equation and is symmetric then it is equivalent to $\psi_j(Px)$ where P is the particle exchange operator. For N particles, there are N! ways of permuting them i.e.,

$$\sum_P \psi_j(Px_i) = N!\,\psi_j(x_i) \text{ if } \psi_j \text{ is symmetric}$$

$$= 0 \text{ if not .} \qquad 3.3.3$$

In line with this argument we have

$$\sum_P \rho(Px,x') = \sum_j^{all} \sum_P \psi_j(Px)\,\psi_j^*(x')e^{-\beta E_j}$$

$$= N! \sum_j^{sym.} \psi_j(x)\psi_j^*(x')e^{-\beta E_j}$$

or

$$\sum_P \rho(Px,x') = N!\,\rho_{sym}(x,x'). \qquad 3.2.4$$

Further, for a system of many particles which start out from a certain configuration, although their final configuration seems that of their initial, the identity of some of the particles may have been exchanged. That means by now the initial state of one particle may have become the final state of any other particle. With these arguments at hand we can write

$$Z_{sym} = \frac{1}{N!}\sum_P \int d^N\bar{r}(0) \int_{\bar{r}_i(0)}^{P\bar{r}_i(0)} \left(\exp\left\{-\left(\frac{m}{2\hbar}\int_0^U \sum_j \dot{\bar{r}}_j^2\,du + \frac{1}{2\hbar}\sum_{j,k}\int_0^U V(|\bar{r}_j-\bar{r}_k|)\,du\right\}\right)$$

$$\cdot\, D^N\bar{r}(u). \qquad 3.2.5$$

At high temperatures this expression should reduce to a classical result and the symmetrization should have no observable consequences. To illustrate this idea consider the motion of a single particle from its initial point to a final point a distance ℓ away. According to eq. (3.2.5), this is a motion from the initial point $\bar{r}_i(0)$ to the permuted position $P\,\bar{r}_i(0)$, and the contribution of this permutation is proportional to $\exp(-m\ell^2kT/2\hbar^2)$, thus decreasing with increasing temperature or spacing between the particles. Hence unless the particles are extremely close together, no permutation in the sum is important even the simplest interchange between two atoms - in comparison with the identity permutation which leaves all atoms in their location. Since only the identity permutation makes a significant contribution to the summations, all that remains for our consideration is the factor $1/N!$.

On the other hand, for Fermi particles the expression analogous to eq. (3.2.5) is also easily written down. However, the evaluation of the sum is difficult, such as for liquid H_e^3. This is so because the contribution of a single permutation is either positive or negative. Besides, the contributions of different permutations have got different magnitudes. It is thus difficult to sum an alternating series of large terms which are decreasing slowly in magnitude when a precise analytic formula for each term is not available.

3.3 The Use of Second Quantized Hamiltonian in Path Integrals

We consider an application to Bose statistics. Let us, therefore, deal with the simple Hamiltonian

$$H = \hbar\omega\, a^+ a \qquad 3.3.1$$

where a and a^+ are the annihilation and creation operators obeying the commutation relation

$$\{a, a^+\} = 1 \,. \qquad 3.3.2$$

Their action on a state of n particles, $|n\rangle$ is

$$a\,|n\rangle = \sqrt{n}\,|n-1\rangle, \quad a^+\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \qquad 3.3.3$$

whence

$$a^+ a\,|n\rangle = n\,|n\rangle \qquad 3.3.4$$

and a^+a is called the number operator. It tells us the total number of particles in a given state.

In the basis $|n\rangle$ H is diagonal and the propagator is easily obtained for

$$\langle m|\exp(-\frac{iH}{\hbar}t)\,|n\rangle = \exp(-in\omega t)\ \delta_{mn}. \qquad 3.3.5$$

We shall, however, make matters a little more complicated by using the system of coherent states

$$|\alpha\rangle = \frac{1}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \exp(-\tfrac{1}{2}|\alpha|^2)\,|n\rangle \qquad 3.3.6$$

where α is any complex number.

The following are a few facts about coherent states:

$|\alpha\rangle$ is an eigenfunction of the annihilation operator a with eigenvalue α i.e.,

$$a|\alpha\rangle = \alpha|\alpha\rangle \quad \text{or} \quad \langle\alpha|a^+ = \langle\alpha|\,\overset{*}{\alpha}. \qquad 3.3.7a$$

Scalar product of two coherent states

$$\langle\alpha|\alpha'\rangle = \frac{1}{\pi}\exp(-\tfrac{1}{2}|\alpha'|^2 - \tfrac{1}{2}|\alpha|^2 + \overset{*}{\alpha}\,\alpha') \qquad 3.3.7b$$

i.e., two different states are not orthogonal.

The completeness relation

$$\int \langle\lambda|\alpha\rangle\langle\alpha|\mu\rangle d^2\alpha = \langle\lambda|\mu\rangle$$

where $d^2\alpha = d(R_e\,\alpha)\,d(I_m\,\alpha)$. Finally,

$$\int \exp\,(-\gamma|\alpha|^2 + \lambda\,\bar{\alpha} + \mu\,\alpha)\ \frac{d^2\alpha}{\pi} = \frac{1}{\gamma}\exp\,(\frac{\lambda\,\alpha}{\gamma}) \qquad 3.3.7c$$

where $\gamma > 0$, is integral identity.

We look for the propagator $\langle\alpha|\exp(-\frac{iH}{\hbar}s)|\alpha'\rangle$ interms of the coherent states. The paramater s could be the time t or $-i\hbar\beta$ to get the denSity matrix in statistical mechanics, or could be a complex paramater in general.

The procedure is familiar. Break the full propagator into short time propagators and use the composition property. Thus the parameter s is devided into steps of width $\Delta s = s/n$, where the initial point corresponds to $s = 0$.

$$\langle\alpha|\exp(-i\omega a^+ a s)|\alpha'\rangle$$

$$= \int\langle\alpha|1-i\omega a^+ a\,\Delta s\,|\alpha_{n-1}\rangle\langle\alpha_{n-1}|1-i\omega a^+ a\,\Delta s|\alpha_{n-2}\rangle\cdots\langle\alpha_1|1-i\omega a^+ a\,\Delta s|\alpha'\rangle$$

$$d^2\alpha_1 \ldots d^2\alpha_{n-1}\,. \qquad 3.3.8a$$

Here we have n short time propagators but n-1 integrations. Using eq. (3.3.7a) we have for a typical short-time propagator

$$\langle x_{j+1}|1-i\omega a^+ a\,\Delta s\,|\alpha_j\rangle = (1-i\omega\alpha^*_{j+1}\alpha_j\Delta s)\langle\alpha_{J+1}|\alpha_j\rangle$$

$$= \frac{1}{\pi}\exp\{-\tfrac{1}{2}|\alpha_j|^2+(1-i\omega\Delta s)\alpha^*_{j+1}\alpha_j$$

$$-\tfrac{1}{2}|\alpha_{j+1}|^2\}$$

to order Δs.

Substituting the above expression in eq. (3.3.8a) we obtain

$$\langle\alpha|\exp(-i\omega a^+ a s)|\alpha'\rangle$$

$$\simeq \int\exp|-\tfrac{1}{2}|\alpha'|^2+(1-i\omega\Delta s)\alpha_1^*\alpha'-|\alpha_1|^2+(1-i\omega\Delta s)\alpha_2^*\alpha_1-|\alpha_2|^2$$

$$+\ldots-|\alpha_{n-1}|^2+(1-i\omega\Delta s)\alpha^*\alpha_{n-1}-\tfrac{1}{2}|\alpha|^2\}\,\frac{1}{\pi}\prod_{j=1}^{n-1}\frac{1}{\pi}\,d^2\alpha_j\,. \qquad 3.3.8b$$

All the integrals can be performed using eq. (3.3.7c) and the result is

$$<\alpha|\exp(-i\omega a^{+} as)|\alpha'> \simeq \frac{1}{\pi}\exp\{-\tfrac{1}{2}|\alpha|^2+(1-i\omega\tfrac{s}{n})^n \alpha^*\alpha' -\tfrac{1}{2}|\alpha'|^2\} \quad 3.3.8c$$

which in the limit $n \to \infty$ leads to the exact propagator in terms of coherent states:

$$<\alpha|\exp(-i\omega a^{+} a s)|\alpha'>$$

$$= \frac{1}{\pi}\exp\{-\tfrac{1}{2}|\alpha|^2 + e^{-i\omega s}\alpha^*\alpha' -\tfrac{1}{2}|\alpha'|^2\} \quad 3.3.8d$$

Next we apply this result to determine the density matrix.

$$<\alpha|\rho|\alpha'> = \frac{<\alpha|\exp(-i\ a^{+}as)\alpha'>}{\int<\alpha|\exp(-i\ a^{+}a)|\alpha> d^2\alpha}$$

$$= \{1-\exp(-i\omega s)\}^{-1}\frac{1}{\pi}\exp\{-\tfrac{1}{2}|\alpha|^2+e^{-i\omega s}\alpha^*\alpha'-\tfrac{1}{2}|\alpha'|^2\} \quad 3.3.9$$

where $s = -ih\beta = -ih/kT$.

The average occupation number is given as

$$<a^{+}a> = \mathrm{Tr}\ \rho a^{+}a = \int <\alpha|\rho|\alpha'><\alpha'|a^{+}a|\alpha> d^2\alpha'\, d^2\alpha$$

which in view of eq. (3.3.9) and the result $<\alpha'|a^{+}a|\alpha> = \alpha'^{*}\alpha<\alpha'|\alpha>$ leads to

$$<a^{+}a> = \frac{1}{\exp(\frac{-h\omega}{kT})-1} \quad 3.3.10$$

the well known Bose function.

It is posssible to develop (obtain) the Fermi function by a similar approach. We know that the classical picture of quantum mechanical amplitudes of Bose oscillators is given by the coherent states considered here. To get a similar picture of Fermi operators we should consider their coherent states. In this case even if coherent states exist, corresponding eigenvalues are no longer complex numbers because of the anti-commutation properties of the Fermi operators. Thus to be consistent the eigenvalues have to be anti-commutable with each other. Such peculiar c numbers are known as Grassman variables. We are not prepared to discuss them in this work.[16,17]

CHAPTER FOUR

THE VARIATIONAL METHOD FOR THE PATH INTEGRAL

4.1 A Minimum Principle

The variational technique is based on the following inequality

$$\langle e^{-x} \rangle \geq e^{-\langle x \rangle} \qquad 4.1.1$$

where x is a real random variable and $\langle x \rangle$ is its weighted average.

This follows from the fact that the curve of e^{-x} is concave upwards. If we imagine a number of weights to lie along this cuve, the center of gravity lies above this curve. The vertical height of this center of gravity is the average vertical position $\langle e^{-x} \rangle$. It exceeds $e^{-\langle x \rangle}$, the ordinate of the curve at the position of the center of gravity. Using this inequality we proceed in a manner reminiscent of the way the variational method is developed in Schrodinger's mechanics.

Suppose we wish to evaluate the free energy F of a system. We know from chapter four that

$$Z = e^{-\beta F} = \int_{-\infty}^{\infty} \left(\int_{x'}^{x'} \exp(-S/\hbar)\, Dx(u) \right) dx'. \qquad 4.1.2$$

Assume that some other s' can be found which satisfies two conditions: One, s' is simple enough that expressions such as $\int e^{-S'/\hbar} Dx(u)$ or $\int G\, e^{-S'/\hbar}\, Dx(u)$ for simple functionals G can be evaluated. Second, the important paths in the integrals $\int e^{-S/\hbar} Dx(u)$ and $\int e^{-S'/\hbar} Dx(u)$ are similar, i.e., s' and s are similar when they are both small. Now suppose F' is the free energy associated with s'. our aim is to find the minimum possible action s', using the minimization procedure to be set up here so that we have an upper limit to the true free energy F. So now we have

$$e^{-\beta F'} = \int_{-\infty}^{\infty} \int_{x'}^{x'} \exp(-s'/\hbar)\, Dx(u)\, dx' \,. \qquad 4.1.3$$

Using eqs. (4.1.2) and (4.1.3) one has

$$e^{-\beta(F-F')} = \int_{-\infty}^{\infty} \int_{x'}^{x'} e^{-s/\hbar}\, Dx(u)\, dx' \Big/ \int_{-\infty}^{\infty} \int_{x'}^{x'} e^{-s'/\hbar} Dx(u)\, dx'$$

or

$$e^{-\beta(F-F')} = \int_{-\infty}^{\infty} \int_{x'}^{x'} e^{-(s-s')/\hbar} e^{-s'/\hbar}\, Dx(u)\, dx' \Big/ \int_{-\infty}^{\infty} \int_{x'}^{x'} e^{-s'/\hbar} \cdot Dx(u)\, dx' \,. \qquad 4.1.4a$$

Thus $e^{-\beta(F-F')}$ is the average value $\langle e^{-\frac{(s-s')}{\hbar}} \rangle$ over all paths with the same initial and final points where each path is given a weight $e^{-s'/\hbar}\, Dx(u)$. Then applying eq. (4.1.1) to (4.1.4a) (real action assumed) we obtain

$$e^{-\beta(F-F')} \geq e^{\langle -\frac{(s-s')}{\hbar} \rangle} \qquad 4.1.4$$

whence

$$F \leq F' + 1/\beta\hbar \langle s-s' \rangle = F' + \delta \qquad 4.1.5$$

where

$$\delta = \frac{1/\beta h \int_{-\infty}^{\infty} \int_{x'}^{x'} (s-s') e^{-s'/\hbar} Dx(u)\, dx'}{\int_{-\infty}^{\infty} \int_{x'}^{x'} e^{-s'/\hbar}\, Dx(u)\, d\, x'} \,. \qquad 4.1.6$$

Eq. (4.1.5) is the minimum principle we were seeking. It says that if we calculate $F' + \delta$ for various "actions" s', the calculation which gives the smallest result is closest to the true free energy F. Actually F is obtained for s' = s. But we can guess that if s and s' differ in some sense to a first order of smallness then the deviation of $F' + \delta$ from F must be of second order.

Thus the procedure consists in starting with a reasonable form of s' with some undetermined parameters. Then one calculates $F'+\delta$. The parameters are to be varied so as to minimize this quantity. This gives the best guess to F.

The same minimal principle can be used to find an approximate value for the ground state energy E_0 of the system. Recall that

$$Z = e^{-\beta F} = \sum_{j=0}^{\infty} e^{-\beta E_j} . \qquad 4.1.7$$

If the temperature of the system becomes lower and lower i.e. β increasing, terms involving higher values of energy become negligible. Here the contribution of the term with the lowest energy $e^{-\beta E_0}$ is the largest.

$$\lim_{\beta \to \infty} Z = e^{-\beta E_0} . \qquad 4.1.8$$

Hence starting with this approximate value and following the previous procedure (we now replace F by E_0) we finally arrive at

$$E_0 \leq E_0' + \delta \qquad 4.1.9$$

However, to obtain eq. (4.1.9), we disregard the need that the paths return to the starting point which was the case in the calculation of F. This is so because the density matrix $\rho(x,x')$ is also dominated by $e^{-\beta E_0}\psi_0(x)\psi_0^*(x')$ in the limit $\beta\to\infty$. The dependence on x' and x now enters as a multiplying factor but does not affect the exponential nature of the function. It is the exponential behaviour which is fundamental to the evaluation of E_0 by this method.

The variational technique as used in the Schrodinger theory can be obtained from this formulation as shown in detail in the book by Feynman and Hibbs. We shall not describe it here. However, one important feature must be noted. The fact that the action be real excludes the case of a particle in a magnetic field. How to include complex actions in the present approach is still an open question. But one suspects that such a simple generalization should exist.

4.2 An Application of the Variation Theorem

Let us now see the application of eq. (4.1.5) to a one dimensional one particle problem. For this case

$$S = \int_0^U \{ \frac{m\dot{x}^2(u)}{2} + V(x(u)) \} du \cdot \qquad 4.2.1$$

The partition function is written as

$$e^{-\beta F} = \int_{-\infty}^{\infty} \int_{x'}^{x'} (\exp\{-\frac{1}{\hbar}\int_0^U [\frac{m\dot{x}^2(u)}{2} + V(x(u)] du\})Dx(u)\,dx'. \qquad 4.2.2$$

Here we first fix $x(0) = x'$ and $x(U) = x(0)$ and do the path integral over all paths, then vary x'. As we have pointed out in chapter four, in the classical limit of high temperature we approximate $V(x(u))$ by $V(x')$ to obtain

$$e^{-\beta F} = \sqrt{\frac{mkT}{2\pi\hbar^2}} \int_{-\infty}^{\infty} e^{-\frac{V(x')}{kT}} dx' \cdot \qquad 4.2.3$$

But now we would like to improve on this classical result. First since $x(0)$ and $x(U)$ are equal we use an average

$$\bar{x} = \frac{1}{U} \int_0^U x(u)\, du \qquad 4.2.4$$

in place of $x(0)$. Second, the deviation of the path from the classical straight line may be taken into account by some average $V(x)$ over the path rather than by a constant $V(x')$. We then use a trial functional

$$s' = \int_0^U \frac{m}{2} \dot{x}^2(u)\, du + U\, w(\bar{x}) \cdot \qquad 4.2.5$$

$w(\bar{x})$ is an undetermined function which is to be varied later to minimize eq. (4.1.5). The corresponding partition function will be

$$e^{-\beta F'} = \int_{x'}^{x'} (\exp\{-[\frac{1}{\hbar} \int_0^U \frac{m}{2}\dot{x}^2(u)\, du + \beta w(\bar{x})]\})\, Dx(u) \qquad 4.2.6a$$

or

$$e^{-\beta F'} = \int_{-\infty}^{\infty} d\bar{x} \underset{(\text{fixed } \bar{x})}{\int_{x'}^{x'}} (\exp\{-[\frac{1}{\hbar} \int_0^U \frac{m}{2}\dot{x}^2(u)\, du + \beta w(\bar{x})]\})\, Dx(u) \cdot \qquad 4.2.6b$$

Let $y = x - x'$; $\dot{y}(u) = \dot{x}(u)$. Then,

$$\bar{e}^{\beta F'} = \int_{-\infty}^{\infty} d\bar{x}\, e^{-\beta w(\bar{x})} \int_{y=0}^{y=0} \left(\exp\{-\frac{m}{2\hbar}\int_0^U \dot{y}^2 du\}\right) Dy(u) \qquad 4.2.6c$$

which is the same as the path integral of a free particle except for the first factor. So using the result from chapter two one has

$$\bar{e}^{\beta F'} = \sqrt{\frac{mkT}{2\pi\hbar^2}} \int_{-\infty}^{\infty} e^{-\frac{w(y)}{kT}} dy \,. \qquad 4.2.6d$$

Next we calculate <s-s'>. From eqs. (4.2.1) and (4.2.5) we have

$$\frac{1}{U} < s-s' > = \frac{1}{U} \int_{x'}^{x'} \left\{ \int_0^U V(x(u))du - Uw(\bar{x}) \right\} e^{-s'/\hbar} Dx(u) \Big/ \int_{x'}^{x'} \bar{e}^{s'/\hbar} Dx(u)$$

$$= \frac{\frac{1}{U}\int_0^U du\left(\int_{x'}^{x'} V(x(u))e^{-s'/\hbar} Dx(u)\right) - \int_{x'}^{x'} w(\bar{x})e^{-s'/\hbar} Dx(u)}{\int_{x'}^{x'} e^{-s'/\hbar} Dx(u)} \,.$$

Consider the first term in the numerator. The path integral here is independent of U so that we can take any value of u, in particular u = 0. The result is

$$\frac{1}{U} < s-s' > = < V(x(0)) > - < w(\bar{x}) > \qquad 4.2.7$$

To transform further we use the following result*.

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* This is obtained by using the transformation

$$x(u) = a_0 + \sum_{n=1}^{\infty} (a_n \cos\frac{2\pi nu}{\beta} + b_n \sin \frac{2\pi nu}{\beta}$$

$$\int \left(\exp\{-\frac{m}{2\hbar}\int_0^U \dot{x}^2(u)\,du\}\exp\{-\frac{i}{\hbar}\int_0^U f(u)x(u)du\}\right)Dx(u)$$

$$= \sqrt{\frac{2\pi m}{\hbar U}}\;\delta\left(\int_0^U f(u)du\right)\exp\{\frac{1}{4m}[\int_0^U\int_0^U |u-u'|f(u)f(u')\,du\,du'$$

$$+\frac{2}{U}(\int_0^U u\,f(u)du)^2]\}. \qquad 4.2.8$$

Next we write

$$\langle V(x(0))\rangle = \int_{x'}^{x'} (V(x(0))\exp\{-\frac{m}{2\hbar}\int_0^U \dot{x}^2(u)du\}\exp\{\frac{U}{\hbar}w(\bar{x})\})Dx(u)$$

$$= \int_{\infty}^{\infty} K(y)\,\exp\{-\frac{U}{\hbar}\,w(y)\}\,dy \qquad 4.2.9$$

where

$$K(y) = \int_{x'}^{x'} V(x(0))\,\exp\{\frac{-m}{2\hbar}\int_0^U \dot{x}^2(u)du\}\,Dx(u). \qquad 4.2.10$$

Such that $y = \bar{x}$. That is in eq. (4.2.9) we first do the path integral keeping $\bar{x}$ fixed. Eq. (4.2.10) may be written as

$$K(y) = \int_{x'}^{x'} V(x(0))\,\exp\{-\frac{m}{2\hbar}\int_0^U \dot{x}^2(u)du\}\,\delta(\bar{x}-y)\,Dx(u). \qquad 4.2.11$$

Then we use the Fourier transform

$$V(x) = \int_{-\infty}^{\infty} V(q)\,e^{iqx}\,d_q\,. \qquad 4.2.12$$

It follows that

$$K(y) = \int_{-\infty}^{\infty} V(q)dq\int_{-\infty}^{\infty} dk\int_{x'}^{x'} \exp\{iqx(0)\}\,\exp\{ik(\bar{x}-y)\}$$

$$\exp\{-\frac{m}{2\hbar}\int_0^U \dot{x}^2(u)\,du\}\,Dx(u) \qquad 4.2.13$$

where we have also Fourier transformed the delta function in eq. (4.2.11); factors such as 2π are neglected here. Now use eq. (4.2.4) in eq. (4.2.13 to write

$$K(y) = \int_{-\infty}^{\infty} V(q)dq \int_{-\infty}^{\infty} dk\, e^{-iky} \int_{x'}^{x'} e^{iqx(0)} \exp\{\frac{ik}{U}\int_0^U x(u)du\}$$

$$\cdot \exp\{-\frac{m}{2\hbar}\int_0^U \dot{x}^2(u)\, du\} Dx(u) \cdot \qquad 4.2.14$$

As can be seen the path integral part of this equation can be brought into the form of eq. (4.2.8) if we define

$$f(u) = q\delta(u-0) + \frac{k}{U} \cdot \qquad 4.2.15$$

Since

$$\int_0^U f(u)\, x(u)du = q\, x(0) + \frac{k}{U}\int_0^U x(u)du \cdot \qquad 4.2.16$$

Using eq. (4.2.15) into eq. (4.2.8) we have

$$\int_0^U f(u)\, du = q + k \qquad 4.2.17$$

$$\int_0^U uf(u)du = \frac{kU}{2} \qquad 4.2.18$$

$$\int_0^U du \int_0^U |u-u'|\, f(u)f(u')\, du' = 2\int_0^U du \int_0^U (u-u) f(u')\, du' f(u)$$

$$= (\frac{k^2}{3} + kq)U \cdot \qquad 4.2.19$$

Use eqs. (4.2.17), (4.2.18) and (4.2.19) in eq.(4.2.8) and also in the path integral part of eq. (4.2.14) to write the latter as

$$K(y) = \int_{-\infty}^{\infty} dq\, V(q) \int_{-\infty}^{\infty} dk\, \exp(-iky)\,\delta(q+k)\, \exp\{\frac{\hbar U}{4m}(\frac{k^2}{3} + kq + \frac{k^2}{2})\}$$

$$\int_{-\infty}^{\infty} dk\, V(-k)\, \exp(-iky)\, \exp(\frac{-\hbar k^2 U}{24m}) \qquad 4.2.20$$

Using the inverse Fourier transform we find that

$$K(y) = \int_{-\infty}^{\infty} dk \exp(-iky) \int_{-\infty}^{\infty} V(z) \exp(ikz) \exp\left(-\frac{\hbar k^2 U}{24m}\right) dz$$

$$= \int_{-\infty}^{\infty} dz\, V(z) \exp\left\{-\frac{6m}{\hbar U}(y-z)^2\right\}. \qquad 4.2.21$$

Including all the factors that have been ignored we have

$$K(y) = \sqrt{\frac{6mkT}{\pi\hbar^2}} \int_{-\infty}^{\infty} dz\, V(z) \exp\left\{-\frac{6mkT(y-z)^2}{\hbar^2}\right\}. \qquad 4.2.22$$

Thus $K(y)$ is $V(z)$ averaged over a Gaussian. The root mean square of the Gaussian spread is $\hbar/\sqrt{12mkT}$. If $T \to \infty$, the Gaussian becomes a delta function and $K(y) \to V(y)$.

Summarizing the results obtained so far we have

$$F \leq F' + 1/\beta h \langle s - s' \rangle_{s'} \qquad 4.2.23a$$

$$e^{-\beta F'} = \sqrt{\frac{mkT}{2\pi h^2}} \int_{-\infty}^{\infty} \exp\left\{-\frac{w(y)}{kT}\right\} dy \qquad 4.2.23b$$

$$\frac{1}{\beta h} \langle s-s' \rangle_{s'} = \int_{-\infty}^{\infty} \{K(y) - w(y)\} e^{-\beta w(y)} dy \Big/ \int_{-\infty}^{\infty} e^{-\beta w(y)} dy. \qquad 4.2.23c$$

We ask what is the best choice of $w(y)$? Let us change $w(y) \to w(y) + \eta(y)$.

Using the last three equations above we find

$$\delta F' = \int_{-\infty}^{\infty} \eta\, e^{-\beta w} dy \Big/ \int_{-\infty}^{\infty} e^{-\beta w} dy \qquad 4.2.24$$

$$\delta \frac{1}{\beta h} \langle s-s' \rangle = \int_{-\infty}^{\infty} e^{-\beta w}\{-\beta\eta(K-w) - \eta\} dy \Big/ \int_{-\infty}^{\infty} e^{-\beta w} dy$$

$$+ \int_{-\infty}^{\infty} e^{-\beta w}(K-w)\, dy \int_{\infty}^{\infty} \beta\eta e^{-\beta w} dy \Big/ \left(\int_{-\infty}^{\infty} e^{-\beta w} dy\right)^2 \qquad 4.2.25$$

Thus

$$\delta \; (F' + 1/\beta\hbar \; \langle s-s' \rangle_{s'}) = 0 \qquad 4.2.26$$

leads to

$$W(y) = \mathcal{K}(y) \qquad 4.2.27$$

which is the best choice of W(y). And eq. (4.2.23c) yields

$$\langle s-s' \rangle_{s'} = 0$$

so that from eq. (4.2.23a)

$$F \leq F_{c\ell,\mathcal{K}} \qquad 4.2.28$$

where $F_{c\ell,\mathcal{K}}$ is the classical free energy with the potential V(y) replaced by $\mathcal{K}(y)$. Alternatively,

$$e^{-F_{c\ell,\mathcal{K}}} = \sqrt{\frac{mkT}{2\pi h^2}} \int_{-\infty}^{\infty} e^{-\mathcal{K}(y)/kt} \, dy \qquad 4.2.29$$

$F_{c\ell,\mathcal{K}}$ is better approximation than the ordinary classical form $F_{c\ell}$ in eq. (4.2.2)

4.3 Effective Classical Parition Functions

We present a method due to Feynman and Kleinert[19] by which a quantum mechanical partition function can be approximated from below by an effective classical partition function.

The partition function of a system is given by

$$Z = e^{-\beta F} = \int (\exp \{- \int_0^\beta [\frac{\dot{x}^2(t)}{2} + V(x(t))] \, dt\}) \, Dx(t) \qquad 4.3.1$$

where we have used system of units in which m = 1, ħ = 1.

Since the paths involved are periodic we may use a Fourier transform of the paths

$$x(t) = x_0 + \sum_{n=1}^{\infty} (x_n \; e^{i\omega_n t} + \text{c.c.}), \; \omega_n = 2\pi n/\beta . \qquad 4.3.2$$

Using eq. (4.3.2) in eq. (4.3.1) we have

$$Z = \int \frac{dx_0}{\sqrt{2\pi\beta}} \prod_{n=1}^{\infty} \int \frac{dx_n^{\text{real}} \, dx_n^{\text{im}}}{\pi/\beta\omega_n^2} \; \exp\{-\beta \sum_{n=0}^{\infty} \omega^2 |x_n|^2 - \int_0^{\beta} V(x(t))dt\} . \qquad 4.3.3$$

The x_n appear implicitly in the argument of V. If all the integrals except $n = 0$ are done we will get

$$Z = \int \frac{dx_0}{\sqrt{2\pi\beta}} \; e^{-\beta W(x_0)} . \qquad 4.3.4$$

Of course, this result can be obtained in high temperature limit, that is $W(x) \to V(x_0)$ as $T \to \infty$ and

$$Z \to Z_{c\ell} = \int \frac{dx_0}{\sqrt{2\pi\beta}} \; \exp\{-\beta V(x_0)\} . \qquad 4.3.5$$

Eq. (4.3.4) is identical to eq. (4.3.5) and thus we refer to $W(x_0)$ as the effective classical potential and the integral eq. (4.3.4) as the effective classical partition function.

The integrals over all x_n, $n \neq 0$, collected in $W(x_0)$ are, in general, impossible to perform. However, for smooth potentials $V(x)$, there exists a simple way of evaluating these integrals approximately to a very high accuracy, leading to an upper bound for $W(x_0)$, to be denoted by $W_1(x_0)$, and to be found accroding to the following rules.

(1) Calculate a smeared version of the potential $V(x)$ as follows:

$$V_{a^2}(x) = \int \frac{dx'}{\sqrt{2\pi a^2}} \exp\{-\frac{1}{2a^2}(x-x')^2\} V(x') \qquad 4.3.6$$

with as an yet unknown parameter a^2.

(2) Introduce a second parameter Ω and form the auxilary potential

$$\tilde{w}_1(x_0,a^2,\Omega) = (1/\beta)\ell n \frac{\sin h\beta\Omega/2}{\beta\Omega/2} - \frac{\Omega^2}{2}a^2 + V_{a^2}(x_0) \cdot \qquad 4.3.7$$

(3) Consider a^2,Ω as functions of x_0 and calculate at each x_0, the minimum of $\tilde{w}_1(x_0,a^2(x_0),\Omega(x_0))$ with respect to the parameters $a^2(x_0)$ and $\Omega(x_0)$. The result is the approximate effective classical potential

$$w_1(x_0) = \min_{a^2(x_0),\Omega(x_0)} \{\tilde{w}_1(x_0,a^2(x_0),\Omega(x_0))\} \cdot \qquad 4.3.8$$

The minimization with respect to Ω gives the following relation between Ω and a^2

$$a^2 = (1/\beta\Omega^2)\{\beta\Omega/2 \cot h(\beta\Omega/2) - 1\} \qquad 4.3.9$$

while the minimization in a^2 determines Ω^2 as a function of the smeared potential

$$\Omega^2(x_0) = 2\frac{\partial V_{a^2}(x_0)}{\partial a^2} = \frac{\partial^2 V_{a^2}(x_0)}{\partial x_0^2} . \qquad 4.3.10$$

Let us now see how these rules come about.

Expanding $V(x(t))$ into Taylor's series about x_0 we have

$$V(x(t)) = V(x_0) + \frac{\partial V}{\partial x}\Big|_{x_0} \{x(t)-x_0\} + \tfrac{1}{2}\frac{\partial^2 V}{\partial x^2}\Big|_{x_0} \{x(t)-x_0\}^2 + \ldots \qquad 4.3.11a$$

Since x_0 is the average position of the system we assume $\frac{\partial V}{\partial x}\Big|_{x_0} = 0$.

$$V(x(t)) = V(x_0) + \tfrac{1}{2}\frac{\partial^2 V}{\partial x^2}\Big|_{x_0} \{x(t)-x_0\}^2 + \ldots \qquad 4.3.11b$$

Let us now approximate $V(x(t))$ by the following function

$$V(x(t)) = L_1(x_0) + \frac{\Omega^2(x_0)}{2}\{x(t) - x_0\}^2 \qquad 4.3.11c$$

where $\Omega^2(x_0)$ denotes an arbitary local curvator of the potential and $L_1(x_0)$ is a trial potential depending on x_0. Then the corresponding trial partition function becomes

$$Z_1 = e^{-\beta F_1} = \int (\exp\{-\int_0^\beta dt\, \{\frac{\dot{x}(t)}{2} + \frac{\Omega^2(x_0)}{2}\{x(t)-x_0\}^2\} - \beta L_1(x_0)\})\, Dx(t). \qquad 4.3.12$$

As shown in appendix A_5 we calculate Z_1 as

$$Z_1 = \int \frac{dx_0}{\sqrt{2\pi\beta}} \frac{\beta\Omega(x_0)/2}{\sinh\{\frac{\beta\Omega(x_0)}{2}\}} e^{-\beta L_1(x_0)} . \qquad 4.3.13$$

It is straight forward to calculate within the partition function Z_1 the expectation of the difference between the true and the trial potential

$$\langle\{V(x(t)) - \frac{\Omega^2(x_0)}{2}\{x(t)-x_0\}^2 - L_1(x_0)\}\rangle_1$$

where

$$< A >_1 = \frac{1}{Z_1} \int (A \exp\{ \int_0^{\beta} \{\frac{\dot{x}^2(t)}{2} + \frac{\Omega^2(x_0)}{2}\{x(t)-x_0\}^2\} - \beta L_1(x_0)dt\}) \cdot \quad 4.3.14$$

Fourier transforming the potential and using the Fourier representation of the position from eq. (4.3.2) we write

$$V(x(t)) = \frac{1}{2\pi} \int dq\, V(q) \exp\{ iq [x_0 + \sum_{n=1}^{\infty}(x_n e^{i\omega_n t} + c.c.)]\} \quad 4.3.15$$

so that

$$<V(x(t))>_1 = \frac{1}{Z_1} \int \frac{dx_0}{\sqrt{2\pi\beta}} \prod_{n=1}^{\infty} \frac{dx_n^{real}\, dx_n^{im}}{\pi/\beta\omega_n^2} \int \frac{dq}{2\pi} V(q) \exp\{-\beta \sum_{n=1}^{\infty}\{\omega_n^2 + \Omega^2(x_0)\}|x_n|^2$$

$$-\beta L_1(x_0) + iq\{x_0 + \sum_{n=1}^{\infty}(x_n e^{i\omega_n t} + c.c)\}\} \quad 4.3.16$$

in which all x_n, $n \neq 0$ can again be integrated out. The result as seen from appendix A_5 is

$$< V(x(t)) >_1 = \int \frac{dx_0}{\sqrt{2\pi\beta}} \frac{\beta\Omega(x_0)/2}{\sinh\{\beta\Omega(x\ )2\}} e^{-\beta L_1(x_0)} V_{a^2(x_0)}(x_0) \quad 4.3.17$$

where $V_{a^2(x_0)}(x_0)$ is the smeared potential eq. (4.3.6) with

$$a^2(x_0) = \frac{2}{\beta} \sum_{n=1}^{\infty} \frac{1}{\omega_n^2 + \Omega^2(x_0)} \quad 4.3.18$$

which can be summed up to give eq. (4.3.9). The Gaussian potential $\frac{1}{2}\Omega^2(x_0)\ \{x(t)-x_0\}^2$ can be considered as a particular case of $V(x(t))$ and its smeared version $V_{a^2(x_0)}(x_0)$ becomes simply $\frac{1}{2}\,\Omega^2(x_0)\,a^2(x_0)$. Hence

$$<V(x(t)) - \frac{\Omega^2(x_0)}{2}\,\{x(t)-x_0\}^2 - L_1(x_0)>$$

$$= \frac{1}{Z_1}\int \frac{dx_0}{\sqrt{2\pi\beta}}\,\frac{\beta\Omega(x_0)/2}{\sin h\{\beta\Omega(x_0)/2}\,e^{-\beta L_1(x_0)}\,\{V_{a^2(x_0)}(x_0) - \frac{\Omega^2(x_0)}{2}\,a^2(x_0) - L_1(x_0)\}\,. \qquad 4.3.19$$

The unknown functions $\Omega^2(x_0)$, $L_1(x_0)$ are now determined by using the extremal principle explained in section 4.2. Thus based on the inequality (4.1.1) we write

$$Z > Z_1 \exp\{-<\int_0^\beta dt\,\{V(x(t)) - \frac{\Omega^2(x_0)}{2}\,\{x(t)-x_0\}^2\} - \beta L_1(x_0)>_1\} \qquad 4.3.20$$

i.e., the true partition function is bounded from below. Using eqs. (4.3.13) and (4.3.19) and making variations in $\Omega(x_0)$ and $L_1(x_0)$ we see that the best lower bound is obtained when the integrand of eq. (4.3.19) vanishes. This gives

$$L_1(x_0) = V_{a^2(x_0)}(x_0) - \frac{\Omega^2(x_0)}{2}\,a^2(x_0)\,. \qquad 4.3.21$$

Feynman and Kleiner applied the above procedure to two cases where the answers are exactly known and found remarkably good fits for the free energies. Before their work several attempts were made[20-25] to improve the original Feynman calculation presented in section 4.2. However, the effective classical potential obtained here seems to provide much better result than these calculations. We shall not pursue the matter further except to note that a Gaussian provides a very good approximation to many known smooth potentials.

CHAPTER FIVE

A SURVEY OF OTHER APPLICATIONS

5.1 Introduction

The previous chapters essentially conclude our studies for this project. However, for the sake of completeness and to emphasize the power of this approach we survey in this chapter a few other applications of the formalism. Many of these works have been done in the past few years and could not readily be a part of such a limited study. But all the same they help us provide the perspective for our future studies. This chapter is presented just in this spirit.

5.2 Non Local Quadratic Actions[7]

Such actions arise in many physical applications. They have the general form:

$$s = \frac{1}{2}\int_0^T dt\,\dot{x}^2 - \frac{1}{2}\int_0^T dt\int_0^T ds\,G(t,s)x(t)x(s) + \int_0^T f(t)x(t)dt \qquad 5.2.1$$

where G(t,s) is a symmetric function of the times t and s while f(t) is some time dependent external force. G(t,s) represents a phenomenological way of characterizing memory effects. They arise when a given system interacts with a larger system such as a heat bath, for example. In these problems one is usually interested in the time evolution of the coordinates of the system (e.g. a particle) which is described by an "average propagator" obtained by averaging the propagator of the total system over the coordinates of the particle. This is the reduced description of the single particle behaviour and it gives rise to non-local selfinteraction terms in the action functional associated with the average propagator. The resulting path integral contains Gaussian integrals and can be performed exactly. We shall now illustrate these general remarks with specific examples.

a) <u>The Polaron Problem:</u>[26-27,6]

Consider an electron moving in a polar crystal. The electron interacts with ions which are not rigidly fixed. This distorts the lattice in the neighbourhood of the electron. When the electron moves about the region of distortion moves with it resulting in self-induced polarization. The electron plus its associated distortion is called a polaron. In this phenomenon the energy of the electron is lowered whereas its effective mass is increased. The distortion so created takes time to die out i.e., the ions take time to relax. Now this distortion acts back on the electron at a later time. In effect, the electron interacts with its past. This generates a non-local self interaction. Feynman studied an idealized version of this problem. The Lagrangian of the total system consists of a sum of the Lagrangian of the free electrons, the Lagrangian of the free phonons and the phonon-electron interaction potential. The dynamics of this system can be described by a path integral over electron and phonon coordinates. The Lagrangian of the system being quadratic in the phonon coordinates, the path integration over these coordinates can be done exactly.

The phonon variables are thus eliminated. The problem, now reduces to the path integral of an effective non-local action functional s involving only the electron coordinates:

$$S = \frac{1}{2}\int_0^\beta \dot{\bar{r}}^2\,dt - \frac{\alpha}{\sqrt{8}}\int_0^\beta dt\int_0^\beta \frac{\exp\{-(t-t')\}}{\bar{r}(t)-\bar{r}(t')}\,dt' \cdot \qquad 5.2.2$$

This is then the functional for the partition function where α is the phonon-electron coupling constant.

The path integral for this action cannot be done. So one has to choose a suitable trial functional S' and apply the variational technique. Feynman chose a functional

$$S' = \frac{1}{2}\int_0^\beta \dot{\bar{r}}^2\,dt + \frac{C}{2}\int_0^\beta dt\int_0^\beta \{\bar{r}(t)-\bar{r}(t')\}^2\exp\{-\omega(t-t')\}dt'. \qquad 5.2.3$$

The parameters C and ω are variational quantities chosen to obtain the lowest upper bound for the ground state energy, i.e.,

$$E \leq E_0 + \frac{1}{\hbar\beta} < s-s' > , \ \beta \to \infty \cdot \qquad 5.2.4$$

The polaron problem has been extensively studied.[28,29]

b) Electronic Spectrum in disordered systems[30-37]

The problem here is the study of the electronic density of states in an amorphous solid where the electrons interact with randomly distributed ions. This problem is relevan from a fundamental point of view as well as the point of view of technology. Semiconductor devices critically depend on the electronic density of states in the band gap region. The basic aim is to obtain the electron propagator from which the density of states follow via a Fourier transform with respect to time as indicated in chapter one. Edward and Gulyaev[35] formulated the problem as follows. They considered an electron in the field of N scattering centres (ions) in a volume V. The electron propagator is

$$k(\bar{r}'',T;\bar{r}',0) = \int \left(\exp\left\{\frac{i}{\hbar}\int_0^T \left(\tfrac{1}{2}m\dot{\bar{r}}^2 - \eta\sum_j V(\bar{r}-\bar{R}_j)\right)dt\right\}\right) D\bar{r}(t) \qquad 5.2.5$$

where $\bar{r}$ is the electron coordinate, $\bar{R}_j$'s are the ion positions and $V(\bar{r}-\bar{R}_j)$ is the potential between the electron and the jth ion. The ions are assumed randomly distributed and therefore their probability distribution $P(\bar{R})d^3\bar{R}$ is given by

$$P(\bar{R})d^3\bar{R} = \prod_j d^3\bar{R}_j/V) \cdot \qquad 5.2.6$$

In the limit the number of ions $N\to\infty$, $V\to\infty$ but the density ρ of ions remains finite; the propagator averaged over all ionic configurations or Green's function becomes

$$G = \int \left(\exp \frac{i}{\hbar}\int_0^T \frac{m}{2}\dot{\bar{r}}^2 dt + \rho\int\left\{\exp\left[-\frac{i}{\hbar}\int_0^T \eta\, V(\bar{r}-\bar{R})dt\right\}-1\right]d^3\bar{R}\right\}\right) D\bar{r}(t) \cdot \qquad 5.2.7$$

For analytical simplicity one considers dense scatterers but weak i.e., $\rho\to\infty$, $\eta\to 0$, but $\rho\eta^2$ remains finite. In such a case one obtains

$$G = \int \exp\left\{\frac{i}{\hbar}\int_0^T \frac{m}{2}\dot{\bar{r}}^2 dt - \rho\, \eta^2/2\hbar^2 \int_0^T dt \int_0^T dt'\, W(\bar{r}(t)-\bar{r}(t'))\right\} D\bar{r}(t)$$

where 5.2.8

$$W = \int V(\bar{r}(t) - \bar{R})\, V(\bar{r}(t') - \bar{R})\, d^3\bar{R} \; .$$

Again the problem becomes one of path integrating a non-local action functional. The non-locality arises due to the averaging over the ionic configuration. The actual form of W depends on the electron-ion interaction potential.

c) The Propagation of Waves in Random Media

As the wave propagates through the medium its amplitude $\bar{A}(\bar{r},t)$ at any space-time point and its frequency ω are affected by the fluctuations in the medium. These fluctuations can be large or small. The path integral formalism is able to handle both. This problem is of interest in atmospheric optics as well as astronomy.[36]

5.3 Path Integrals in Polar Coordinates[7]

We have discussed path integrals in rectangular coordinates. The choice of a coordinate system depends on the symmetry of a given problem. It is thus natural to enquire if path integrals can be handled in other coordinate systems. As a matter of fact, a tremendous amount of work has been done in this direction. The propagator can be evaluated for polar coordinates provided the angular coordinates can be separated from the radial ones by means of an appropriate expansion in terms of standard polynomials. One can thus deal with the free particle, harmonic oscillator, inverse square potential as well as some non central potentialis.

We briefly outline one such example.[37,7] A charged particle in a harmonic potential subjected to a uniform magnetic field B say in the Z direction. The equation of motion is

$$m(\ddot{\bar{r}} + \Omega^2\bar{r}) = e(\dot{\bar{r}} \times \bar{B}) \cdot \qquad 5.3.1$$

Assuming $\bar{B}$ along the Z direction the corresponding Lagrangian is

$$L = \frac{m}{2}\dot{r}^2 + m\,\omega\,(x\dot{y} - y\dot{x}) - \frac{m}{2}\Omega^2 r^2 \qquad 5.3.2$$

where $\omega = eB/2m$. We can write this Lagrangian in a convenient form

$$L = L_0(z,\dot{z}) + L^{\perp}(\dot{x},\dot{y},x,y) \cdot \qquad 5.3.3$$

L_0 is the Lagrangian corresponding to the z - motion

$$L_0 = \frac{m}{2}(\dot{z}^2 - \Omega^2 z^2) \qquad 5.3.4$$

while L is the Lagrangian corresponding to the motion in a plane perpendicular to the z - axis

$$L^{\perp} = \frac{m}{2}(\dot{x}^2 + \dot{y}^2) + m\omega(x\dot{y} - y\dot{x}) - \frac{m}{2}\Omega^2(x^2 + y^2) \cdot \qquad 5.3.5$$

Hence, the propagator factorizes as

$$K = k_0(z",t";z',t')\; K^{\perp}(x",y",t";x',y',t') \qquad 5.3.6$$

where k_0 corresponds to the Lagrangian in eq. (5.3.4) and it is the propagator of the simple harmonic oscillator which can be written down immediately using the method of chapter two. $K^{\perp}$ is the propagator associated with the planar motion characterized by the Lagrangian in eq. (5.3.5). The problem of evaluating this propagator can be done using plane polar coordinates. Here we write

$$L = \frac{m}{2}\left(\dot{r}^2 + r^2\dot{\theta}^2 - \Omega^2 r^2 + 2\omega r^2\dot{\theta}\right). \qquad 5.3.7a$$

To make it radially symmetric we use a linear transformation $\varphi = \theta + \omega t$. Then

$$L^{\perp} = \frac{m}{2}\left(\dot{r}^2 + r^2\dot{\varphi}^2 - (\Omega^2 + \omega^2) r\right). \qquad 5.3.7b$$

This is the Lagrangian of a harmonic oscillator with frequency $\Omega' = \sqrt{\Omega^2 + \omega^2}$ and using the polar coordinate formalism one can show that

$$K^{\perp} = \left(\frac{m\Omega'}{2\pi i\hbar \sin\Omega' T}\right)^{\frac{1}{2}} \exp\left\{\frac{im\Omega}{2\hbar\sin\Omega' T}\left(r''^2 + r'^2\right)\cos\Omega' T - 2r'r''\cos\left(\theta'' - \theta' + \omega T\right)\right\} \qquad 5.3.8$$

where $T = t'' - t'$. The complete propagator is obtained using eq. (5.3.6).

Replacing T by $-i\hbar\beta$ one gets the density matrix $\rho(r'', r'; \beta)$. The partition function is obtained by setting $r'' = r'$ and integrating ρ over all values of r' i.e.,

$$Z(\beta) = \int_0^{\infty} \rho(r', r'; \beta)\, dr' \equiv \left\{8 \sinh\left\{\frac{\beta\hbar}{2}(\Omega' + \omega)\right\} \sinh\left\{\frac{\beta\hbar}{2}(\Omega' - \omega)\right\} \sinh\frac{\beta\hbar\Omega}{2}\right\}^{-1}. \qquad \ldots \quad 5.3.9$$

We can then obtain the density of states $n(\varepsilon)$ from

$$Z(\beta) = \int_0^\infty n(\varepsilon)\, \exp(-\beta\varepsilon)\, d\varepsilon; \qquad 5.3.10$$

recall that the partition function is the Laplace transform of the density of states. Using the inverse Laplace transform we find

$$n(\varepsilon) = \sum_{n_1, n_2, n_3} \delta(\varepsilon - \varepsilon_{n_1, n_2, n_3}) \qquad 5.3.11$$

with

$$\varepsilon_{n_1,n_2,n_3} = (n_1 + \tfrac{1}{2})\hbar(\Omega'+\omega) + (n_2 + \tfrac{1}{2})\hbar(\Omega'-\omega) + (n_3 + \tfrac{1}{2})\hbar\Omega \,. \qquad 5.3.12$$

This is equivalent to the Zeeman effect exhibited by a harmonically bound charge.

We can also use the partition function to evaluate some other quantities. For example, consider ions on a lattice modelled as independent harmonic oscillators each of frequency Ω subjected to a uniform magnetic field $\mathbf{B}$ applied along the Z direction. Since each ion oscillates independently, the single particle partition function given by eq.(5.3.10) is sufficient for obtaining the thermodynamic properties of the system. Thus using this result it is possible to evaluate the free energy F, the lattice energy E, the specific heat C and the magnetization per particle $M = -\partial F/\partial \mathbf{B}$ of the medium. This rather unrealistic model has very interesting properties. For example it shows that the ionic lattice at low fields is diamagnetic.

We note that non Cartsian coordinates have found a use with non-spherically symmetric potentials. The calogero[38] problem is one such problem. Here three particles of equal mass interact pairwise via harmonic and inverse square potentials. By a suitable coordinate transformation this problem is converted into a free particle problem plus a part which can be solved in plane polar coordinates. Another problem is that of an isotropic oscillator in an inverse square potential.[7]

5.4 General Coordinate Transformations

This method widens the class of exactly solvable problems considerably. The basic idea is to look for coordinate transformations which convert the given Lagrangian into the class of previously solved problems. One then makes a transformation $x \to f(q)$ followed by a time transformation $t \to t'$. A very important problem solved thereby is the Coulomb problem.[39-42] The non-trival task is the evaluation of the radial propagator given by

$$K^{j} = (r''r')^{d_j} \; K_{\gamma_j}(r'',r';T) \qquad 5.4.1$$

where the supscript $j(=2,3)$ indicates the 2 and 3 dimensional cases. The constants d_j and γ_j are given by $d_2 = -\frac{1}{2}$, $d_3 = -1$, $\gamma_2 = \ell$, $\gamma_3 = \ell + \frac{1}{2}$. One is then led to an effective one dimensional radial Lagrangian

$$L = \frac{m}{2}\dot{r}^2 - \left\{ \frac{(\gamma_j^2 - 1/4)\hbar^2}{2mr^2} + \frac{e^2}{r} \right\} \qquad 5.4.2$$

so that

$$V_{eff} = \frac{A}{r} + B/r^2 \qquad 5.4.3$$

using the transformation $r = q^2$ followed by $dt/dt' = 4q^2$, this is changed to the problem involving potential terms of the type $A/q^2 + Bq^2 + c$. The answer for this problem is known.

5.5 Constrained Path Integrals

Constrained motions are often of interest. Examples are the particle in a box and the rigid rotator. As a rule the propagator for such a system is obtained by relating the system to another unconstrained system for which the propagator is available. This may be achieved by using a suitable transformation so that the motion of our system becomes unconstrained. Next the propagator of the unconstrained system is evaluated whereby the propagator of the constrained system is obtained by using the relation between the two systems. Another type of constraint appears when a particle moves in a multiply connected region such as the case of the motion of a particle in the Bohm Aharonov problem.

The simplest type of constrained problems is described by a quadratic action of the type

$$S = \int_0^T \{\frac{m}{2}\dot{x}^2 - \frac{\omega^2(t)}{2}x^2\}\, dt, \quad 0 < x < \infty \qquad 5.5.1$$

Instead one solves the propagator K_g for the functional $s + s'$ where $s' = -\int_0^T (g/x^2)dt$, $0 < x < \infty$. The propagator k_g is easily obtained by the usual procedure. Finally, the propagator to the functional in eq. (5.5.1) is obtained by taking the limit $g \to 0$. K_g does not go over to the usual harmonic oscillator propagator. This feature of path integrals is called the "Klauder Phenomena"[43] and is very welcome. We expect this in quantum mechanics where the singular part of a potential eliminates some of the formal solutions of the Schrodinger equation as for example in the case of the half-oscillator where the even parity solutions are eliminated.

The problem of the rigid rotator[7] can be solved using such an approach. Three other problems can be related to the rigid rotator by the general coordinate transformation technique. These are the Scharf,[44] Puschl-Teller[45] and Rosen-Morse[46] potentials. Amusingly enough the problem of a particle in a box has been successively solved only recently[48] using the technique of general coordinate transformation.

Now let us come back to the second type of constrained problem mentioned above. This is the motion of a system in a multiply connected region (space). Such spaces arise due to the presence of singularity around which the paths pass. The paths which cannot be deformed into each other are said to belong to different homotopy classes. A simple example is that of a free particle in a plane where the origin is a singular point. A path between two points r" and r' cannot pass through this singularity. It can go around it once, twice, etc. A path which encircles this singularity m times is homotopically different from the one that encircles it n times. The number of turns around a singularity is called the winding number and takes values 0, ±1, ±2... The presence of the solenoid in the Bohm-Aharonov problem makes the space multiply connected. A similar problem arises in a polymer which is a large number of repeated molecular chains called monomers.

5.6 Invariants in Time-dependent Problems

Finally since path integrals are generally designed for time dependent problems an interesting problem is the search for invariants for time dependent problems. The hope always is that their knowledge can simplify the problem as does that of the integrals of motion for time independent Hamiltonians. This approach in fact is proving to be extremely fruitful. Lewis and Riesenfeld[48] showed that for a quantum system characterized by a time-dependent Hamiltonian operator $H(t)$ and a Hermitian invariant operator $I(t)$ the general solution of the time dependent Schrodinger equation is given by

$$\psi(\bar{r},t) = \Sigma\, C_n \exp\{i\alpha_n(t)\}\psi_n(\bar{r},t) \qquad 5.6.1$$

where $\psi_n(\bar{r},t)$ are the normalized eigenfunctions of the invariant operator I, i.e,

$$I\psi_n = \lambda_n \psi_n \qquad 5.6.2$$

where the eigenvalues are time independent. The expansion coefficients are constant and the time dependent phases are given by

$$\hbar \frac{\partial}{\partial t} \alpha_n(t) = \langle \psi_n | i\hbar \partial/\partial t - H | \psi_n \rangle . \qquad 5.6.3$$

They used this result for the problem of a time dependent oscillator and a charged particle in a time varying electromagnetic field. An important relation between the invariant and the Feynman propagator follows. We have

$$C_n = \exp\{-i\alpha_n(t)\} \int \psi_n^* \psi d^3\bar{r} \qquad 5.6.4$$

i.e.,

$$\psi(\bar{r}'',t') = \sum_n \exp\{-i\alpha_n(t')\} \{\int \psi_n^*(\bar{r},t')\psi(\bar{r},t')d^3\bar{r}\}$$

$$\cdot \exp\{i\alpha_n(t'')\} \psi_n(\bar{r}'',t'')$$

$$= \int d^3\bar{r}\{\sum_n \exp\{i(\alpha_n(t'')-\alpha_n(t'))\} \psi_n^*(\bar{r}'.t')\psi_n(\bar{r}'',t'')$$

$$\cdot \psi(\bar{r}',t')\}$$

$$= \int d^3\bar{r}' k(r'',t''; \bar{r}',t') \psi(\bar{r}',t'), \quad t''>t' \qquad 5.6.5$$

From this we deduce the expansion formula for the propagator of the time dependent Hamiltonian i.e.,

$$k(\bar{r}'',t'';\bar{r}',t') = \sum_n \exp\{i(\alpha_n(t'')-\alpha_n(t'))\}\psi_n^*(\bar{r}',t')\psi_n(\bar{r}'',t'')$$

$$t''>t' \qquad 5.6.6$$

For the time dependent problem, the conserved quantity is the invariant I rather than the Hamiltonian H and the propagator admits a natural expansion in terms of the eigenfunctions of the invariant operator. The existence of the invariant I greatly simplifies the derivation of the propagator. We shall not go into further details.

At this point we would have to stop rather abruptly the exposition of the path integral technique, for, a real narration of all its achievements is well beyond the scope of the present work.

EPILOGUE

We have attempted a basic exposition of this elegant and powerful technique in relation to non relativistic quantum mechanics and statistical mechanics. Feynman's hope in initiating this approach has not been belied. The effectiveness of this method enhances with the evaluation of each new propagator. Central to this presentation have been Gaussian path integrals. The technique of general co-ordinate transformation and time rescaling is proving to be very valuable as it is even able to deal with originally non integrable problems. Currently this method is employed in discussing quantum mechanics on curved spaces and Gauge theories. One area where no systematic work is still available is the quantum mechanics of compound potentials where the Schrodinger theory has answers rather readily available. This is an area we wish to explore in future.

Appendix A_1

We present a method due to Abe in which the path integral formulation of the propagator arises out of the Schrodinger formalism.

Let the Hamiltonian of a system be given by

$$H(\bar{r}) = -\frac{\hbar^2}{2m}\nabla^2 + V(\bar{r}) \qquad (1)$$

We have

$$\{i\hbar\frac{\partial}{\partial t} - H(\bar{r})\}\,\psi(\bar{r},t) = 0 \qquad (2)$$

whose solution is

$$\psi(\bar{r},t) = \exp\{-\frac{it}{\hbar}H(\bar{r})\}\,\psi_0(\bar{r}) \qquad (3)$$

where $\psi_0(\bar{r})$ is the initial wave function of the system.

We can write eq. (3) as

$$\psi(\bar{r},t) = \int \exp(-\frac{it}{\hbar}H)\delta^3(\bar{r}-\bar{r}')\psi_0(\bar{r}')d^3\bar{r}' = \int K(\bar{r},t;\bar{r}',0)\psi_0(\bar{r}')d^3\bar{r}' \qquad (4)$$

whence

$$K(\bar{r},t;\bar{r}',0) = \exp(-\frac{it}{\hbar}H)\delta^3(\bar{r}-\bar{r}') \qquad (5)$$

We know that $\delta^3(\bar{r}-\bar{r}') = \langle\bar{r}|\bar{r}'\rangle$ and thus

$$K(\bar{r},t;\bar{r}',0) = \langle\bar{r}|\exp(-\frac{it}{\hbar}H(\bar{r}))|\bar{r}'\rangle \qquad (6)$$

But

$$\exp\{-\frac{it}{\hbar}H(\bar{r})\} = \lim_{n\to\infty}\{1 - \frac{itH(\bar{r})}{\hbar n}\}^n \qquad (7)$$

Now we write

$$K_n(\bar{r},t;\bar{r}',0) = \int\langle\bar{r}|(1-\frac{i\varepsilon}{\hbar}H)|\bar{r}_{n-1}\rangle\langle\bar{r}_{n-1}|(1-\frac{i\varepsilon}{\hbar}H)|\bar{r}_{n-2}\rangle$$

$$\langle\bar{r}_{n-2}|(1-\frac{i\varepsilon}{\hbar}H)|\bar{r}_{n-3}\rangle\cdots\langle\bar{r}_1|(1-\frac{i\varepsilon}{\hbar}H)|\bar{r}'\rangle d^3\bar{r}_1\cdots d^3\bar{r}_{n-1}$$

(8)

Where we have divided the time into steps of width $\varepsilon = t/n$. We need

$$K = \lim_{n \to \infty} K_n \tag{9}$$

In eq. (8) we have n short time propagators of the form

$$< \bar{r}_{j+1} | 1 - \frac{i\varepsilon}{\hbar} H(\bar{r}_{j+1}) | \bar{r}_j > = \{1 - \frac{i\varepsilon}{\hbar} H(\bar{r}_{j+1})\} \delta(\bar{r}_{j+1} - \bar{r}_j) \tag{10}$$

and n-1 3-D integrations.

Fourier transforming the δ-function we have

$$\delta(\bar{r}_{j+1} - \bar{r}_j) = \frac{1}{(2\pi)^3} \int d^3\bar{K} \; \exp\{ i\bar{K}.(\bar{r}_{j+1} - \bar{r}_j)\} \tag{11}$$

combining eqs. (1), (10) and (11) and noting that ε is infinitesimal we immediately obtain

$$< \bar{r}_{j+1} | 1 - \frac{it}{\hbar} H(\bar{r}_{j+1}) | \bar{r}_j >$$

$$= \frac{1}{(2\pi)^3} \int d^3\bar{k} \exp\{ - \frac{i\hbar k^2}{2m} \varepsilon - \frac{i\varepsilon V(\bar{r}_j)}{\hbar} \} \exp\{ i\bar{k}.(\bar{r}_{j+1} - \bar{r}_j)\}$$

$$= (\frac{m}{2\pi i\hbar\varepsilon})^{3/2} \{\exp \frac{i\varepsilon}{\hbar} [\frac{m}{2} (\frac{r_{j+1} - r_j}{\varepsilon})^2 - V(\bar{r}_j)]\}\} \tag{12}$$

The integration on $\bar{k}$ in eq. (12) is trivally done by completing the square. If we use the above result in eq. (9) we have the desired expression

$$K_n = (\frac{m}{2\pi i\hbar\varepsilon})^{3/2} \int \exp\{\frac{i\varepsilon}{\hbar} \sum_{j=0}^{n-1} [\frac{m}{2} (\frac{\bar{r}_{j+1} - \bar{r}_j}{\varepsilon})^2 - V(\bar{r}_j)]\}$$

$$\prod_{j=1}^{n-1} (\frac{m}{2\pi i\hbar\varepsilon})^{3/2} d^3\bar{r}_j \tag{13}$$

where $\bar{r}_0 = \bar{r}'$ and $r_n = \bar{r}$.

Notice that eq. (13) contains the Lagrangian explicitly in descrete form although we started with the Hamiltonian formalism. In the limit $n \to \infty$, the sequence k_n goes to the required propagator. Then introducing the Feynman notation of path integrals we have

$$k(\bar{r},t;\bar{r}',0) = \int_{\bar{r}'}^{\bar{r}} \exp\{\frac{iS\{\bar{r}(t)\}}{\hbar}\} D\vec{r}(t)$$

where $S\{\bar{r}(t)\} = \int_0^t \{\frac{m}{2}\dot{\bar{r}}^2(t) - V(\bar{r}(t))\}\,dt = \int_0^t L dt$ and

$$Dr(t) = \lim_{n\to\infty} (\frac{m}{2\pi i\hbar\varepsilon})^{3/2} \prod_{j=1}^{n} (\frac{m}{2\pi i\hbar\varepsilon})^{3/2} d^3\bar{r}_j$$

Note also that the integration measure has come out automatically in this derivation. This should be contrasted with Feynman's original derivation based on Dirac's suggesti

Appendix A_2

The Fourier Method for Evaluating Path Integrals:

The paths $y(t)$ are written as a Fourier sine series with a period of T

$$y(t) = \sum_n a_n \sin \frac{n\pi t}{T}$$

We regard the paths as functions of the coefficients a_n. Here we have a linear transformation with a constant Jacobian J, independent of ω, m and h. But we are not interested in the evaluation of J since we can always recover the correct factor at the end. This, as we see depends on the result for $\omega = 0$, $A(T)=A(t)=\sqrt{m/2\pi i\hbar t}$

$$\int_0^T \dot{y}^2(t)\,dt = \sum_n \sum_m \frac{n\pi}{T} \frac{m\pi}{T} a_n a_m \int_0^T \cos\frac{n\pi t}{T} \cos\frac{m\, t}{T} dt$$

$$= \frac{T}{2} \sum_n a_n^2 \left(\frac{n\pi}{T}\right)^2$$

Similarly,

$$\int_0^T y^2 dt = \frac{T}{2} \sum_n a_n^2$$

So now the multiple integral eq.(2.2.1) becomes

$$A_N(T) = J\int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} \{\exp[\sum_{n=1}^{N} \frac{im}{2\hbar}((\frac{n}{T})^2 - \omega^2) a_n^2]\} \frac{da_1}{B} \cdots \frac{da_N}{B}$$

where $B = \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{\frac{1}{2}}$. for the n^{th} variable

$$\int_{-\infty}^{\infty} \{\exp[\frac{im}{2\hbar}(\frac{n^2\pi^2}{T^2} - \omega^2) a_n^2]\} \frac{d^a n}{B} = \left(\frac{n^2\pi^2}{T^2} - \omega^2\right)$$

Thus doing the integral over all variables a_n we get

$$A_N(T) = J \prod_{n=1}^{\infty} \left(\frac{n^2\pi^2}{T^2} - \omega^2\right)^{-\frac{1}{2}} = J \prod_{n=1}^{N} \left(\frac{n^2\pi^2}{T^2}\right)^{-\frac{1}{2}} \prod_{n=1}^{N} \left[1-\frac{\omega^2 T^2}{n^2\pi^2}\right]^{-\frac{1}{2}}$$

In the limit $N\to\infty$, $\prod_{n=1}^{N} \left[1-\frac{\omega^2 T^2}{n^2\pi^2}\right] = \left(\frac{\sin\omega T}{\omega T}\right)^{-\frac{1}{2}}$ and collecting all the factors which do not depend on ω into a single constant C we have

$$A(T) = C\left(\frac{\sin\omega T}{\omega T}\right)^{-\frac{1}{2}}$$

For a free particle, $\omega = 0$, $A(T) = \sqrt{m/2\pi i\hbar T}$

whence for the harmonic oscillator

$$A(T) = \left(\frac{m\omega}{2\pi i\hbar\sin\omega T}\right)^{\frac{1}{2}}$$

Appendix A_3

The Classical Action for the Simple Harmonic Oscillator:

Here the Lagrangian is given by

$$L = \frac{m}{2}(\dot{x}_{cl}^{2} - \omega^2 x_{cl}^{2})$$

corresponding to a classical trajectory. The equation c motion is

$$\ddot{x}_{cl} + \omega^2 x_{cl} = 0$$

with solution

$$x_{cl}(t) = A\sin\omega t + B\cos\omega t$$

Applying the initial condition $x_{cl}(t_a) = x_a$ and $x_{cl}(t_b) = x$ and solving the resulting equations we find

$$A = \frac{x_b\cos\omega t_a - x_a\cos\omega t_b}{\sin\omega(t_b - t_a)}, \quad B = \frac{x_a\sin\omega t_b - x_b\sin\omega t_a}{\sin\omega(t_b - t_a)}$$

Now

$$s_{cl} = \int_{t_a}^{t_b} L(x_{cl}, \dot{x}_{cl}, t)\,dt = \int_{t_a}^{t_b} \left(\frac{m}{2}\dot{x}_{cl}^2 - \frac{m}{2}\omega^2 x_{cl}^2\right)dt$$

Then using the expression for x_{cl} we find

$$s_{cl} = \frac{m\omega^2}{2}\int_{t_a}^{t_b}[(A^2 - B^2)\cos 2\omega t - 2AB\sin 2\omega t]\,dt$$

$$= \frac{m\omega^2}{2}\left[\frac{(A^2 - B^2)}{2\omega}\sin 2\omega t + \frac{AB}{\omega}\cos 2\omega t\right]_{t_a}^{t_b}$$

or

$$s_{cl} = \frac{m\omega^2}{2}\left[\frac{(A^2 B^2)}{2\omega}(\sin 2\omega t_b - \sin 2\omega t_a) + AB(\cos 2\omega t_b - \cos 2\omega t_a)\right]$$

Substituting the expressions for A and B and simplify we finally get

$$S_{cl} = \frac{m\omega}{2\sin\omega T}\{(x_a^2+x_b^2)\cos\omega T - 2x_a x_b\}$$

From eq. (4.1.20) we have

$$Z = \int_{-\infty}^{\infty} \exp\left[-\frac{U}{\hbar} V(\bar{x})\right] d\bar{x} \int_{-\infty}^{\infty} \frac{dk}{2\pi} \int_{y(0)}^{y(U)} \left(\exp\left\{-\frac{1}{\hbar}\int_0^U \left[\frac{m}{2}\dot{y}'^2 + \frac{V''}{2} y^2 + iky\right] du\right\}\right) DY(U)$$

The integrand of the path integral has the same form as the path integral for a forced harmonic oscillator if we assume that the frequency is given by $\omega^2 = -V''/m$. Let us expand each path $y(u)$ about the path that makes the largest contribution to Z, i.e. the "classical path" y_{cl} and we write $y(u) = y_{cl}(u) + y^*(u)$ where $y^*(0) = y^*(U) = 0$. Applying the method used in chapter 2 we can write the above path inegral as

$$I = F(U) \int_{-\infty}^{\infty} \exp(-"s_{cl}"/\hbar) dy(0),$$

since we have to inegrate over all possible initial confifu-tion of the system. For the path integral F(u) we have

$$F(U) = \int_0^0 \left(\exp\left\{-\frac{1}{\hbar}\int_0^U \left[\frac{m}{2}\dot{y}^{*2} + \frac{V''}{2} y^{*2} + iky^*\right]\right\}\right) Dy^*(u)$$

From eq. (2.2.21C) one has

$$"s_{cl}" = \frac{m\omega}{2\pi\sin\omega U}\left[\{y^2(0) + y^2(U)\}\cos\omega U - 2y(0)y(U) + \frac{2y(0)}{m\omega}\int_0^U f(u)\sin(U-u)du + \frac{2y(U)}{m\omega}\int_0^U f(u)\sin\omega u du - \frac{2}{m^2\omega^2}\int_0^U\int_0^u f(u)f(u')\sin\omega(U-u)\sin\omega u' du' du\right], \omega^2 = \frac{V''(\bar{x})}{m}$$

However we have to take $y(0) = y(U) = y'$. Also A is seen that

$$"s_{cl}" = \frac{m\omega}{2\sin\omega U}[2y'^2(\cos\omega U-1) + \frac{2iky'}{m\omega}\int_0^U \sin\omega(U-u)du$$

$$+ \frac{2iky'}{m\omega}\int_0^U \sin\omega u du + \frac{2k^2}{m^2\omega^2}\int_0^U\int_0^u \sin\omega(U-u)\sin\omega u' du' du]$$

After integrating and simplifying the resulting expression we get

$$"s_{cl}" = \frac{m\omega(\cos\omega U-1)}{\sin\omega U}(y' - \frac{ik}{m\omega^2})^2 - \frac{Uk^2}{2m\omega^2}$$

or

$$"s_{cl}" = -\frac{m\omega(1-\cos\omega U)}{\sin\omega U}(y' - \frac{ik}{m\omega^2})^2 - \frac{uk^2}{2m\omega^2}$$

$$I = F(U)\int_{-\infty}^{\infty} \exp[-\frac{m\omega(1-\cos\omega U)}{\hbar\sin\omega U}(Y' - \frac{ik}{m\omega^2})^2 - \frac{Uk^2}{2\hbar m\omega^2}]dy'$$

By making a change of variable, say $v = y' - \frac{ik}{m\omega^2}$ and integrat we can get

$$I = F(U)\sqrt{\frac{\pi\hbar}{m\omega}}\sqrt{\frac{\sin\omega U}{1-\cos\omega U}}\exp(-Uk^2/2\hbar m\omega^2)$$

$$= \tfrac{1}{2}F(U)\sqrt{\frac{\pi\hbar}{m\omega}}(\tan\frac{\omega U}{2})^{-\frac{1}{2}}\exp(-Uk^2/2\hbar m\omega^2)$$

Next consider the integral

$$I' = \frac{1}{2\pi}\int_{-\infty}^{\infty} I dk$$

we will get

$$I' = \frac{\hbar}{2\sqrt{2}}F(U)\left(\frac{\omega}{U}\right)^{\frac{1}{2}}(\tan\frac{\omega U}{2})^{-\frac{1}{2}}$$

To first order in V" or second order in ω we have

$$I' = \frac{\hbar}{2\sqrt{2}} F(U) (\frac{}{U})^{\frac{1}{2}} [\frac{\omega U}{2} + \frac{1}{3}(\frac{\omega U}{2})^3]^{-\frac{1}{2}}$$

$$= \frac{\hbar F(U)}{2U} (1 + \frac{\omega^2 U^2}{12})^{-\frac{1}{2}}$$

$$= C(U) (1 + \frac{\omega^2 U^2}{12})^{-\frac{1}{2}} , \quad C(U) = \frac{\hbar F(U)}{2U}$$

and to the order indicated we write

$$I' = C(U) (1 - \frac{\omega^2 U^2}{24}) = C(U) [1 - \frac{U^2 V''(\bar{x})}{24m}]$$

or

$$I' = C(U) \exp[- \frac{U^2 V''(\bar{x})}{24m}]$$ again to the same order.

Now using the equation at the very begining together with this result Z becomes

$$Z = C(U) \int_{-\infty}^{\infty} \exp(-[\frac{U}{\hbar} V(\bar{x}) + \frac{U^2 V''(\bar{x})}{24m}]) d\bar{x}$$

But in the limit of applicability of the classical expression this result must reduce to eq. (4.1.15) whence

$$C(U) = \sqrt{m/2\pi\hbar U}$$

Therefore

$$Z = \sqrt{m/2\pi\hbar U} \int_{-\infty}^{\infty} \exp(-[\frac{U}{\hbar} V(\bar{x}) + \frac{U^2 V''(\bar{x})}{24m}]) d\bar{x}$$

$$Z = \sqrt{mkT/2\pi\hbar^2} \int_{-\infty}^{\infty} \exp(-\beta [V(\bar{x}) + \frac{\beta\hbar^2 V''(\bar{x})}{24m}]) d\bar{x}$$

Appendix A_5

We have

$$Z_1 = \int_{x(0)}^{x(\beta)=x(0)} \exp[-\int_0^\beta dt\{\frac{\dot{x}^2(t)}{2} + \frac{\Omega^2(x_o)}{2}[x(t)-x_o]^2\} - \beta L_1(x_o)] \quad (1)$$

$$x(t) = x_o + \sum_{n=1}^{\infty} (x_n e^{i\omega_n t} + x_n^* e^{-\omega_n t}), \ \omega_n = 2\pi n/\beta \quad (1)$$

$$= x_o + 2\sum_{n=1}^{\infty} (x_n^r \cos\omega_n t - x_n^i \sin\omega_n t), \ r\text{-real}, \ i - \text{imaginary} \quad (2)$$

This gives

$$\int_0^\beta [x(t)-x_o]^2 dt = 2\sum_{n=1}^{\infty} |x_n|^2, \ \int_0^\beta \dot{x}^2(t)dt = 2\sum_{n=1}^{\infty} \omega_n^2 |x_n|^2 \quad (3)$$

i.e. $$Z_1 = \int_{-\infty}^{\infty} \frac{dx_o}{\sqrt{2\pi\beta}} \prod_{n=1}^{\infty} \int_{-\infty}^{\infty} \frac{dx_n^r \, dx_n^i}{\pi/\beta\omega_n^2} \exp\{-\beta\sum_{n=1}[\omega_n^2 + \Omega^2(x_o)]|x_n|^2 - \beta L_1(x_o)\} \quad (4)$$

We have simple Gaussian integrals over x_n^r and x_n^i which give

$$Z_1 = \int_{-\infty}^{\infty} \frac{dx_o}{\sqrt{2\pi\beta}} \prod_{n=1}^{\infty} \frac{\omega_n^2}{\omega_n^2 + \Omega^2(x_o)} \exp(-\beta L_1(x_o))$$

$$= \int_{-\infty}^{\infty} \frac{dx_o}{\sqrt{2\pi\beta}} \prod_{n=1}^{\infty} \frac{1}{1+[\frac{\beta\Omega(x_o)}{2\pi n}]^2} \exp[-\beta L_1(x_o)]$$

$$= \int_{-\infty}^{\infty} \frac{dk_o}{\sqrt{2\pi\beta}} \frac{\beta\Omega(x_o)/2}{\sinh[\beta\Omega(x_o)/2]} \exp[-\beta L_1(x_o)] \quad (5)$$

The average value of $V(x(t)$ with respect Z_1 is found as follows:

$$V(x(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} V(q) \exp(iqx) dx \tag{6}$$

so that

$$\langle V(x(t))\rangle_1 = \frac{1}{Z_1} \int_{-\infty}^{\infty} \frac{dx_o}{\sqrt{2\pi\beta}} \prod_{n=1}^{\infty} \int_{-\infty}^{\infty} \frac{dx_n^r \, dx_n^i}{\pi/\beta\omega_n^2} \int_{-\infty}^{\infty} \frac{dq}{2\pi} \exp\{-\beta \sum_{n=1}^{\infty}$$

$$[\omega_n^2 + \Omega^2(x_o)]|x_n|^2 - \beta L_1(x_o) + iq[x_o + 2\sum_{n=1}^{\infty}(x_n^r \cos\omega_n t - x_n^i \sin\omega_n t)]\} V(q) \quad \cdots (7)$$

The exponent in the variables x_n^r and x_n^i is simplified to give

$$-\beta \sum_{n=1}^{\infty} [\omega_n^2 + \Omega^2(x_o)]\{(x_n^r - \frac{iq\cos\omega_n t}{\beta[\omega^2+\Omega^2(x_o)]})^2 + (x_n^i + \frac{iq\sin\omega_n t}{\beta[\omega^2+\Omega^2(x_o)]})^2\}$$

$$- \sum_{n=1}^{\infty} \frac{q^2}{\beta[\omega^2+\Omega^2(x_o)]}$$

At this stage define $u_n = x_n^r - \frac{iq\cos\omega_n t}{\beta[\omega_n^2+\Omega^2(x_o)]}$, $y_n = x_n^i + \frac{iq\sin\omega_n t}{\beta[\omega_n^2+\Omega^2(x_o)]}$

The result is (once again we have simple Gaussian integrals)

$$\langle V(x(t))\rangle_1 = \frac{1}{Z_1} \int_{-\infty}^{\infty} \frac{dx_o}{\sqrt{2\pi\beta}} \frac{\beta\Omega(x_o)/2}{\sinh[\beta\Omega(x_o)/2]} \exp[-\beta L_1(x_o)] \int_{-\infty}^{\infty} \frac{dq}{2\pi} V(q) \exp(\frac{a^2 q^2}{2} + iqx_o) \tag{8}$$

where

$$a^2 = \frac{2}{\beta} \sum_{n=1}^{\infty} \frac{1}{\omega^2+\Omega^2(x_o)} \tag{9}$$

Making inverse Fourier transform the 2^{nd} integral in (8) becomes

$$I = \int_{-\infty}^{\infty} \frac{dq}{2\pi} \exp(iqx_o) \int_{-\infty}^{\infty} V(x')\exp(-iqx')\exp(-\frac{a^2q^2}{2})dx'$$

or

$$I = \int_{-\infty}^{\infty} \frac{dx'}{2\pi} V(x') \int_{-\infty}^{\infty} \exp\{-\frac{a^2}{2}[q-\frac{i(x_o-x')}{a^2}]^2 - \frac{(x_o-x')^2}{2a^2}\}dq$$

$$= \int \frac{dx'}{\sqrt{2\pi a^2}} V(x')\exp[-\frac{1}{2a^2}(x_o-x')^2]$$

which is the smeared version of the potential $V(x)$, i.e.

$$V_a^2(x_o) = \int \frac{dx'}{\sqrt{2\pi a^2}} V(x')\exp[-\frac{1}{2a^2}(x_o-x')^2] \qquad (10)$$

using this result in (8) we finally get

$$\langle V(x(t))\rangle_1 = \frac{1}{Z_1} \int \frac{dx_o}{\sqrt{2\pi\beta}} \frac{\beta\Omega(x_o)/2}{\sinh[\beta\Omega(x_o)/2]} V_{a^2}(x_o) \qquad (11)$$

Note that the Jacobian of the transformation can be found to be $\Pi\beta\omega_n^2|\pi$. Also, we have used the result

$$\prod_{n=1}^{\infty} \frac{1}{1+[\beta\Omega(x_o)]^2} = \frac{\beta\Omega(x_o)/2}{\sinh[\beta\Omega(x_o)/2]} .$$

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DECLARATION

THIS THESIS IS MY ORIGINAL WORK AND HAS NOT BEEN PRESENTED FOR A DEGREE IN ANY OTHER UNIVERSITY.

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