CHAPTER I

USEFUL FUNDAMENTAL CONCEPTS

Before going into the actual subject of this work concerning path integrals, it may be useful to recall some of the theoretical background underlying the theory to be developed.

Motion in Classical Mechanics

A classical mechanical system is described by a set of generalized coordinates $q_1, \ldots, q_N$, the associated velocities, $\dot{q}_1, \ldots, \dot{q}_N$, and a Langrangian[Goldstein 1980, Landau 1976]

$$L\left(q_i\left(t\right), \dot{q}_i\left(t\right), t\right). \tag{1.1}$$

The dot denotes the time derivative. The Lagrangian governs the dynamics and is, at most, a quadratic function of $\dot{q}_i$. The time integral

$$S[q_i] = \int_{t_a}^{t_b} dt\, L\left(q_i\left(t\right), \dot{q}_i\left(t\right), t\right) \tag{1.2}$$

over the Lagrangian along an arbitrary path $q_i\left(t\right)$ is called the *action* of this path. The path $q_i\left(t\right)$ that is actually chosen by the system as a function of time is called the classical path, $q_i{}^{cl}\left(t\right)$. It has the property of extremizing the action in comparison with all neighboring paths

$$q_i\left(t\right) = q_i{}^{cl}\left(t\right) + \delta q_i\left(t\right) \tag{1.3}$$

with fixed end points $q(t_b)$, $q(t_a)$. To express this property formally one introduces the *variation* of the action as the linear term in $\delta q_i(t)$ of the changes of $S[q_i]$.

$$\delta S[q_i] \equiv \left\{ S[q_i + \delta q_i] - S[q_i] \right\}_{lin} . \tag{1.4}$$

The extremal principle for the classical path is then

$$\delta S[q_i]\big|_{q_i(t)=q_i^{cl}(t)} = 0 \tag{1.5}$$

for all variations of the path around the classical path, $\delta q_i(t) \equiv q_i(t) - q_i^{cl}$, which vanish at the end points:

$$\delta q_i(t_a) = \delta q_i(t_b) = 0 . \tag{1.6}$$

Since the action is a time integral of a Lagrangian, this extremality property can be phrased in terms of differential equations. Let us calculate the variation of $S[q_i]$ explicitly,

$$\delta S[q_i] = \left\{ S[q_i + \delta q_i] - S[q_i] \right\}_{lin}$$

$$= \int_{t_a}^{t_b} dt \left\{ L(q_i(t) + \delta q_i(t), \dot{q}_i(t) + \delta \dot{q}_i(t), t) - L(q_i(t), \dot{q}_i(t), t) \right\}_{lin}$$

$$= \int_{t_a}^{t_b} dt \left\{ \frac{\partial L}{\partial q_i} \delta q_i(t) + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i(t) \right\}$$

$$= \int_{t_a}^{t_b} dt \left\{ \frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} \right\} \delta q_i(t) + \frac{\partial L}{\partial \dot{q}_i} \delta q_i(t) \Big|_{t_a}^{t_b} . \tag{1.7}$$

The last expression arises by partially integrating the $\delta \dot{q}_i$ term. Here, repeated indices are understood to be summed. The end point terms at t_a and t_b may be dropped, due to (1.6). Thus we find, for the classical orbit $q_i^{cl}(t)$, the so-called *Euler-Lagrange equations:*

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial q_i} \tag{1.8}$$

There is an alternative formulation of classical dynamics which is based on a Legendre transformed function of the Lagrangian called the *Hamiltonian*

$$H(p_i(t), q_i(t), t) \equiv \frac{\partial L}{\partial \dot{q}_i}\dot{q}_i(t) - L(q_i(t), \dot{q}_i(t), t). \tag{1.9}$$

Its value at any time is identified with the energy of the system. According to the general theory of Legendre transformations, the natural variables in H are no longer $q_i(t)$ and $\dot{q}_i(t)$, but $q_i(t)$ and the generalized momenta $p_i(t)$ defined by the equations

$$p_i(t) \equiv \frac{\partial}{\partial \dot{q}_i}L(q_i(t), \dot{q}_i(t), t). \tag{1.10}$$

In order to specify the Hamiltonian $H(p_i(t), q_i(t), t)$ in terms of its proper variables $p_i(t), q_i(t)$, the equations (1.10) for $p_i(t)$ have to be solved for $\dot{q}_i(t)$,

$$\dot{q}_i(t) = v_i(p_i(t), q_i(t), t), \tag{1.11}$$

and inserted into (1.9), giving H as

$$H(p_i(t), q_i(t), t) = p_i(t)v_i(p_i(t), q_i(t), t) - L(q_i(t), v_i(p_i(t), q_i(t)), t). \tag{1.12}$$

Expressed in terms of H, the action becomes a functional of $p_i(t)$ and $q_i(t)$.

$$S[p, q] = \int_{t_a}^{t_b} dt\,[p_i(t)\dot{q}_i(t) - H(p_i(t), q_i(t), t)]. \tag{1.13}$$

This is the so-called *canonical form* of the action. The classical orbits, now specified by $p_i^{cl}(t), q_i^{cl}(t)$, extremize the action in comparison with all neighboring orbits,

where $q_i(t)$ is varied except at fixed end points , and $p_i(t)$ is varied without restriction :

$$q_i(t) = q_i^{cl}(t) + \delta q_i(t), \qquad \delta q_i(t_a) = \delta q_i(t_b) = 0,$$
$$p_i(t) = p_i^{cl}(t) + \delta p_i(t). \tag{1.14}$$

This gives a variation

$$\delta S[p,q] = \int_{t_a}^{t_b} dt \left[\delta p_i(t) \dot{q}_i(t) + p_i(t) \delta \dot{q}_i(t) - \frac{\partial H}{\partial p_i} \delta p_i - \frac{\partial H}{\partial q_i} \delta q_i \right]$$

$$= \int_{t_a}^{t_b} dt \left\{ \left(\dot{q}_i(t) - \frac{\partial H}{\partial p_i} \right) \delta p_i - \left(\dot{p}_i(t) + \frac{\partial H}{\partial q_i} \right) \delta q_i \right\}$$

$$+ p_i(t) \delta q_i(t) \Big|_{t_b}^{t_b} \tag{1.15}$$

Form this we find the *Hamilton equations* of motion for the classical orbits,

$$\dot{p}_i = -\frac{\partial H}{\partial q_i},$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i}. \tag{1.16}$$

These agree with the Euler-Lagrange equations (1.8) via (1.10), as can easily be varified.

Time Displacement Operator

In terms of the bra and ket notation, the Schrödinger equation can be expressed in a basis independent way as an operator equation [Sakurai 1985, Kleinert 1990]

$$\hat{H} \big| \Psi(t) \big\rangle \equiv H(\hat{p}, \hat{x}, t) \big| \Psi(t) \big\rangle = i \hbar \partial_t \big| \Psi(t) \big\rangle, \tag{1.17}$$

to be supplemented by the following specifications of the operators,

$$\widehat{\mathbf{p}} \equiv -i\hbar\partial_x \, , \qquad (1.18)$$

$$\widehat{\mathbf{x}} \equiv \mathbf{x} \, . \qquad (1.19)$$

If the Hamiltonian operator has the special form $H = H(\widehat{p}, \widehat{x})$, i.e., if it contains no explicit time dependence, the basis independent Schrödinger equation (1.17) can be integrated to find the wave function $|\Psi(t)\rangle$ at any time t_b, given the state at any other time t_a

$$|\Psi(t_b)\rangle = e^{-i(t_b - t_a)\widehat{H}/\hbar}|\Psi(t_a)\rangle . \qquad (1.20)$$

The operator

$$\widehat{U}(t_b, t_a) = e^{-i(t_b - t_a)\widehat{H}/\hbar} \qquad (1.21)$$

is called the *time displacement operator*. Its inverse is obtained by interchanging the order of t_b and t_a:

$$\widehat{U}^{-1}(t_b, t_a) \equiv e^{i(t_b - t_a)\widehat{H}^{\dagger}/\hbar} = \widehat{U}^{\dagger}(t_b, t_a) . \qquad (1.22)$$

As an exponential of i times a hermitian operator, $\widehat{U}$ is a unitary operator, with the defining relation

$$\widehat{U}^{\dagger} = \widehat{U}^{-1} . \qquad (1.23)$$

Indeed,

$$\widehat{U}^{\dagger}(t_b, t_a) = e^{i(t_b - t_a)\widehat{H}^{\dagger}/\hbar}$$

$$= e^{i(t_b - t_a)\widehat{H}/\hbar} = \widehat{U}^{-1}(t_b, t_a) . \qquad (1.24)$$

If $H(\widehat{p}, \widehat{x}, t)$ depends explicitly on time, the integration of the Schrödinger equation (1.17) is somewhat more involved. The solution may be found iteratively : For $t_b > t_a$ the time integral is sliced into a large number $N+1$ of small pieces of

thickness ε with $\varepsilon \equiv (t_b - t_a)/(N+1)$, slicing once at each time $t_n = t_a + n\varepsilon$ for $n = 1, \ldots, N$. Then we use the Schrödinger equation (1.17) to relate the wave function in each slice approximately to the previous one:

$$|\Psi(t_a + \varepsilon)\rangle \approx \left(1 - \frac{i}{\hbar} \int_{t_a}^{t_a + \varepsilon} dt\, \hat{H}(t)\right)|\Psi(t_a)\rangle,$$

$$|\Psi(t_a + 2\varepsilon)\rangle \approx \left(1 - \frac{i}{\hbar} \int_{t_a + \varepsilon}^{t_a + 2\varepsilon} dt\, \hat{H}(t)\right)|\Psi(t_a + \varepsilon)\rangle,$$

$$\vdots$$

$$|\Psi(t_a + (N+1)\varepsilon)\rangle \approx \left(1 - \frac{i}{\hbar} \int_{t_a + N\varepsilon}^{t_a + (N+1)\varepsilon} dt\, \hat{H}(t)\right)|\Psi(t_a + N\varepsilon)\rangle. \quad (1.25)$$

In this way we find the approximate time development

$$|\Psi(t_b)\rangle = \left(1 - \frac{i}{\hbar} \int_{t_N}^{t_{N+1}} dt'_{N+1}\, \hat{H}\left(t'_N\right)\right)$$

$$\times \left(1 - \frac{i}{\hbar} \int_{t_{N-1}}^{t_N} dt'_N\, \hat{H}\left(t'_N\right)\right)$$

$$\times \ldots \times \left(1 - \frac{i}{\hbar} \int_{t_a}^{t_1} dt'_1\, \hat{H}\left(t'_1\right)\right)|\Psi(t_a)\rangle. \quad (1.26)$$

Hence the time displacement operator is given approximately by the product

$$\hat{U}(t_b, t_a) \approx \left(1 - \frac{i}{\hbar} \int_{t_N}^{t_{N+1}} dt'_{N+1}\, \hat{H}\left(t'_{N+1}\right)\right) \times \ldots \times \left(1 - \frac{i}{\hbar} \int_{t_a}^{t_1} dt'_1\, \hat{H}\left(t'_1\right)\right). \quad (1.27)$$

The product can be multiplied out and we find in the limit $N \to \infty$ the series

$$\widehat{U}(t_b, t_a) = 1 - \frac{i}{\hbar} \int_{t_a}^{t_b} dt \ \widehat{H}(t) + \left(\frac{-i}{\hbar}\right)^2 \int_{t_a}^{t_b} dt_2 \int_{t_a}^{t_2} dt_1 \widehat{H}(t_2) \widehat{H}(t_1)$$

$$+ \left(\frac{-i}{\hbar}\right)^3 \int_{t_a}^{t_b} dt_3 \int_{t_a}^{t_3} dt_2 \int_{t_a}^{t_2} dt_1 \widehat{H}(t_3) \widehat{H}(t_2) \widehat{H}(t_1) + \ldots \quad . \quad (1.28)$$

This is known as Neumann-Liouville expansion.

Notice that each integral has the time arguments in the Hamiltonian operators ordered causally: Operators with later times stand to left of those with earlier times.

Propagator as The Time Displacement Amplitude

By construction, $\widehat{U}(t_b, t_a)$ has some important properties which we now list [Sakurai 1985, Kleinert 1990]:

a) *Fundamental composition law*

If two time translations are performed after each other, then the corresponding operators $\widehat{U}$ are related by the operator product,

$$\widehat{U}(t_b, t_a) = \widehat{U}(t_b, t') \widehat{U}(t', t_a), \qquad t' \ \varepsilon \ (t_b, t_a). \qquad (1.29)$$

For time independent Hamiltonians, with $\widehat{U}(t_b, t_a)$ given by (1.21), this is trivial to see. It makes the $\widehat{U}$ operators a representation of the abelian group of time translations.

b) *Unitarily*

Initially, the time displacement operator $\widehat{U}(t_b, t_a)$ is derived only for the *causal* time arguments, with t_b later than t_a. We may, of course, define $\widehat{U}(t_b, t_a)$ also for

the *anticausal* case, with t_b earlier than t_a. To be consistent with the above composition law (1.29), we must have

$$\widehat{U}(t_b, t_a) = \widehat{U}(t_a, t_b)^{-1}. \tag{1.30}$$

Indeed, if we consider two states of successive times

$$|\Psi(t_a)\rangle = \widehat{U}(t_a, t_b)|\Psi(t_b)\rangle \tag{1.31}$$

the order of succession is inverted by multiplying both sides by $\widehat{U}^{-1}(t_a, t_b)$:

$$|\Psi(t_b)\rangle = \widehat{U}(t_a, t_b)^{-1}|\Psi(t_a)\rangle. \tag{1.32}$$

This is the time displacement operator $\widehat{U}(t_b, t_a)$ from a later time t_a to an earlier time t_b.

For the case that the Hamiltonian is independent of time, where the time displacement operator is known explicitly,

$$\widehat{U}(t_b, t_a) = e^{-i(t_b - t_a)\widehat{H}/\hbar}, \qquad t_b < t_a, \tag{1.33}$$

it is in accordance with (1.30), and obviously unitary, as observed before in (1.23),

$$\widehat{U}(t_b, t_a) = \widehat{U}(t_a, t_b)^{-1} = \widehat{U}^{\dagger}(t_a, t_b), \qquad t_b < t_a. \tag{1.34}$$

c) *Schrödinger equation for* $\widehat{U}(t_b, t_a)$

Since $U(t_b, t_a)$ gives the relation between arbitrary wave functions at different times,

$$|\Psi(t_b)\rangle = \widehat{U}(t_b, t_a)|\Psi(t_a)\rangle, \tag{1.35}$$

the Schrödinger equation (1.17) implies that the operator $\widehat{U}$ satisfies the equations

$$\hbar i \partial_t \widehat{U}(t, t_a) = \widehat{H}\widehat{U}(t, t_a),$$

$$\hbar i \partial_t \widehat{U}(t, t_a)^{-1} = -\widehat{U}(t, t_a)^{-1}\widehat{H}. \tag{1.36}$$

In the subsequent development, an important role will be played by the matrix elements of the time displacement operator in the localized basis states,

$$(x_b t_b | x_a t_a) = \langle x_b | \widehat{U}(t_b, t_a) | x_a \rangle . \qquad (1.37)$$

They will be referred to as *time displacement amplitudes*. The functional matrix $(x_b t_b | x_a t_a)$ is also called the *propagator*.

The operator equations (1.36) imply that propagators satisfy the Schrödinger equation

$$[H(-i\hbar\partial_{x_b}, x_b, t_b) - i\hbar\partial_{t_b}](x_b t_b | x_a t_a) = 0 . \qquad (1.38)$$

For the quantum mechanics of nonrelativistic particles, only propagators from earlier to later times will be relevant. It is therefore convenient to introduce the so-called *causal propagator* or *retarded propagator*:

$$(x_b t_b | x_a t_a) \equiv \begin{cases} \langle x_b | \widehat{U}(t_b, t_a) | x_a \rangle & t_b > t_a , \\ 0 & t_b < t_a . \end{cases} \qquad (1.39)$$

Since this differs from (1.38) only for $t_b < t_a$ and all formulas to be written down in the subsequent text will be used only for $t_b > t_a$, our notation does not distinguish between the two amplitudes.

The Partition Function

Consider a physical system without explicit time dependence in the Hamiltonian. Let it have a constant number of particles N. If it is brought in contact with a thermal reservoir at a temperature T then, after equilibrium is reached, its thermodynamic properties can be obtained through the following rules [Feynman and

Hibbs 1965, Kleinert 1990] : At the level of classical mechanics, each volume element in phase space

$$\frac{dp\,dq}{h} = \frac{dp\,dq}{2\pi\hbar} \tag{1.40}$$

is occupied with a probability

$$e^{-H(p,\,q)/k_B T} \;, \tag{1.41}$$

where k_B is the Boltzmann constant

$$k_B = 1.3806221 \times 10^{-16}\,\text{erg / Kelvin}\,. \tag{1.42}$$

The quantity $1/k_B\,T$ which has the dimension of an inverse energy is commonly denoted by β.

The integral over the probabilities of all phase space elements,

$$Z_{cl}(T) \equiv \int \frac{dp\,dq}{2\pi\hbar}\,e^{-H(p,\,q)/k_B T}\,, \tag{1.43}$$

is called *classical partition function*. It contains all classical thermodynamic information of the system. Of course, for a general Hamiltonian system with many degrees of freedom, $\int dp\,dq/2\pi\hbar$ means the product $\prod\limits_{n}\int dp_n\,dq_n/2\pi\hbar$.

In quantum statistics, the Hamiltonian is replaced by the operator $\widehat{H}$ and the integral over phase space by the trace in the Hilbert space. This leads to the *quantum statistical partition function*

$$Z(T) \equiv \text{tr}\left(e^{-H(\widehat{p},\,\widehat{q})/k_B T}\right) \equiv \text{tr}\left(e^{-\widehat{H}/k_B T}\right). \tag{1.44}$$

In terms of all eigenstates $|n\rangle$ of the Hamiltonian, we can also write the partition function as

$$Z(T) = \sum_{n} e^{-E_n/k_B T}\,, \tag{1.45}$$

where E_n is the energy eigenvalue of the nth state.

At this point we make an important observation: The quantum partition function is related in a very simple way to the quantum mechanical time displacement operator. To emphasize this relation we shall define the trace of this operator as the *quantum mechanical partition function*:

$$Z_{QM}(t_b, t_a) \equiv \text{tr}\left(\widehat{U}(t_b, t_a)\right) = \text{tr}\left(e^{i(t_b-t_a)\widehat{H}/\hbar}\right). \tag{1.46}$$

Obviously the quantum statistical partition function $Z(T)$ may be obtained from the quantum mechanical one by continuing the time interval $t_b - t_a$ the negative imaginary value

$$t_b - t_a = -\frac{i\hbar}{k_B T} \equiv -i\hbar\beta. \tag{1.47}$$

For this simple formal reason the trace of the time displacement operator is sufficient to understand also all thermodynamic equilibrium properties of a quantum system.

Given a partition function $Z(T)$ at a fixed particle number N, the *free energy* is defined by

$$F(T) = -k_B T \ln Z(T).$$
$$\text{or} \qquad Z(T) = e^{-F(T)/k_B T}, \tag{1.48}$$

and the *internal energy* is defined by

$$E = \text{tr}\left(\widehat{H}e^{-\widehat{H}/k_B T}\right)/\text{tr}\left(e^{-\widehat{H}/k_B T}\right). \tag{1.49}$$

It may be obtained from the partition function $Z(T)$ by forming the temperature derivative

$$E = -\frac{1}{Z}k_B T^2 \frac{\partial}{\partial T} Z(T) = -k_B T^2 \frac{\partial}{\partial T} \ln Z(T). \tag{1.50}$$

In terms of the free energy (1.48), this becomes

$$E \;=\; -T\,\frac{\partial}{\partial T}F(T) + F(T)\,. \qquad (1.51)$$

In thermodynamic considerations, another quantity of fundamental interest is the entropy, which is defined directly by

$$S(T) \;=\; -\frac{\partial}{\partial T}F(T) \qquad (1.52)$$

and then

$$F \;=\; E - TS\,. \qquad (1.53)$$

At this point we have made some important observations that will be useful from now on.