THE ACTION PRINCIPLE IN STATISTICAL MECHANICS

by

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ABSTRACT

The role of the classical action (i.e. the time integral of the Lagrangian) is studied in statistical mechanics by taking as paradigms two simple systems, viz., the linearly damped particle (LDP) and the linearly damped harmonic oscillator (DHO). Both of these systems can be described by means of an exact Lagrangian which forms the basis of a self-consistent dynamical theory, Hamilton's equations being satisfied. The action can be calculated as a quadratic function of the position and the time. While the minimum number of assumptions is made in both cases, a new viewpoint is introduced whereby the dissipative term in the Lagrangian is made physically transparent. We propose that the aforementioned term be understood as a natural metric, and that the particle (LDP or DHO) is thus moving in a curved space.

A consistent formulation of quantum mechanics can be made, and although no alteration is caused to the physics, the formalism is developed in a rigorous manner. A complete quantum description can be given either in the Schrödinger picture, or by means of the functional integral method of Feynman, in which the action is of paramount importance.

Finally the irreversible statistical mechanics is developed using the quantum propagator to find the time-dependent density matrix. Two possible ways of doing this are shown, and the connexion between this work and the standard theory of Brownian motion is pointed out. The

entropy and average energy are also calculated and it is shown that for very large times a pure state results.

A comparison is made with the work of several authors who have used the same Lagrangian, and a discussion given of the differences that exist. Alternative methods of describing the LDP and DHO are reviewed, and notable agreement is found with the early (1943) work of Chandrasekhar.

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This thesis is dedicated to the memory of my parents.

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INTRODUCTORY SURVEY

In this work we have set out an attempt to solve one of the oldest problems in physics, namely that of how to describe the dissipation of energy, especially in statistical mechanics. The emphasis throughout our study is on the rôle that the classical action plays in such a process, since we know that equilibrium thermodynamics in particular can be developed from the action based formalism of Feynman path integration. The treatment of dissipation conventionally ascribes the losses as resulting from two distinguishable sets of forces: systematic mechanical ones, and random ones which must be treated in a statistical fashion. We wish to concentrate our attention on the systematic forces and include them in Lagrangian theory, then using the Feynman propagator to extend the description to finite temperatures, or in other words to a theory of irreversible statistical mechanics.

To this end we concentrate our attention on two simple classical systems which exhibit dissipation of energy, namely the damped harmonic oscillator (DHO) and the linearly damped particle (LDP), and try to phrase these problems in the language of the Lagrangian formalism. This generalization turns out to be very simple, and both the LDP and DHO Lagrangians are found to be quadratic functions of the velocity and position, which smoothly reduce to the quadratic Lagrangians of a free particle and simple harmonic oscillator (SHO) respectively as the damping is switched off. The

description of dissipation by such quadratic Lagrangians is the simplest way of achieving decay in time. We then attempt to give as complete a description of the problem as possible, studying in turn the classical, quantal and statistical mechanical behavior using the classical action as the basic function characterizing the evolution of these systems. In all these disciplines we expect to find evidence of dissipation of energy, and in the finite temperature case that we are dealing with an irreversible phenomenon.

The equations of motion for the LDP and DHO have been discussed within the framework of Newtonian Mechanics for well over two centuries, whereas a Lagrangian-Hamiltonian description did not make an appearance until comparitively recently. Kanai, writing in 1948, seems to have been the first to attempt a solution of the quantum problem including the type of dissipation envisaged above. At present the problem of losses is of great importance in the quantum theory of coherent optics, and the DHO is often introduced here as a simple model of a lossy cavity.

In Chapter 1 we introduce our dissipative models and set up the appropriate Lagrangian functions. Hence one can find the Hamiltonian and the action function in a consistent way. At this point we indicate a novel interpretation of the way in which the damping features in the problem by introducing the tensor calculus of curvilinear coordinates. This helps us to find an expression for the momentum which

is decreasing in time, in contrast to the work of others where this generalized momentum increases with time. Then we can find a suitable expression for the energy. Having found the Hamiltonian, we devote Chapter 2 to a solution of the Schrödinger equation. First a consistent formalism is developed, avoiding difficulties associated with the definition of the position-momentum commutator. Then the Schrödinger equation is solved by means of a unitary transformation to comoving coordinates. The wavefunctions are found, and thence the average of the Hamiltonian and total "energy" may be found. It turns out for the DHO in particular, that there is a one to one correspondence between states of the DHO and the SHO which is obtained in the limit $\gamma \to o$. Since the quantum mechanical problem can be solved, we can pass with confidence to the path integral description of the damped systems, using the classical Lagrangian to find the quantum propagator. We obtain the propagators for LDP and DHO and show that they obey the rules for propagators, that they tend to the relevant undamped propagators as the damping is switched off, and that they are consistent with the wavefunction describing the quantum problem.

Finally in Chapter 4 we deal with the statistical mechanics of an ensemble of such dissipative systems. The aim is to find a density matrix which contains the damping in a way which guarantees the agreement of the expressions for the potential and kinetic energies with those given by

other theories of dissipation. It is hoped that the well-known analytic continuation methods of quantum statistical mechanics can be applied to give the density matrix at finite temperature from a knowledge of the (zero temperature) quantum propagator. We introduce the influence functional formalism and show how the ideas in this theory enable a density matrix to be constructed by propagation of the initial conditions. We then show how to calculate the mean energy and the entropy. In the entire discussion, a knowledge of the action is of fundamental importance. Even to write down the explicit form of the Schrödinger equation, we first must have the Lagrangian, since the Hamiltonian which is implied by it cannot be found in any other way (other than trial and error).

Considering the simplicity of our models for dissipating systems, the above programme has been reasonably successful in giving results in accord with our knowledge of how such systems behave in practice.

During the years over which this work was undertaken, much of the physics dealt with above has also been studied by other authors, and much of it has been published elsewhere by Denman (1973, 1974) and Papadopoulos (1973, 1974). Some of the results of these authors have influenced this work. Nonetheless, the Lagrangian at the heart of this work was deduced independently, and the ideas relating to tensor calculus are original. The results of the finite temperature calculation are entirely new.

CHAPTER ONE

DISSIPATION IN CLASSICAL MECHANICS

1.1 Introduction

The dissipating systems which we wish to study have the following classical equations of motion in one dimension, where a dot denotes time differentiation:

LINEARLY DAMPED PARTICLE (L.D.P.):

$$m\ddot{x} + \lambda\dot{x} = 0 \tag{1}$$

DAMPED HARMONIC OSCILLATOR (D.H.O):

$$m\ddot{x} + \lambda\dot{x} + kx = 0 \tag{2}$$

Both equations are second order differential equations for the position of the particle, mass m, as a function of time. λ is the viscosity constant, and k the spring constant whence the undamped frequency, ω_0, is defined:

$$\omega_0 = \left(\frac{k}{m}\right)^{\frac{1}{2}} \tag{3}$$

In both cases, an attempt is made to replace the viscous or damping effect of an interacting collection of particles (henceforth referred to as the bath) on a single selected heavy particle by a systematic force. Experimentally it is found that this force is velocity dependent and always opposes the motion, so that λ must be positive. Equations (1) and (2) are satisfactory approximations to the actual situation provided the velocity of the particle

is low.

Solution of the above equations is elementary. We note down a solution of each for boundary conditions as indicated.

L.D.P.

$$x(t) - x_0(t=0) = \frac{p_0}{\lambda}\left(1 - e^{-\frac{\lambda t}{m}}\right) \tag{4}$$

$$\dot{x}(t=0) = \frac{p_0}{m},$$

where t is the time variable, p_0 is the initial momentum, and $x = x_0$ at time zero.

D.H.O.

The behavior of the solution here is dependent on the relationship between the quantities ω_0^2 and $\gamma^2 = (\frac{\lambda}{2m})^2$. We distinguish three cases:

(i) $\omega_0^2 > \gamma^2$ (Underdamping)

$$x(t) = x_0 e^{-\gamma t} \cos Wt, \tag{5a}$$

with $W^2 = \omega_0^2 - \gamma^2$

(ii) $\omega_0^2 = \gamma^2$ (Critical damping)

$$x(t) = x_0 e^{-\gamma t} \tag{5b}$$

and (iii) $\omega_0^2 < \gamma^2$ (Overdamping)

$$x(t) = x_0 e^{-\gamma t} \cosh W't \tag{5c}$$

with $W'^2 = \gamma^2 - \omega_0^2$.

We have in each case considered the particle to be at the position x_o at time zero. In all three cases the particle displacement gradually shrinks to zero.

However, the above statements comprise the entire analysis which can be made by Newtonian mechanics: it is not possible to arrive at a rigorous expression for the energy, and indeed the Hamiltonian formalism is inapplicable, since the system described by x(t) is not conservative.

The best that can be done is to argue as follows (Landau and Lifschitz, 1960): the energy of the LDP is totally kinetic, so that $E \approx \frac{1}{2}mx^2 = \frac{p_o^2}{2m} e^{-2\gamma t}$, which decays in time as it should. For a DHO with very small damping, one expects the energy to be proportional to the square of the displacement, as is the case for a simple harmonic oscillator (SHO). Then for initial energy E_o, one can show that $E(t) \approx E_o e^{-2\gamma t}$.

However, in order to use the LDP and DHO to gain insight into the general problem of dissipation, it is necessary to have a more fundamental way of ascertaining the energy, bearing in mind that the same type of decay as above must emerge from such a theory. Early attempts were made to develop a Lagrangian theory incorporating dissipation. Rayleigh introduced the ad hoc formalism of the dissipative function, whence dissipation could be included in the usual Euler-Lagrange equations by adding in the velocity derivative of this function:

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{x}}\right) - \frac{\partial \mathcal{L}}{\partial x} = -\frac{\partial R}{\partial \dot{x}} \,,$$

where $\mathcal{L}$ is the Lagrangian $\mathcal{L}(\dot{x},x)$ without dissipation, and R the dissipative function,

$$R = \frac{\lambda \dot{x}^2}{2}.$$

R is clearly positive definite. Then for the DHO the quantity

$$\frac{d}{dt}\left(\frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2\right) = -2R \qquad \forall t$$

is clearly monotonically decreasing as $t \to \infty$, and the left hand side of this equation may be regarded as the time derivative of the energy of the oscillator.

Nonetheless, this theory lies outside the scope of Lagrange-Hamilton formalism since the dissipative forces are not derivable from a potential and therefore Hamilton's equations are not correctly obtained.

1.2 Lagrangian Theory of Dissipation

Starting from first principles, we have succeeded in finding a Lagrangian function which enables a complete and consistent description of the classical dynamics to be given. Not surprisingly, we are not the first to discover such a Lagrangian, the first being Heinrich Helmholtz in 1887. A partial list of contributors to the theory includes Kanai

(1948), Havas (1957), Kerner (1958), Stevens (1958), Bopp (1962), Denman (1966), Marcuse (1970) and Papadopoulos (1973).

Our problem may be enunciated thus: we have the equations of motion (1) and (2), and wish to find a function $\mathcal{L}(\dot{x}, x, t)$ such that its substitution in the Euler-Lagrange equation

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{x}}\right) - \frac{\partial \mathcal{L}}{\partial x} = 0$$

will reproduce the equations of motion exactly. We seek $\mathcal{L}(\dot{x}, x, t)$ in the general form

$$\mathcal{L}(\dot{x}, x, t) = g(t)\left\{\tfrac{1}{2}m\dot{x}^2 - \tfrac{1}{2}kx^2\right\},$$

substitute in the Euler-Lagrange equation, and by comparison induce what form g(t) should have. It may be immediately verified that

$$g(t) = Ce^{\frac{\lambda t}{m}}$$

for both DHO and LDP Lagrangian functions, with C an arbitrary constant set equal to 1, since it cannot alter the dynamics in any way. (We neglect the trivial case C = 0.)

Then we note:

$$\mathcal{L}_{L.D.P.}(\dot{x}, t) = e^{\frac{\lambda t}{m}}\frac{m\dot{x}^2}{2} \qquad (6)$$

and

$$\mathcal{L}_{D.H.O.}(\dot{x}, x, t) = e^{\frac{\lambda t}{m}}\left\{\frac{m\dot{x}^2}{2} - \frac{kx^2}{2}\right\} \qquad (7).$$

There is a striking similarity to the undamped processes when LDP becomes a free particle, and DHO reduces to a SHO.

Since the two functions (6) and (7) satisfy the Euler-Lagrange equation, we can call them the Lagrangians for our systems. Now are they unique, indeed is there only a single function g(t) which is generated by the procedure mentioned above? This question has been investigated in detail (Havas, 1957), and in fact the Lagrangians above are not unique. There are other so-called q-equivalent Lagrangians and Hamiltonians (Currie and Saletan, 1966) which will generate the correct equation of motion for q, but not for p. For our purposes, we shall restrict ourselves to the above Lagrangians (6) and (7) since (i) they are the only ones among the q-equivalent Lagrangians displaying explicit time dependence; (ii) they satisfy Hamilton's equations, and (iii) lead to the standard commutation relations in quantum mechanics[†]. (See §2.2)

Of course, it is always true in classical mechanics that one can add on to any Lagrangian a function which is a total time derivative of an arbitrary function of the coordinates only, without altering the physical situation in any way. Our statement of uniqueness embraces such a possibility.

[†] The situation as regards the uniqueness of the quantum mechanical Hamiltonian is even more complicated. It so happens that the position and momentum operators will only give the correct commutation for a certain subset of q-equivalent Hamiltonians. It is only the Hamiltonians which are related to one another by unitary transformations that should be regarded as physically relevant. See Razavy (1972).

From equations (6) and (7), we define the generalized momentum p,

$$p = \frac{\partial \mathcal{L}}{\partial \dot{x}},$$

$$p = e^{\frac{\lambda t}{m}} m\dot{x} \tag{8}$$

for both LDP and DHO.

The Hamiltonian is the Legendre transform of the Lagrangian with respect to the variable $\dot{x}$, viz.,

$$H = \dot{x}\frac{\partial \mathcal{L}}{\partial \dot{x}} - \mathcal{L},$$

and writing this Hamiltonian in terms of the independent variables p, x, we find

$$H_{L\cdot D\cdot P\cdot}(p) = e^{-\frac{\lambda t}{m}} \frac{p^2}{2m} \tag{9}$$

and

$$H_{D\cdot H\cdot O\cdot}(p,x) = e^{-\frac{\lambda t}{m}} \frac{p^2}{2m} + e^{\frac{\lambda t}{m}} \frac{kx^2}{2} \tag{10}.$$

It may be verified directly that Hamilton's equations are satisfied. As is generally the case, the generalized momentum p, and the kinematical momentum $m\dot{x}$ are different. p_{DHO} behaves pathologically, diverging with time irrespective of the type of motion, whereas the kinematical momentum decreases. On the other hand P_{LDP} remains constant, whereas $(m\dot{x})_{LDP}$ decreases. Thus, while H_{LDP} above decreases with time, H_{DHO} does not always do so, and depending on the relation between ω_o^2 and γ^2, may either oscillate, decrease

or remain constant. Thus for the DHO, an ad hoc definition of the energy based on the kinematical momentum is made (Kerner, 1958; Denman, 1966):

$$E_{D.H.O.} = e^{-2\gamma t} H_{D.H.O.} \qquad (11).$$

This "energy" is equal to the sum of "kinetic energy", $\frac{1}{2}m\dot{x}^2$, and the "potential energy" $\frac{1}{2}kx^2$, and always decreases with time.

To complete this discussion, it is worth studying the equation of motion (2) further, from the point of view of constants of the motion. Since the equation is time-translation invariant, i.e. replacing t by t+b for constant b does not alter the form of the equation of motion, a constant of the motion exists. However it should not be supposed that this automatically demands conservation of energy. To find this constant for the DHO (Denman, 1968; Denman and Buch, 1973), we set

$$u = \frac{\dot{x}}{x},$$

and then integrate equation (2), to find the constant c:

$$C = \ln\left[(\dot{x}+\gamma x)^2 + W^2x^2\right] - \frac{2\gamma}{W}\tan^{-1}\left[\frac{\gamma x+\dot{x}}{Wx}\right] \qquad (12),$$

and for $\omega_o^2 > \gamma^2$, may write,

$$C = \ln\left[Wx(0)\right]^2.$$

To make the meaning of this constant more transparent, set

$$a = \dot{x} + \gamma x$$
$$b = \omega x.$$

Then
$$a = -\omega x_0 e^{-\gamma t} \sin \omega t,$$
$$b = \omega x_0 e^{-\gamma t} \cos \omega t.$$

If we now change to polar coordinates (ρ, ϕ) such that

$$\rho^2 = a^2 + b^2,$$

or
$$\rho^2 = \omega^2 x^2(0) e^{-2\gamma\phi/\omega} \tag{14}$$

where

$$\phi = -\tan^{-1}\left(\frac{a}{b}\right).$$

Then equation (13) can be written as

$$C = \ln(\rho^2) + \frac{2\gamma\phi}{\omega} \tag{15}.$$

From equation (13) it may be seen that C is related to the initial energy of the oscillator; indeed when $\gamma \to 0$, the argument of the logarithm is essentially the energy of the SHO of frequency ω_0.

On the other hand, equation (15) is the plane polar coordinate representation of a logarithmic spiral. This is the same type of curve as the phase-space trajectory of the oscillator for phase-space variables of the position and kinematical momentum (Marion, 1965), since the variables a and b are related to these by a linear transformation. The constant, C, above is therefore equal to the initial

value of the radius vector (see Figure 1).

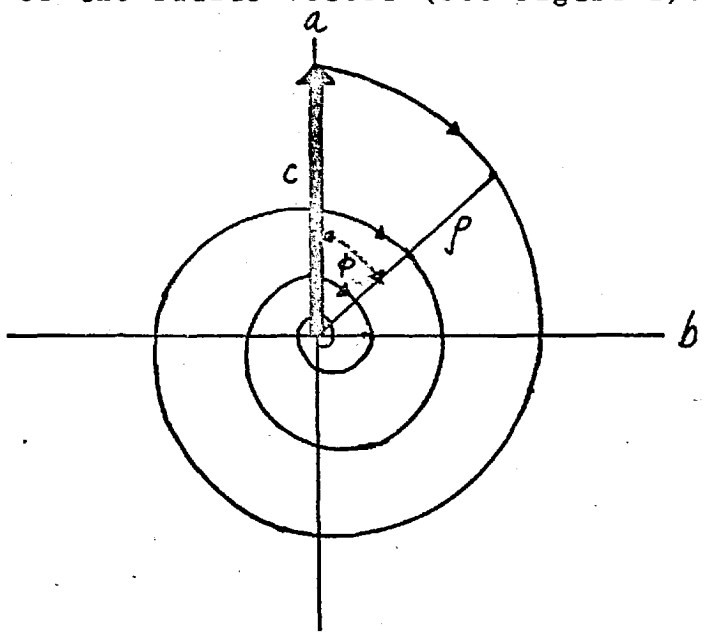

Fig. 1 Phase space trajectory of the DHO. Arrows indicate direction of evolution.

Therefore, although a constant of the motion exists, it only refers to the initial state of the system and does not give any direct information about the general evolution in time. All that can be said is that a different such constant corresponds to each different initial condition.

1.3 Curvilinear Coordinates

A 3-space is completely described by its line element

$$ds^2 = g_{ij}\, dx^i\, dx^j, \quad i,j = 1,2,3 \tag{16}$$

where g_{ij} is the metric tensor, $\{dx^i\}$ are the contravariant coordinate displacements, and we have used the Einstein summation convention. The inverse of the metric tensor is g^{ij}; therefore

$$g_{kj}\, g^{ji} = \delta^{i}_{k},$$

where δ^{i}_{k} is Kronecker's delta:

$$\delta^{i}_{k} = 0, \qquad i \neq k.$$

$$\delta^{i}_{i} = 1. \qquad \text{(no sum)}$$

The elements g_{ij} may be explicitly time and co-ordinate dependent.

The kinetic energy, T, is defined by

$$T = \frac{m}{2}\left(\frac{ds}{dt}\right)^{2},$$

$$\text{i.e.} \quad T = \frac{m}{2}\, g_{ij}\, \dot{x}^{i}\dot{x}^{j} \tag{17},$$

so that in the presence of a scalar potential $V(x^{i})$, the Lagrangian is written as

$$\mathcal{L}(\dot{x}^{i}, x^{i}, t) = \frac{m}{2}\, g_{ij}\, \dot{x}^{i}\dot{x}^{j} - V(x^{i}) \tag{18}.$$

Comparing equations (6), (7) and (18) we now assert that the integrating factor $e^{\frac{\lambda}{m}t}$ can be identified with the metric tensor elements in (18). Although we have confined our study thus far to one dimension, no complications arise when three dimensions are studied - the same identification is possible. Therefore we shall continue to work in one dimension, using sub and superscripts solely to distinguish contravariant and covariant quantities where necessary.

We write

$$g_{ij} = e^{\frac{\lambda t}{m}} \delta_{ij} ,$$

$$g^{ij} = e^{-\frac{\lambda t}{m}} \delta^{ij} \qquad (19),$$

and the motion is now visualized as taking place in a curved space. This accords well with Eddington's (1965) idea that forces acting on a particle can be incorporated into a metric; thus into the geometry.*

Thus we have

$$\mathcal{L}_{L.D.P.}(\dot{x}^i, t) = \frac{m}{2} g_{ij}(t) \dot{x}^i \dot{x}^j$$

$$\mathcal{L}_{D.H.O.}(\dot{x}^i, x^i, t) = \frac{m}{2} g_{ij}(t) \dot{x}^i \dot{x}^j - \frac{k}{2} g_{ij}(t) x^i x^j \qquad (20).$$

Note that

$$g_{ij} x^i x^j = x_i x^i \qquad (21)$$

is valid because the metric tensor is not coordinate dependent.

The line element of our 3-space is

$$ds^2 = e^{\frac{\lambda t}{m}} \left(dx_1^2 + dx_2^2 + dx_3^2 \right) \qquad (22)$$

where the "curvature" arises solely from the damping. Incidentally, the de Sitter line element of general relativity

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* Denman and Kupferman (1973) have indicated that the problem of a particle subjected to quadratic friction may be construed in similar fashion: an exponential integration factor with argument $\operatorname{sgn}(\dot{x})\lambda x$ is introduced.

theory (Tolman, 1934), viz.,

$$d\sigma^2 = e^{\frac{2t}{R}}\left(dx_1^2 + dx_2^2 + dx_3^2\right) - dt^2,$$

bears close resemblance to the line element (22). Our 3-space may thus be viewed as a constant time segment of a de Sitter universe.*

In general Tensor calculus, the invariant volume element, dV, is given by

$$dV = \sqrt{g(t)}\, dx_1\, dx_2\, dx_3 = d_t x,$$

where

$$g(t) = \det g_{ij} = e^{2\delta t}$$

in our case.

The LDP is now to be regarded as a free particle moving in a "curved" space, and its path is therefore a geodesic. (Although our time dependent metric implies zero spatial curvature, we still refer to the space as curved).

The geodesic condition is

$$\delta \int ds = 0,$$

and from equation (22) we thus find the geodesics are given by

$$m\ddot{x} + \lambda\dot{x} = 0,$$

which is exactly the equation for the L.D.P.. In this

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* We shall not pursue this cosmological analogy further here. In Newtonian Cosmology (Bondi, 1968) a basic requirement is the conservation of energy, and we certainly cannot fulfill this here.

curved space, geodesics are curves - no longer straight lines as would be found in a space with constant metric tensor elements.

From the fact that $x_i = g_{ij}\, x^j$, we see that

$$\dot{x}_i = \frac{\lambda}{m} x_i + g_{ij}\, \dot{x}^j \tag{23}$$

and that x_i satisfies the equation

$$m\ddot{x}_i - \lambda \dot{x}_i = 0 \tag{24}$$

Therefore the time evolution of x_i and x^i is different - both for LDP and DHO - the magnitude of x_i grows with time whereas x^i decreases, as is experimentally observed. Therefore x^i describes the true situation, and we shall therefore always calculate solely with x^i. Henceforth, x will denote x^i wherever a superscript is not vital.

The (covariant) generalized momentum

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{x}^i} \tag{25}$$

which increases with time, is an independent variable in any Hamiltonian theory. We can therefore write down its associate vector, the contravariant quantity

$$p^i = g^{ij} p_j \tag{26}$$

and this momentum <u>always decreases</u> with time (LDP and DHO) as would be found for the kinematic momentum $m\dot{x}^i$.

We therefore construct the quantity

$$E = \delta_{ij} \frac{p^i p^j}{2m} + \delta_{ij} \frac{m\omega_0^2 x^i x^j}{2} \tag{27}$$

by analogy with the expression for the energy of the SHO. For the LDP we obviously do not include the second term on the right. This quantity, E, has the same value as equation (11).

The Hamiltonian follows rigorously from equation (10) as

$$H(p_i, x^i) = g^{ij}\frac{p_i p_j}{2m} + V(x^i) \qquad (28).$$

Hamilton's equations are once again satisfied.

1.4 Canonical Transformation of Coordinates

We briefly examine the following important change of coordinates; following Bopp (1962):

$$x \longrightarrow z = xe^{\gamma t} \qquad (29).$$

This transformation, which appears at first sight to be merely a change of scale, is in fact a true canonical transformation, as will be shown below for the case of the DHO.

Under the above change of variable, the Lagrangian $\mathcal{L}(\dot{x}, x)$ is transformed to

$$\mathcal{L}(\dot{z}, z) = \frac{1}{2}m\dot{z}^2 - \frac{\lambda}{2}\dot{z}z - \frac{m}{2}W^2z^2 \qquad (30),$$

which is no longer explicitly time dependent. W is as defined earlier.

The canonical momentum is

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{z}},$$

or

$$\pi = m\dot{z} - \frac{\lambda z}{2} \tag{31}.$$

The new Hamiltonian H' is once again given as the Legendre transform of $\mathcal{L}(\dot{z},z)$:

$$H'(\pi,z) = \frac{\pi^2}{2m} + \gamma \pi z + \frac{m\omega_0^2 z^2}{2} \tag{32}.$$

We can write equation (30) in the more transparent form

$$\mathcal{L}(\dot{z},z) = \frac{1}{2}m\dot{z}^2 - \frac{1}{2}mW^2z^2 - \frac{1}{4}\frac{d}{dt}(z^2),$$

and since the last term is a total time derivative of a function of the coordinates only, this Lagrangian is equivalent to the Lagrangian

$$\mathcal{L}(\dot{z},z) = \frac{1}{2}m\dot{z}^2 - \frac{1}{2}mW^2z^2, \tag{33}$$

which is the Lagrangian of a SHO of frequency W. Furthermore the Hamiltonian H' shows no explicit time dependence. The transformation (29) is thus to a set of comoving coordinates in which our dynamic functions $\mathcal{L}$, H' show no damped behaviour.

Since $\pi = pe^{-\gamma t}$ (33)

the Poisson bracket, $\{\pi,z\}$, equals unity, thus confirming that the transformation, whilst time dependent, is canonical.

The generator of the transformation is

$$F = pz\,e^{-\alpha t} \tag{34a}$$

which satisfies the usual conditions (Landau and Lifschitz, 1960) viz.,

$$H' - H = \frac{\partial F}{\partial t} \tag{34b}$$

and $$\Pi = -\frac{\partial F}{\partial z}\,. \tag{34c}$$

1.5 Action

The last dynamical function we wish to calculate is the action, obtained as the time integral of the Lagrangian:

$$A(x',t';x,t) = \int_t^{t'} d\bar{t}\; \mathcal{L}(\dot{x}, x, \bar{t}) \tag{35}$$

where the particle motion commences at time t from position x, and terminates at t' at position x'. The action is thus the generator of the classical motion, and satisfies the two relations

$$\frac{\partial A}{\partial x'} = p'$$

(p' being expressed in terms of t'),

and

$$\frac{\partial A}{\partial t} = -H(p',x')\,.$$

For a given system the action is evaluated as follows: having solved the e.o.m. for x(t), one writes the Lagrangian

as a function of time only, and thus (in principle) can carry out the time integration. The resulting expression is then written as a function of the initial and final position and time variables. Below we list the essential features of this procedure carried out for the LDP and DHO.

LDP

$$\mathcal{L}(t) = e^{-\frac{\lambda t}{m}} \frac{p_o^2}{2m},$$

so that

$$A(x,t;x_o,t=0) = \frac{\lambda (x-x_o)^2}{2\left(1-e^{-\lambda t/m}\right)}, \qquad (36),$$

and we note that as $\lambda \to 0$, this goes smoothly over to the expression for a free particle.

DHO

Without loss of generality, we only consider $\omega_o^2 > \gamma^2$.

$$\mathcal{L}(t) = \frac{1}{2} m x_o^2 \left(\gamma \cos Wt + W \sin Wt\right)^2 - \frac{1}{2} k x_o^2 \cos^2 Wt,$$

so that

$$A(x',t';x,t) = \frac{mW}{2}\left[\left(x'^2 e^{2\gamma t'} + x^2 e^{2\gamma t}\right)\frac{\cos WT}{\sin WT} - \frac{2x e^{\gamma t} x' e^{\gamma t'}}{\sin WT} + \right.$$

$$\left. + \frac{\gamma}{W}\left(x^2 e^{2\gamma t} - x'^2 e^{2\gamma t'}\right)\right], \qquad (37)$$

where $T = t' - t$.

For $\omega_o^2 < \gamma^2$, we write $W' = iW$ and substitute in

equation (37), resulting in the replacement of sines and cosines by the relevant hyperbolic functions.

Again, as $\lambda(\gamma) \to 0$, equation (36) goes over smoothly to the expression for a SHO.

A brief calculation using the relation $H = \frac{-\partial A}{\partial t}$ shows consistency with our earlier expression for H.

It is important to note that the quadratic Lagrangians both yield quadratic action functions.

1.6 Conclusion

We have developed a complete and consistent description of damping insofar as it is understood in classical mechanics, namely that energy is lost but no sink of energy is described in the formalism.

Both Lagrangian and Hamiltonian theories are constructed, and their respective descriptions are concordant with one another. The Hamiltonian is the basis for the subsequent Schrödinger picture of the problem, while the Lagrangian is the basis of the path integral one.

The introduction of the metric as suggested by the form of the Lagrangian, gives a means of identifying those position and coordinate variables which behave as do the experimentally observed ones. Hence we arrive at a value for the energy showing the correct time dependence.

By means of a canonical transformation it is shown how the damped system (DHO) is related to the undamped one (SHO).

Lastly, the action has been calculated, both for later use and as a check on the value found for the Hamiltonian. Like the Lagrangian, the action is also a quadratic function.

CHAPTER TWO

DISSIPATION IN QUANTUM MECHANICS

2.1 Introduction

Since the equation basic to quantum mechanics viz., Schrödinger's equation, is reversible in time, it may be concluded that one cannot speak of dissipation for a single particle system on this microscopic level. Yet by contemplating a quantum-mechanical generalization of equations (1) and (2), this is precisely the difficulty that faces us. We note in passing that authors such as de Broglie (1964) and de la Peña Auerbach e.a. (1972), have developed the "hidden variable" theory of quantum mechanics to include the fictitious case of the thermodynamics of a single particle interacting with this hidden thermostat. Our description of the dissipating processes, by focussing attention on the particle itself, attempts such a single particle view, but replaces the effect of the real bath by the unquantized, classical constant λ.

Now, by identifying the damping with the geometry of the space, we are able to introduce dissipation on the microscopic level since there is no difficulty in setting up a general curvilinear quantum theory.

The adoption of this approach means that our description is semi-classical since we only quantize the particle motion, treating the bath classically.

2.2 Formalism of Quantum Mechanics in Curvilinear Coordinates

We assume therefore that the classical DHO (or LDP) is the analogue of a certain one-dimensional quantum system. The observables of this system are functions of the coordinate and momentum operators $\hat{q}$ and $\hat{p}$ respectively. Now a knowledge of the commutation relation between these two operators is generally sufficient for setting up and solving the quantum dynamics completely.

In the case of dissipative systems, Marcuse (1970) has pointed out certain difficulties encountered in attempting to define such a commutation relation, namely that if both coordinate and momentum operators are time dependent $\sim e^{-\gamma t}$, the commutator eventually vanishes, whereas the non-vanishing (indeed constant) nature of this commutator is essential for a quantum description to be given at all times.

Recalling the analogy drawn in §1.3 between our Lagrangian integrating factor and the metric tensor, we note down and adapt the theory of quantum mechanics in curvilinear spaces (de Witt, 1957). We must now distinguish between contravariant and covariant operators.

The <u>scalar</u> commutator of $\hat{p}_i$ and $\hat{q}^j$ is postulated as

$$\frac{i}{\hbar}\left[\hat{p}_k, \hat{q}^j\right] = \delta^j_k = \frac{i}{\hbar}\left[\hat{p}^j, \hat{q}_k\right], \qquad (1)$$

where $\hbar$ is Planck's constant.

The coordinate basis states in Dirac notation, $|q,t\rangle$, are normalized at time t as

$$\langle q', t / q, t \rangle = \delta(q', q, t)$$

$$= g^{-\frac{1}{2}} \delta(q' - q) \qquad (2).$$

Since our space $g_{ij} = e^{\frac{\lambda t}{m}} \delta_{ij}$ has zero spatial curvature ($R \equiv 0$), the momentum operator in coordinate representation is given by*

$$\hat{p}_j = \frac{\hbar}{i} \frac{\partial}{\partial q^j} . \qquad (3)$$

Because the metric tensor is time-dependent, the conservation of the norm of the system wavefunction demands a modified time differentiation operation.

Briefly, one can show that the change in the representation of the state vector $|\psi\rangle$ under the infinitesimal unitary transformation

$$V = 1 + \frac{iH}{\hbar} \delta t$$

where δt is an arbitrary displacement in time, is

$$\langle q', t' + \delta t' / \psi \rangle = \left[1 - \frac{1}{4} \left(\frac{\partial \ln g'}{\partial t} \right) \delta t' \right] \langle q', t' / \psi \rangle +$$

$$+ \frac{i}{\hbar} \langle q', t' / H(t') / \psi \rangle \delta t' \qquad (4),$$

where H is the quantum analogue of the classical Hamiltonian, assuming that it exists.

We observe that the conventional time derivative is replaced by the "conservative" time derivative†

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* See also Trigg (1964) and Charap (1973).

† de Witt's terminology

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \frac{1}{4}\frac{\partial}{\partial t}(\ln g) \qquad (5),$$

which for our metric (equation (19), §1.3) becomes

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \frac{\gamma}{2} \qquad (6).$$

Equation (4) is the Schrödinger equation in the curvilinear space, and from it one can immediately verify that the norm of $\langle q|\psi\rangle \equiv \psi(q)$ is time independent, since the time dependence of the volume element dV is eliminated by the additional term in (6).

In the next section we write down and solve the Schrödinger equation for the D.H.O..

2.3 Solution of the Schrödinger Equation of the DHO

We can now write the Schrödinger equation (4) in the coordinate representation using the representations of the position and momentum operators found in the previous section. We find

$$\left\{-\frac{\hbar}{2m} g^{ij}(t)\frac{\partial}{\partial q^i(t)}\frac{\partial}{\partial q^j(t)} + \frac{m\omega_0^2}{2} g_{ij}(t)\, q^i(t) q^j(t)\right\}\psi(q^i,t) =$$

$$= i\hbar\left\{\frac{\partial\psi}{\partial t}(q^i,t) + \frac{\gamma}{2}\psi(q^i,t)\right\} \qquad (7).$$

The above equation is derived from the classical Hamiltonian (§1.3 equation 28) by appealing to the correspondence principle. In this classical theory, the canoni-

cal momentum is $p_i = \frac{\partial \mathcal{L}}{\partial \dot{x}^i}$.

In general, (Charap, 1973) a quantum theory taking a Lagrangian, $\hat{L}$, as its starting point cannot yield a Hamiltonian by means of a Legendre transform as in the classical case, since differentiation with respect to a quantum operator - $p_i = \frac{\partial \mathcal{L}}{\partial \dot{x}^i}$ means just this, is meaningless. Instead one needs to replace the process of differentiation by a suitable commutation or anti-commutation relation. The Legendre transform relating $\hat{L}$ and $\hat{H}$ is thus written in quantum mechanics as

$$\hat{L} = \frac{1}{2}\left(\hat{P}_i \dot{\hat{q}}^i + \dot{\hat{q}}^i P_i\right) - \hat{H}.$$

In our case, since the Christoffel symbols vanish identically, we can easily relate* $\dot{\hat{q}}^i$ and $\hat{p}_k$ via the Heisenberg equation for $\hat{q}^i$, and thus write down (7) without ambiguity. We now proceed to a rigorous solution of this equation, pointing out the significance of the metric term as we proceed.

The way to solve equation (7) is by changing the variable q by the substitution (one-dimensional)

$$z = qe^{\gamma t}, \quad t \to t \,. \tag{8}$$

As we pointed out previously, this transformation is in fact

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* We have for a particle of unit mass, $\hbar = 1$,

$$\dot{\hat{q}}^i = i\left[\hat{H}, \hat{q}^i\right] = i\left[\frac{g^{ij}\hat{P}_i\hat{P}_j}{2} + V(\hat{q}^i), \hat{q}^i\right]$$

or $$\dot{\hat{q}}^i = \frac{1}{2}\left\{g^{ik}, \hat{P}_k\right\}$$

so that $$\dot{\hat{q}}^i = g^{ik}\hat{P}_k \quad \text{since} \quad g^{ik} = g^{ik}{}_{(t \text{ only})}.$$

a canonical transformation (Kerner, 1958; Bopp, 1962).

In §1.4 we found the change in form of the classical Hamiltonian under such a transformation, but to avoid any ambiguities (specifically: to ensure the Hermiticity of $\hat{H}$), we cannot immediately apply the correspondence principle to equation (32), §1.4. Rather we have to work with the symmetrized form

$$\hat{H} = \frac{\hat{\Pi}^2}{2m} + \frac{\gamma}{2}\left(\hat{\Pi}\hat{z} + \hat{z}\hat{\Pi}\right) + \frac{m\omega_0^2\hat{z}^2}{2} \qquad (9),$$

where $\hat{\pi}$ and $\hat{z}$ are respectively the transformed momentum and coordinate operators.

One can then readily solve equation (7) by applying the commutation relation between $\hat{\pi}$ and $\hat{z}$, then finding the wavefunction, and lastly transforming it back to the x coordinates. To do this one needs to know the quantum transformation analagous to equation (8).

Now, to every classical canonical transformation, there corresponds a unitary transformation in quantum mechanics. Denote this operator by $\hat{U}$. We seek $\hat{U}$ in the form

$$\hat{U} = e^{i\hat{S}} \qquad (10),$$

where $\hat{S}$ is Hermitian, and such that the time-dependence associated with the operators is removed from the Schrödinger equation. Proceeding in this way, but with a different application in mind, Stevens (1958) has found such an operator $\hat{S}$. For our purposes we use this $\hat{S}$, but with opposite

sign*. Accordingly we take

$$\hat{S} = -\frac{\gamma t}{2\hbar}\left(\hat{q}^i \hat{p}_i + \hat{p}_i \hat{q}^i\right) \tag{11},$$

(with no sum on i).

Then using the commutation relation (1), it is easy to show that

$$e^{i\hat{S}}\,\hat{q}\,e^{-i\hat{S}} = e^{-\gamma t}\,\hat{q}, \tag{12a}$$

$$e^{i\hat{S}}\,\hat{q}^2\,e^{-i\hat{S}} = e^{-2\gamma t}\,\hat{q}^2, \tag{12b}$$

and

$$e^{i\hat{S}}\,\hat{p}^2\,e^{-i\hat{S}} = e^{2\gamma t}\,\hat{p}^2 \tag{12c}.$$

What we are doing is to operate on the physical system. The transformed wave function is $|\phi\rangle$:

$$|\phi\rangle = e^{i\hat{S}}\,|\psi\rangle \tag{13a}$$

and

$$\hat{H}' = e^{i\hat{S}}\,\hat{H}\,e^{-i\hat{S}} \tag{13b}$$

is the transformed Hamiltonian.

Now we normalized our states previously by

$$\langle q'|\hat{q}|q\rangle = \delta(q',q,t)\,\hat{q} \equiv e^{-\gamma t}\,\delta(q'-q)\,q.$$

Insert the unit operator

$$I = e^{i\hat{S}}e^{-i\hat{S}}$$

in the left-hand side of this relation:

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* $\hat{0}$ may also be found from first principles from the infinitesimal generator. See de Witt (1957).

$$\langle q'|e^{-i\hat{S}}e^{i\hat{S}}\hat{q}e^{-i\hat{S}}e^{i\hat{S}}|q\rangle = e^{-\gamma t}q\,\delta(q'-q).$$

Now by equation (12a), this is the same as

$$\left(\langle q'|e^{-i\hat{S}}\right)\hat{q}\left(e^{i\hat{S}}|q\rangle\right) = q\,\delta(q'-q). \qquad (14)$$

The transformed coordinate basis states are thus normalized differently - in fact what (14) indicates is that in the transformed system, the metric is effectively the flat space ($g_{ij} = \delta_{ij}$) one. This is in accord with the meaning of equation (8), where the line element in the z system would be (one-dimension)

$$ds^2 = dz^2,$$

so that $g_{11} = 1$.

Therefore we do not operate with the conservative time derivative, $\frac{D}{Dt}$, but with the ordinary time derivative in the transformed system.

Now by inserting the unit operator $I = e^{i\hat{S}}e^{-i\hat{S}}$ in equation (4), we obtain

$$\hat{H}'|\phi\rangle - \hbar\frac{\partial\hat{S}}{\partial t}|\phi\rangle = i\hbar\frac{\partial}{\partial t}|\phi\rangle \qquad (15),$$

so that the generator of the motion (translation in time) is now the operator $\hat{H}' - \hbar\frac{\partial\hat{S}}{\partial t}$ rather than the Hamiltonian itself. This is the analogue of equation (34b) §1.4.

In full we have the equation

$$i\hbar\frac{\partial}{\partial t}|\phi\rangle = \left[\frac{\hat{p}^2}{2m} + \frac{m\omega_0^2\hat{q}^2}{2} + i\hbar\left(\frac{-i\gamma}{2\hbar}\right)\left(\hat{p}\hat{q}+\hat{q}\hat{p}\right)\right]|\phi\rangle \qquad (16),$$

and in the transformed basis $|Q\rangle$ we then have

$$i\hbar \frac{\partial \phi(Q,t)}{\partial t} = \left\{ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial Q^2} + \frac{m\omega_o^2 Q^2}{2} - \frac{i\gamma\hbar}{2}\left(1 + 2Q\frac{\partial}{\partial Q}\right)\right\}\phi(Q,t) \tag{17}$$

a result in agreement with equation (9).

Making the separation of variables

$$\phi(Q,t) = e^{-i\omega' t} e^{-im\gamma Q^2/2\hbar} \chi(Q), \tag{18}$$

then substituting in equation (17), we have

$$\hbar\omega\chi(Q) = -\frac{\hbar^2}{2m}\frac{\partial^2\chi(Q)}{\partial Q^2} + \frac{mW^2Q^2}{2}\chi(Q). \tag{19}$$

This equation is identical to the Schrödinger equation for a harmonic oscillator with frequency $W = (\omega_o^2 - \gamma^2)^{\frac{1}{2}}$. We thus have transformed the system to a frame in which the Schrödinger equation is essentially time independent. This agrees with the result found in §1.4 for the transformed classical system.

If, on the other hand, $\omega_o^2 < \gamma^2$, we can introduce $W'^2 = \omega_o^2 - \gamma^2$ where W' is purely imaginary: $W' = iW$. Solution is now in the range of continuous eigenvalues. For $\omega_o^2 = \gamma^2$, we have the case of a free particle (in transformed coordinates), and a solution is again possible*.

Returning now to the eigenvalue equation (19), we know its solution from elementary quantum mechanics:

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* This has been done by Buch and Denman (1974) for the LDP in the theory of conductivity.

$$\omega_n = W\left(n+\tfrac{1}{2}\right), \quad n = 0, 1, 2 \ldots\ldots \tag{20}$$

are the eigenvalues, and the eigenfunctions are

$$\chi_n(Q) = \left(\sqrt{\pi}\, 2^n n!\right)^{-\frac{1}{2}} e^{-mWQ^2/2\hbar} H_n\left(\sqrt{\tfrac{mW}{\hbar}}\, Q\right), \tag{21}$$

with the $\{H_n(\sqrt{\frac{mW}{\hbar}}Q)\}$ Hermite polynomials of order n. They are a set of complete orthogonal polynomials. The normalisation factor $(\sqrt{\pi}\ 2^n n!)^{-\frac{1}{2}}$ guarantees the normalisation of the $\{\chi_n(Q)\}$ to unity.

The full solution of equation (17) is thus

$$\phi_n(Q,t) = e^{-i\omega_n t} e^{-im\gamma Q^2/2\hbar} \chi_n(Q) \tag{22}.$$

Now

$$\phi(Q) \equiv \langle Q/\phi\rangle = \left(q/e^{-i\hat{S}} e^{i\hat{S}}/\psi\right),$$

by using the replacements indicated earlier; i.e.

$$\phi(Q) = \psi(q), \tag{23}$$

where Q is the coordinate in the system with metric $g_{ij} = \delta_{ij}$.

We know that $q = Qe^{-\gamma t}$, so that

$$\psi_n(q,t) = \left(\sqrt{\pi}\, 2^n n!\right)^{-\frac{1}{2}} e^{-i\omega_n t} e^{-mWq^2 e^{2\gamma t}/2\hbar} e^{-im\gamma q^2 e^{2\gamma t}/2\hbar} H_n\left(\sqrt{\tfrac{mW}{\hbar}}\, q e^{\gamma t}\right) \tag{24}.$$

In the absence of the metric interpretation, we would find $\psi_n(q,t)$ multiplied by the factor $e^{\gamma t/2}$ arising from using ordinary time derivatives in equation (4) (Kanai, 1948; Kerner, 1958; Stevens, 1958; Bopp, 1962; Buch and Denman, 1973). This factor does not alter the observable properties

of the system since it is identical in value to the value associated with dV in the presence of a metric different to δ_{ij}.

Again, since the χ_n were normalized to one, the functions ψ_n are so normalized as well. Furthermore the $\{\psi_n(q,t)\}$ are a complete orthonormal set of functions.

It may be verified by substitution that $\psi_n(q,t)$ is a solution of equation (7). However it is not an eigenfunction of H^*, nor are the $\{\omega_n\}$ eigenvalues of H. This is because equation (7) is only satisfied by the cancellation of identical terms on the right and left hand sides, thus changing the form of H. This also applies to the transformed coordinates: the eigenvalues belong to the operator $H' + \frac{\gamma}{2}(\hat{p}\hat{q} + \hat{q}\hat{p})$. Although the transformed system is related to the time dependent one by a unitary transformation, the eigenvalues are not the same in both systems since $\hat{U}$ is time dependent.

The label n is the same quantum number that would occur in the problem of the undamped oscillator. Since n is not a function of γ, and for $\gamma \to o$ a smooth transition is made to the frequency ω_o, there is thus a one-to one correspondence between the states of the DHO and SHO even though n is not a good quantum number for the DHO Hamiltonian in the metrical coordinates. This absence of mixing of the non-interacting states means that subsequent calculations based on $\psi_n(q,t)$ will possess features of a non-interacting description.

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* Application of H to the function $\psi_n(q,t)$ generates three states: the state ψ_n, and states labeiled n±2. See below.

We now indicate some results to be found for the observables of interest.

2.4 Quantum Mechanical Energy

To explicitly calculate the energy in the state $\psi_n(q,t)$, we cannot simply attempt to identify it with ω_n in the argument of the leading exponential factor in equation (24). Instead we have to explicitly calculate what happens when $\hat{H}$ operates on the wave function $\psi_n(q,t)$ given by equation (24). On the other hand, a comparison of the results in §1.4 for the energy in the transformed system allows us to conclude that in the transformed quantum system the "energy" eigenvalues are given by

$$E_n = \hbar W \left(n+\tfrac{1}{2}\right) \qquad n=0,1,2\ldots\ldots \qquad (25).$$

These are the eigenvalues of the quantum generator of time translations.

To calculate $\hat{H}|\psi>$, we first need the following identities

$$2y\,H_n(y) = H_{n+1}(y) + 2n\,H_{n-1}(y)$$

and $$H_n'(y) = 2n\,H_{n-1}(y),$$

whence one easily shows that

$$\hat{H}\psi_n(q,t) = \frac{\hbar\omega_0^2}{W}\left(n+\tfrac{1}{2}\right)\psi_n(q,t) - \hbar f_n e^{-iWt}\cdot e^{-im\gamma q^2 e^{2\gamma t}/2\hbar}\cdot$$
$$e^{-mWq^2e^{2\gamma t}/2\hbar}\left\{H_{n+2}(\beta q e^{\gamma t})\left(\frac{i\gamma W-\gamma^2}{4}\right)+H_{n-2}(\beta q e^{\gamma t})\,n(n-1)\cdot\right.$$
$$\left.\cdot\left(-\gamma^2-i\gamma W\right)\right\}, \qquad (26)$$

$$\beta = \sqrt{\frac{mW}{\hbar}},$$

where f_n denotes the normalisation constant $(\sqrt{\pi}2^n n!)^{-\frac{1}{2}}$.

Now

$$f_{n+2} = f_n \cdot \tfrac{1}{2}\left[(n+1)(n+2)\right]^{-\frac{1}{2}}$$

and

$$f_{n-2} = f_n \cdot 2 \cdot \left[n(n-1)\right]^{\frac{1}{2}},$$

so that we can rewrite equation (26) as

$$\hat{H}\psi_n(q,t) = \frac{\hbar\omega_0^2}{W}(n+\tfrac{1}{2})\psi_n(q,t) + \sqrt{(n+1)(n+2)}\,\Omega\,\psi_{n+2}(q,t) +$$

$$+\sqrt{n(n-1)}\,\Omega^*\psi_{n-2}(q,t) \qquad (27),$$

where

$$\Omega = (\gamma^2 - i\gamma W)\frac{\hbar}{2W},$$

and Ω^* is the complex conjugate of Ω.

Since the $\{\psi_n\}$ are normalised, we have the expectation value of $\hat{H}$ for the n^{th} wave function:

$$\langle\hat{H}\rangle = \frac{\hbar\omega_0^2}{W}\left(n+\tfrac{1}{2}\right) \qquad (28).$$

This result agrees with that of the authors cited earlier, with the exception of Kanai (1948), but the discrepancy here appears to be a mere typographical error. In

the case of Bopp (1962), the non-Hermitian character of his transformed Hamiltonian (it is not symmetrized) leads to a complex energy.

On the other hand, if we take equation (27) §1.3 as the definition of the energy operator we would find

$$\langle E \rangle = e^{-\frac{\lambda t}{m}} \frac{\hbar \omega_o^2 \left(n+\frac{1}{2}\right)}{W} \qquad (29).$$

This amounts to evaluating $\langle P^2_{\text{kinematic}} \rangle$: this is permitted since $[P, P_{kin}] = 0$. One can recover this result following an heuristic argument due to N. Rivier.

In the classical limit, the energy of the SHO in the comoving coordinates is ε:

$$\mathcal{E} = \tfrac{1}{2} m W^2 z_o^2,$$

where z_o is the maximum displacement.

Since the energy eigenvalues are

$$\mathcal{E}_n = \hbar W \left(n+\tfrac{1}{2}\right)$$

one can say that

$$z_o^2 \sim \frac{2\hbar\left(n+\frac{1}{2}\right)}{mW}.$$

Similarly, it is assumed that the energy in the x-coordinates at given time t is given by $\frac{1}{2}m\omega_0^2 x^2_{max}$, since at the maxima of displacement the "kinetic energy" is zero.

Now $x^2_{max} = z_0^2 e^{-\lambda/m t}$,

so $$\langle E \rangle = \tfrac{1}{2} m \omega_o^2 e^{-\frac{\lambda t}{m}} \frac{2\hbar}{mW}\left(n+\tfrac{1}{2}\right),$$

which is merely equation (29)'. This amounts to saying that

given a quantity with dimension (length)^2 in the comoving coordinates, the relevant expression in the laboratory coordinates is $e^{-\lambda/mt}$ (length)^2*.

Result (27) is an immediate indication that n is not a good quantum number for H, since operation of H on ψ_n does not reproduce only ψ_n, but also ψ_{n+2}, ψ_{n-2}. It may be immediately verified that

$$|\langle\psi_{n+2}|\hat{H}|\psi_n\rangle|^2 = (n+1)(n+2)\,\Omega\Omega^*$$

and $$|\langle\psi_{n-2}|\hat{H}|\psi_n\rangle|^2 = n(n-1)\,\Omega\Omega^*.$$

What this seems to indicate is a preference to "populate" the states ψ with larger n, drawing a closer analogy between the result (27) and the second-quantized theory of stimulated emission. For annihilation and creation operators, a and a^+ respectively, such that

$$[a, a^+] = 1,$$

with

$$a\psi_n(q,t) = \sqrt{n}\,\psi_{n-1}(q,t)$$

$$a^+\psi_n(q,t) = \sqrt{(n+1)}\,\psi_{n+1}(q,t),$$

we can rewrite $\hat{H}$ as

$$\hat{H} = \frac{\hbar\omega_0^2}{W}\left(a^+a + \frac{1}{2}\right) + \Omega a^+a^+ + \Omega^* aa. \qquad (30)$$

Clearly this operator is Hermitian, and as $\gamma \to 0$, it becomes the SHO second-quantized Hamiltonian. This shows how states $\psi_{n\pm2}$ become "populated". We have placed "populate" in inverted commas to stress that n is not in fact equal to the

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* The envelope $e^{-\lambda/mt}$ is a geodesic in the curved space. Riding along on it is going to give a time independent energy. Conversely to leave it, we multiply by $e^{-\lambda/mt}$, c.f. §1.3.

number of quanta - we do not even know what frequency these have - should it be W as indicated by equation (25), or $\frac{\omega_o^2}{W}$ as shown by equation (28)? In the transformed system the frequency of the quanta is W, whereas the expectation value of the Hamiltonian in the n^{th} state gives a shift to $\frac{\omega_o^2}{W}$. There is certainly a basic difficulty here. In fact one author (Stevens, 1958) even regards the basic frequency as being ω_o, and from equation (29) deduces that the quanta are shrinking in time, as does the zero point energy (see below). Furthermore, since as $t \to \infty$, the square of non-metrical wave function†

$$\psi_n(q,t) = e^{\gamma t/2} e^{-iW_n t} e^{-im\gamma q^2 e^{2\gamma t}/2\hbar} e^{-mWq^2 e^{2\gamma t}/2\hbar} H_n(\beta q e^{\gamma t}) \beta_n$$

shrinks into a delta function located at the origin:

$$\lim_{t\to\infty} \int_{-\infty}^{\infty} |\psi_n(q,t)|^2 f(q)\,dq = f(0).$$

Kerner (1958) interprets this as meaning that the oscillator has entered the classical regime in which a vanishing zero-point energy is understandable.

Alternatively, for the value of $\langle \hat{H} \rangle$ given by (28) i.e. the value following formally from the Hamiltonian, we find a zero point energy $\frac{h\omega_o^2}{2W}$, a value in excess of the undamped value $\frac{h\omega_o}{2}$. The interaction with a heat bath represented by the phenomenological damping parameter λ thus seems to

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† Under integration the metrical wave function is also a delta function, and this is all that matters. We find it easier to visualize $\delta(x)$ symbolically rather than $\exp(-\gamma t)\,\delta(x)$.

boost the zero point energy.

To complete the mathematical detail, we note that the position-momentum uncertainty relation $\langle \Delta\hat{p}\Delta\hat{q}\rangle$ is given by the time-independent value

$$\langle \Delta\hat{p}\,\Delta\hat{q}\rangle = \langle (g^{ij}\hat{p}_i\hat{p}_j)^{\frac{1}{2}} (g_{ij}\hat{q}^i\hat{q}^j)^{\frac{1}{2}} \rangle \qquad (31),$$

which equals

$$\langle \Delta\hat{p}\,\Delta\hat{q}\rangle = \frac{\hbar\omega_0}{W}\left(n+\tfrac{1}{2}\right), \qquad (32)$$

a value larger than the minimal value $\hbar\omega_0(n+\frac{1}{2})$, and we again see that the interaction with the bath has increased the uncertainty in the position-momentum relation.

Were we to calculate this uncertainty relation for the operators combined in the scalar form introduced for equation (27) §1.3, we would find a time decaying product

$$\langle \Delta\hat{p}\,\Delta\hat{q}\rangle = (\delta_{ij}\hat{x}^i\hat{x}^j)^{\frac{1}{2}} (\delta_{ij}\hat{p}_i\hat{p}_j)^{\frac{1}{2}}.$$

One might then have concluded that the system had entered the classical régime as $t \to \infty$. This only indicates how careful one has to be before ascribing direct physical meaning to notions like the energy and the number of quanta.

2.5 Other Models of the D.H.O.

Because of its importance in the field of coherent optics many authors have studied the DHO to gain insight into the general problem of losses. Such models usually

assume a Hamiltonian of the form

$$\hat{H} = \hat{H}_{\text{oscillator}} + \hat{H}_{\text{interaction}} + \hat{H}_{\text{bath}} .$$

Various properties are then assigned to the medium e.g. in the case of a lossy cavity (Glauber, 1969; Haake, 1973; Louisell, 1969; Agarwal, 1971) as consisting of a set of oscillators with some spread in frequency, or as consisting of two-state dipoles (Senitzky, 1959). The above procedures and the one adopted here are fundamentally different in that we do not assign any structure to λ and in particular do not quantize the metric tensor $g_{ij} = e^{\frac{\lambda t}{m}} \delta_{ij}$, nor do we need to carry out any decoupling approximation.

On the other hand, the detailed models are successful in obtaining a time-dependent description, showing how the zero-point energy evolves in time, the usual constant value being approached as $t \to \infty$. The constant value is contributed by the random properties associated with the interaction bath. Our metric theory gives a constant value for the zero point energy, whereas the ad hoc theory (viz. that in which $E \to o$ as $t \to \infty$) gives a value tending to zero.

We should also mention the work of Santos (1969) who has constructed a Lagrangian theory of dissipation working from the theory of stochastic quantum mechanics. The only effect of the random forces is to produce a diffusion effect.

The last model we wish to consider is that in which dissipation (damping) is introduced into an oscillating system by the modulation of the oscillation frequency

(Kubo, 1962).

For constant ω, the equation

$$\dot{x}(t) = i\omega x(t), \tag{33}$$

is identical to the equation of motion for a SHO of frequency ω, as can be verified by differentiation of (33) with respect to time, and subsequent substitution of $\dot{x}(t)$ by the value (33).

Now if ω is some (usually random) function of t, $\omega(t)$, carrying out the same procedure as above leads to the real equation

$$\ddot{x}(t) - \frac{\dot{\omega}(t)}{\omega(t)}\dot{x}(t) + \omega^2(t)x(t) = 0 \tag{34},$$

which looks like that describing the DHO.

The modulated frequency, $\omega(t)$, is a stochastic process so that the differential equation (34) is stochastic too, and as such its solution is given by a probability distribution.

For example, with an assumed Gaussian distribution, one can calculate the displacement autocorrelation function $\langle x(t)x^*(o)\rangle$.

This function is found to exhibit a behaviour strongly dependent on the speed of modulation. For fast modulation it shows negative exponential decay with $e^{-\frac{\lambda}{m}t}$, where $\frac{\lambda}{m} <<$ the modulation frequency. For slow modulation, the time dependence is Gaussian. The first type is the one we have

encountered thus far in our studies and represents the situation where the (incoherent) impulses of the surrounding medium have a much shorter lifetime than that of the damped particle.

2.6 Conclusion

We have presented a formalism in which the time-dependent Schrödinger equation may be formulated and solved. The solution to this equation is however not an eigenfunction of the Hamiltonian, nor do we find its eigenvalues. This makes for difficulties in interpreting the averaging of the Hamiltonian in the n^{th} quantum state, where the label n refers to a stationary state, whilst the Schrödinger equation as a whole is manifestly time-dependent. Nonetheless within the strict framework of the formalism we can show that our momentum-position commutation relation is vindicated and that a reasonable value for the zero point - energy is obtained. All the above conclusions are unaltered if no metric identification is made, and the solution as a whole is exact.

On the other hand we can look at the expectation value of the ad hoc definition of the energy, constructed to show a damped behaviour. The zero point energy is then also decaying in time, which is assumed by some to indicate the system enters a classical régime. However, if a sufficiently detailed study is made of the problem, it is seen that the zero point energy remains finite as $t \to \infty$.

The mathematical reason why all the observables in

the rigorous theory turn out to be time-independent is because (both with, and without the metric theory) all integrals are evaluated by means of the transformation $x \exp(\gamma t) \rightarrow z$, which is a transformation to time-independent coordinates. The expansion of the volume element always compensates any decay.

CHAPTER THREE

FUNCTIONAL INTEGRAL THEORY WITH DISSIPATION

3.1 Introduction

The path (functional) integral method in stochastic process theory developed by N. Wiener was introduced into quantum mechanics two decades ago by R.P. Feynman in his doctoral dissertation (Feynman, 1948). A comprehensive review of the topic is to be found in the paper by Gel'fand and Yaglom (1960) and in the monograph by Feynman and Hibbs (1965).

The path integral arises in the stochastic theory as the solution (for specified boundary conditions) of the partial differential diffusion equation. A simple scaling of constants and the substitution of the real time variable by a purely imaginary one has the effect of changing the diffusion equation into the Schrödinger equation, and one can thus state that subject to the same replacements, the Schrödinger equation also possesses a path integral solution.

Feynman's idea was to take this latter statement as the starting point for a description of quantum mechanics. The evolution of a physical system is now written as a sum of weighted probability amplitudes.

In particular the probability amplitude that a single particle initially at position x_a at time t_a will be found at x_b at time t_b is given by the propagator (or Kernel or

Green's function)

$$K(x_b, t_b ; x_a, t_a) = \int_{x_a}^{x_b} \mathcal{D}x(t) \exp \frac{i}{\hbar} \int_{t_a}^{t_b} \mathcal{L}\, dt \quad , \tag{1}$$

where $\mathcal{D}x(t)$ denotes a sum over all paths x(t) joining x_b and x_a subject to $x(t = t_a) = x_a$ and $x(t = t_b) = x_b$.

The time integral in equation (1) is simply the classical action, and the weight function $\exp \frac{i}{\hbar} A(x_b, t_b ; x_a, t_a)$ is termed the Feynman measure.

A first property of $K(b,a) \equiv K(x_b, t_a ; x_a, t_a)$ is that of closure:

$$K(b,a) = \int_{-\infty}^{\infty} dx_c \; K(b,c)\, K(c,a), \tag{2}$$

where $x_b > x_c > x_a$.

Furthermore when $K(b,a)$ depends only on the time difference $T = t_b - t_a$, one has

$$K^*(x_b, x_a ; T) = K(x_a, x_b ; -T), \tag{3a}$$

and

$$\int_{-\infty}^{\infty} dx \; K(x, x' ; T)\, K^*(x, x'' ; T) = \delta(x' - x'') \tag{3b}.$$

The path integral description provides a very compact and elegant picture of the quantum mechanical behavior of a system. Moreover, let $\hbar \to 0$ in equation (1). Then the argument of the exponential will fluctuate greatly from one neighboring path to the next so that these contributions to

the sum will cancel each other. Only when the action is stationary with respect to a change to a neighboring path will a contribution be found - in this case the propagator is proportional to $\exp \frac{iA}{\hbar}$classical . This is exactly what is meant by the extremization of the action in classical mechanics ($\hbar = 0$).

Note that equations (2) and (3) can be immediately generalized to the case where the metric tensor is not flat, but only time dependent as is our $g_{ij}(t)$; one simply includes $d_t x$ in place of dx.

The propagator is also the starting point for a development of equilibrium statistical mechanics. Before considering how this arises, we examine how the propagator may be calculated for our model systems.

3.2 Calculation of Propagators

One can show (Feynman and Hibbs, 1965) that if the Lagrangian is a generalized quadratic,

$$\mathcal{L}(\dot{x},x,t) = a(t)\dot{x}^2 + b(t)\dot{x}x + c(t)x^2 + d(t)\dot{x} + e(t)x + f(t), \quad (4)$$

then

$$K(b,a) = F(t_b,t_a) \exp \frac{i}{\hbar} A(b,a)_{classical},$$

where

$$F(t_b,t_a) = \int_0^0 \mathcal{D}y(t) \exp \frac{i}{\hbar} \int_0^T dt \left\{ a(t)\dot{y}^2 + b(t)\dot{y}y + c(t)y^2 \right\} \quad (5),$$

and the path integration above is over all paths subject to the condition $y(o) = 0 = y(T)$. The limitation to quadratic Lagrangians still covers a large number of systems since the approximation of an interacting system either by a non-interacting one or by a linear interaction is often valid.*

The free particle, SHO, LDP and DHO are exactly of the form (4), and we therefore need only find the conditional propagator (5) to have the full propagator.

The path integration in equation (5) does not in fact need to be carried out, as there is a simple relationship between $F(t_b,t_a)$ and $A(x_b,t_b;\ x_a,t_a)$ in the quadratic Lagrangian case. This was first noticed by Pauli (1962), using the work of Van Vleck (1928). Below we outline a flat space method of calculating $F(t_b,t_a)$ due to Miller (1970).

The starting point of this calculation is the unitarity condition (36). One assumes that $K(b,a)$ can be written as

$$K(b,a) = B(b,a) \exp \frac{i}{\hbar} \phi(b,a),$$

for two functions B and ϕ, and then by applying a stationary phase argument can show that (3b) is satisfied if

$$|B(b,a)| = \left(\frac{i}{2\pi\hbar} \cdot \frac{\partial^2 \phi(b,a)}{\partial x_b \, \partial x_a} \right)^{\frac{1}{2}}.$$

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* c.f. §3.4

This result holds true for any Lagrangian in the limit $\hbar \to 0$, and is exact for quadratic Lagrangians.* de Witt (1957) extended the formula to include the case of curvilinear coordinates. He showed that

$$F(t_b, t_a) = \left(\frac{i}{2\pi\hbar} \, g^{\frac{1}{2}}(t_b) \frac{\partial^2 A_c(b,a)}{\partial^2 x_b \, \partial x_a} \, g^{\frac{1}{2}}(t_a) \right)^{\frac{1}{2}} . \tag{6}$$

Then we have the following results:

(i) free particle

$$F(t_b, t_a) = \left(\frac{m}{2\pi i\hbar T} \right)^{\frac{1}{2}} \tag{7a}$$

with propagator

$$K_F(b,a) = \left(\frac{m}{2\pi i\hbar T} \right)^{\frac{1}{2}} \exp \frac{im(x_b - x_a)^2}{2\hbar T} . \tag{7b}$$

(ii) LDP

$$F(t_b, t_a) = \left(\frac{\lambda e^{-\lambda t/2m}}{2\pi i\hbar \left(1 - e^{-\lambda/m\, t}\right)} \right)^{\frac{1}{2}} \tag{8a}$$

and

$$K_{LDP}(b,a) = \left(\frac{\lambda e^{-\lambda t/2m}}{2\pi i\hbar \left(1 - e^{-\lambda t/m}\right)} \right)^{\frac{1}{2}} \exp \frac{i\lambda (x_b - x_0)^2}{2\hbar \left(1 - e^{-\lambda t/m}\right)} . \tag{8b}$$

(iii) SHO

$$F(t_b, t_a) = \left(\frac{m\omega_0}{2\pi i\hbar \sin \omega_0 T} \right)^{\frac{1}{2}} \tag{9a}$$

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* The case of three dimensions can be found in Bruch and Revercomb (1973).

and

$$K_{SHO}(b,a) = \left(\frac{m\omega_o}{2\pi i\hbar \sin\omega_o T}\right)^{\frac{1}{2}} \exp\frac{im\omega_o}{2\hbar\sin\omega_o T}\left[\left(x_a^2+x_b^2\right)\cos\omega_o T - 2x_a x_b\right] \quad (9b)$$

and

(iv) DHO $(\omega_o^2 > \gamma^2)$

$$F(t_b,t_a) = \left(\frac{mW}{2\pi i\hbar \sin WT}\right)^{\frac{1}{2}} \quad (10a)$$

and

$$K_{DHO}(b,a) = \left(\frac{mW}{2\pi i\hbar \sin WT}\right)^{\frac{1}{2}} \exp\frac{imW}{2\hbar}\left[\left(x_a^2 e^{2\gamma t_a} + x_b^2 e^{2\gamma t_b}\right)\frac{\cos WT}{\sin WT} - \right.$$

$$\left. - \frac{2x_a x_b e^{\gamma(t_a+t_b)}}{\sin WT} + \frac{\gamma}{W}\left(x_a^2 e^{2\gamma t_a} - x_b^2 e^{2\gamma t_b}\right)\right]. \quad (10b)$$

For the case $\omega_o^2 < \gamma^2$, replace sin WT by sinh W'T and cos WT by cosh W'T throughout.

Incidentally, Papadopoulos (1973) has calculated the LDP and DHO propagators without making the metric identification. The propagators are similar to ours and satisfy the same closure relation, but the pre-exponential factors (8a) and (10a) are respectively altered to

$$\left(\frac{\lambda}{2\pi i\hbar\left(1-e^{-\lambda t/m}\right)}\right)^{\frac{1}{2}} \quad \text{and} \quad \left(\frac{mWe^{\gamma t_a+\gamma t_b}}{2\pi i\hbar \sin WT}\right)^{\frac{1}{2}}.$$

All the above propagators, including those of Papadopoulos also satisfy the unitarity condition.

In the next section, as a check and for completeness, we give a direct calculation of the DHO path integral.

3.3 Path Integration for the DHO

The standard way of evaluating path integrals such as (1) is by dividing the time interval T into N segments of length ε such that $N\varepsilon = T$.

At the end of the calculation, the limit $N \to \infty$ is to be taken. Some approximation for the stepwise Lagrangian is then chosen e.g.

$$\mathcal{L}_n = \mathcal{L}\left(\frac{x_n - x_{n-1}}{\epsilon}, \frac{x_n + x_{n-1}}{2}, \frac{t_n + t_{n-1}}{2}\right).$$

Other choices are also possible - see Feynman (1948).

It may then be shown that our path integral takes the form of the following N-fold integral:

$$K(b,a) = \lim_{N\to\infty} \int_{-\infty}^{\infty} \cdots \int dx_1 \, dx_2 \cdots dx_{n-1} \frac{1}{A^N} \exp \frac{i\epsilon}{\hbar} \sum_{n=1}^{N} \mathcal{L}_n \,, \qquad (11)$$

where

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

is a normalization constant whose value is the same as the flat space value, as shown in Appendix 1.

The first result we need is the relevant path integral for the SHO. This is a well-known result but is rarely cal-

culated in full in the texts, and accordingly we present such a calculation below (in flat space).

Because of the periodicity condition in the general definition of $F(t_b, t_a)$, we introduce

$$x(t = j\epsilon) = x_j$$

$$x_j = \sum_{n=1}^{N-1} a_n \sin \frac{n\pi j}{N} \,, \tag{12}$$

and write the action, having made use of the SHO Lagrangian and the definition of $\mathcal{L}_n$, as

$$A(b,a) = \frac{m\epsilon}{2} \sum_{j=1}^{N} \sum_{\substack{n=1 \\ \ell=1}}^{N-1} a_n a_\ell \left[\frac{\left\{ \sin \frac{n\pi j}{N} - \sin \frac{\ell(j-1)\pi}{N} \right\} \left\{ \sin \frac{\ell \pi j}{N} - \sin \frac{m\pi(j-1)}{N} \right\}}{\epsilon^2} - \right.$$

$$\left. - \omega_o^2 \sin \frac{n\pi j}{N} \sin \frac{\ell \pi j}{N} \right]. \tag{13}$$

Now since

$$\sum_{j=1}^{N} e^{ipj\pi/N} = N \delta_{p,0} \,,$$

we reduce equation (13) to

$$A(b,a) = \frac{m\epsilon N}{2} \sum a_\ell^2 \left\{ \frac{1}{\epsilon^2} \left(1 - \cos \frac{\ell\pi}{N} \right) - \frac{1}{2} \omega_o^2 \right\}. \tag{14}$$

The introduction of the Fourier series expansion of the $\{x_i\}$ means that we are now regarding the set $\{a_n\}$ as the

variables of integration, and consequently the propagator is now to be evaluated from

$$F(t_b, t_a) = \lim_{N\to\infty} \frac{1}{A^N} J \int_{-\infty}^{\infty}\cdots\int da_1 \cdots da_{n-1} \exp \frac{im\epsilon N}{2\hbar} \cdot$$

$$\cdot \sum_{l=1}^{N-1} a_l^2 \left\{ \frac{1}{\epsilon^2}\left(1-\cos\frac{l\pi}{N}\right) - \frac{1}{2}\omega_0^2 \right\} \quad , \qquad (15)$$

where J is the Jacobian arising out of the change of variables. The elements of the Jacobian matrix are

$$J_{ik} = \sin \frac{ik\pi}{N} .$$

Muir (1882) evaluated the determinant J above as

$$J \equiv \det J_{ik} = \left(\frac{N}{2}\right)^{\frac{N-1}{2}} .$$

Now using

$$\int_{-\infty}^{\infty}\cdots\int dx_1 \cdots dx_n \exp -\tfrac{1}{2}\beta_{ik} x_i x_k = \frac{\pi^{N/2}}{(\det \beta_{ik})^{\frac{1}{2}}} \quad ,$$

we find

$$F(t_b, t_a) = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^N \left(\frac{N}{2}\right)^{\frac{N-1}{2}} \left(\frac{2\pi i\hbar\epsilon}{mN}\right)^{\frac{N-1}{2}} \prod_{m=1}^{N-1} \left(1-\cos\frac{m\pi}{N} - \frac{1}{2}\omega_0^2\epsilon^2\right)^{-\frac{1}{2}} .$$

Now

$$\prod_{m=1}^{N-1}\left(1-\cos\frac{m\pi}{N} - \frac{1}{2}\omega_0^2\epsilon^2\right) = \prod_{m=1}^{N-1}\left(1-\cos\frac{m\pi}{N}\right) \prod_{m=1}^{N-1}\left(1 - \frac{\frac{1}{2}\omega_0^2\epsilon^2}{1-\cos\frac{m\pi}{N}}\right) ,$$

and since (Gradshteyn and Ryzhik, 1965)

$$\prod_{k=1}^{N-1} 2\left(1-\cos\frac{k\pi}{N}\right) = N,$$

we have

$$\prod_{m=1}^{N-1}\left(1-\cos\frac{m\pi}{N}-\frac{1}{2}\omega_o^2\epsilon^2\right)=\frac{N}{2^{N-1}}\prod_{m=1}^{N-1}\left\{1-\frac{\frac{1}{2}\omega_o^2\epsilon^2}{1-\cos\frac{m\pi}{N}}\right\}.$$

Write $1-\cos\frac{m\pi}{N} = 2\sin^2\frac{m\pi}{2N}$, and apply the identity

$$2N\left(1-\frac{\sin^2\theta}{\sin^2\frac{\pi}{2N}}\right)\left(1-\frac{\sin^2\theta}{\sin^2\frac{\pi\cdot 2}{2N}}\right)\cdots\left(1-\frac{\sin^2\theta}{\sin^2\frac{\pi(N-1)}{2N}}\right)=\frac{\sin 2N\theta}{\sin\theta}$$

(Jolley, 1922), by identifying θ with $\frac{1}{2}\omega_o\epsilon$. Hence

$$\prod_{m=1}^{N-1}\left(1-\frac{\frac{1}{4}\omega_o^2\epsilon^2}{\sin^2\frac{m\pi}{2N}}\right)=\frac{\sin 2N\cdot\frac{1}{2}\omega_o\epsilon}{2N\frac{1}{2}\omega_o\epsilon}\underset{\epsilon\to 0}{=}\frac{\sin\omega_o T}{\omega_o T}.$$

The complete expression above is then

$$\prod_{m=1}^{N-1}\left(1-\cos\frac{m\pi}{N}-\frac{1}{2}\omega_o^2\epsilon^2\right)^{-\frac{1}{2}}=\frac{1}{N^{\frac{1}{2}}\left(\frac{1}{2}\right)^{\frac{N-1}{2}}}\left(\frac{\omega_o T}{\sin\omega_o T}\right)^{\frac{1}{2}}.$$

Insertion into the expression for $F(t_b,t_a)$ shows full agreement with equation (9a) as is required.

To proceed further in the calculation of $K_{DHO}(b,a)$, we use the results of §1.4, making the transformation $z = xe^{\gamma t}$ as before.

The Lagrangian to be inserted in the transformed path integral is now

$$\mathcal{L}(\dot{z},z) = \frac{1}{2}m\dot{z}^2 - \frac{\lambda}{2}\dot{z}z - \frac{1}{2}mW^2z^2.$$

For the classical path, the Lagrangian is taken without the term in λ for the reason pointed out before in §1.4. We now proceed to calculate $F(t_b,t_a)$ for the DHO, and since the sum is over all possible paths, including the classical one, the full Lagrangian must be retained in the time-integral since the λ term is only irrelevant on the unique least action path. This causes no mathematical difficulty since the λ term is an exact time derivative and may immediately be integrated out.

Specifically we have

$$F(t_b,t_a) = \int_0^0 \mathcal{D}z(t) \left\{ \exp\frac{i}{\hbar}\int_0^T dt\left(\frac{1}{2}m\dot{z}^2 - \frac{1}{2}mW^2z^2\right)\right\}\left\{\exp\frac{i\gamma}{2\hbar}(z_a^2 - z_b^2)\right\} \quad (16).$$

The remaining path integral is exactly that found above for the SHO with W replacing ω_0. There is no Jacobian shown explicitly in (16) - it is in fact equal to 1, since no additional factors need be introduced in the metrical form of equation (5) to make the above transformation.

Finally, combining all the terms and transforming back to the {x,t} coordinates, we recover equations (10a) and (10b), the exponential in (16) which involves γ being absorbed into the classical action exponent to give the full $A_{DHO}(b,a)$.

3.4 Observables in the Path Integral Method

Feynman (1948) and Pauli (1962) have shown that for all systems in the classical limit, and generally for systems described by a quadratic Lagrangian, the propagator satisfies

$$i\hbar \frac{\partial K(b,a)}{\partial t_b} = H(b) K(b,a) + i\hbar \delta(x_b - x_a)\, \delta(t_b - t_a), \quad (17)$$

and that it therefore contains the same information as the wave function for the system. [H(b) means that the operators in H only affect the "b" coordinates.] Equation (17) is consistent with our definition of K(b,a) only for $t_b > t_a$. We see that K(b,a) is quite formally the Green's function of the differential equation (7) §2-3.

When H is time independent, the solution K(b,a) can be written in terms of the energy eigenfunctions $\{\phi_n(x)\}$ as

$$K(b,a) = \sum_{n=0}^{\infty}{}' \phi_n(x_b)\, \phi_n^*(x_a)\, e^{-\frac{iE_n}{\hbar}(t_b - t_a)}, \quad (18)$$

E_n being the energy eigenvalues.

The importance of equation (19) lies in the fact that knowing K(b,a) we should in principle also know $\{\phi_n\}$ and vice versa.

As a tentative way of generalizing equation (19) to include time-dependent systems such as those discussed earlier, we absorb the time-evolution factor back into the wave functions, writing

$$K(b,a) = \sum_{n=0}^{\infty} \psi_n(x_b,t_b)\,\psi_n^*(x_a,t_a)\,, \qquad (19)$$

the $\{\psi_n\}$ being solutions of the time-dependent Schrodinger Equation.

Using equation (24), §2.3, we see that expression (19) takes the form

$$K(b,a) = \exp\left(-\frac{im\gamma}{2\hbar}\left(x_b^2 e^{2\gamma t_b} - x_a^2 e^{2\gamma t_a}\right)\right)\exp\left(-\frac{mW}{2\hbar}\left(x_b^2 e^{2\gamma t_b} + x_a^2 e^{2\gamma t_a}\right)\right).$$

$$\cdot \sum_{n=0}^{\infty} e^{-iW_n(t_b-t_a)/\hbar}\left(\ell_n\right)^2 H_n\left(\beta x_b e^{\gamma t_b}\right) H_n\left(\beta x_a e^{\gamma t_a}\right) \qquad (20)$$

Now, since* (Magnus, Oberhettinger and Soni, 1966)

$$\sqrt{1-z^2}\,e^{-\frac{x^2-y^2}{}} \sum_{m=0}^{\infty}\left(\frac{z^m}{2^m m!}\right) H_m(x) H_m(y) = e^{-\left(x^2+y^2-2xyz\right)/1-z^2} \qquad (21)\,,$$

we can evaluate the sum in equation (20) and obtain

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* This is Mehler's formula. It is also given in Morse and Feshbach (1965), but appears with the wrong sign in the square root on the LHS.

$$K(b,a) = \left(\frac{mW}{2\pi i\hbar \sin WT}\right)^{\frac{1}{2}} \exp\frac{imW}{2\hbar}\left[\left(x_b^2 e^{2\gamma t_b} + x_a^2 e^{2\gamma t_a}\right)\frac{\cos WT}{\sin WT} - \right.$$

$$\left. - \frac{2x_a x_b e^{\gamma(t_a+t_b)}}{\sin WT} + \frac{\gamma}{W}\left(x_a^2 e^{2\gamma t_a} - x_b^2 e^{2\gamma t_b}\right)\right] \qquad (22)$$

which is the result for the propagator found in (10b) above. Clearly this procedure is reversible, relying only on the connection offered by Mehler's formula. The same applies to the undamped oscillator. As to finding the eigenvalues, given the propagator, we can proceed following Burton and de Borde (1955) by trying to generalize the formula

$$\int_{-\infty}^{\infty} dx\; K(x,t;x,t=0) \equiv \sum_{n=0}^{\infty} e^{-iE_n t/\hbar} \;, \qquad (23)$$

which follows from equation (18).

For the SHO, the LHS of equation (23) may be evaluated, and is equal to

$$\sum_{n=0}^{\infty} e^{-i\omega_0 t\,(n+\frac{1}{2})} \;,$$

whence we can equate the arguments of order n to recover the well-known result

$$E_n = \hbar\omega_0\,(n+\tfrac{1}{2}).$$

In the case of the DHO, the x variables always feature in conjunction with the exponential time factor $\exp(\gamma t)$. We have terms like $x_a^2 \exp(2\gamma t_a)$, $x_b^2 \exp(2\gamma t_b)$, and recalling

the metric description, realise that these are equal to the norms of $x^i(a)$ and $x^i(b)$ respectively. We denote these by $X^2(a)$ and $X^2(b)$. Then we can write

$$K(X(a),X(b),T)=\left(\frac{mW}{2\pi i\hbar\sin WT}\right)^{\frac{1}{2}}\exp\frac{imW}{2\hbar}\left[\left\{X^2(a)+X^2(b)\right\}\frac{\cos WT}{\sin WT}-\right.$$

$$\left.-\frac{2X(a)X(b)}{\sin WT}+\frac{\delta}{W}\left\{X^2(a)-X^2(b)\right\}\right]. \qquad (24)$$

Then the trace procedure of equation (24) can be carried out as

$$\int_{-\infty}^{\infty}dX\,K(X,X,T)=\sum_{n=0}^{\infty}e^{-iW_nT}, \qquad (25)$$

which can be seen from the form of $\psi_n(x,t)$. Unfortunately this yields no more information than in the SHO example, since we merely obtain the eigenvalue appearing in the transformed equation (19) of §2.3.

In standard many-body theory (Brown, 1967), expectation values can be found directly from the Green's function, no knowledge of the eigenfunctions being necessary. For a system of single particles, the Green's function $G(\kappa,\tau)$ (in momentum representation) allows a direct expression for the ground state energy, $\langle E\rangle = \langle T\rangle + \langle V\rangle$, to be found. $\langle T\rangle$ and $\langle V\rangle$ are the respective expectation values of the kinetic and potential energies.

Since

$$\lim_{\tau\to-0}G(\kappa,\tau)=-in_\kappa, \qquad (26)$$

where n_k is the occupation number of the k^{th} momentum state, <T> is given by

$$\langle T \rangle = i \sum_k \frac{k^2}{2m} (-i n_k). \tag{27}$$

Further, from the equation of motion for $G(k,\tau)$, it can be shown that

$$\langle T \rangle + 2\langle V \rangle = -\sum_k \lim_{\tau \to -0} \frac{\partial G(k,\tau)}{\partial \tau}. \tag{28}$$

Thus <T> and <V> are known, and <E> can be found.

For the Feynman propagators, in coordinate representation, the statement equivalent to equation (26) is

$$\lim_{t_b \to t_a} K(x_b, t_b; x_a, t_a) = \delta(x_b - x_a), \tag{29}$$

and in the situation where $g_{ij} = g_{ij}(t)$, we obtain

$$\lim_{t_b \to t_a} K(x_b, t_b; x_a, t_a) = \delta(x_b, x_a, t_a). \tag{30}$$

In the momentum representation defined by

$$K(k_b, t_b; k_a, t_a) = \int_{-\infty}^{\infty} \int d_{t_a} x_a \, d_{t_b} x_b \, e^{i k_b x_b + i k_a x_a} K(x_b, t_b; x_a, t_a), \tag{31}$$

(k_b is the covariant momentum; x_b is contravariant as before: the quantity $k_b \cdot x_b$ is thus a scalar product) when $t_b \to t_a$,

we find,

$$\lim_{t_b \to t_a} K(k_b, t_b; k_a, t_a) = e^{\gamma t_a} \delta(k_b - k_a) . \qquad (32)$$

In contradistinction with (26), we have a singular distribution, only one "k" state being occupied. We are dealing with a single particle, rather than the many non-interacting particles described by $G(k,\tau)$ above. There is insufficient information in equations (30) and (32) to enable us to find a value for the energy compatible with the description of §2.4. This conclusion was also reached by Montroll (1952), whose value for the energy of a general system is once again given in terms of the system wave function.

For us the practical value of the propagator lies in its use as a check on the solution of the Schrödinger equation, and more importantly in determining the statistical mechanical properties of the system.

We had hoped, moreover, that a finite temperature formalism could be found by analytic continuation of the propagator in the same way as is done in conventional many body theory (Abrikosov e.a, 1965). All our attempts in this direction have been fruitless, the essential difficulty being that ours is a single particle theory.

3.5 Conclusion

We have shown how damping maybe included in the path integral formalism of Feynman. Since this theory is Lagrangian (action) based, our Lagrangian incorporating damping

is particularly easy to introduce into this formalism.

We first showed how to modify the formulae of the flat space theory to include any time-dependent metric tensor. Then, having established the propagator for the SHO by a direct method, we were able to explicitly calculate the DHO propagator. This is in accordance with the value to be found from the Van Vleck-Pauli-de Witt formulae.

Furthermore, the propagator so found (for overdamped and underdamped) motion is exactly the same as that to be found by building the propagator from the wave-functions. Most important of course is the fact that there are no approximations in these calculations: the quadratic nature of the Lagrangian means all our formulae are exact.

However, the path integral method as developed here is of little use in calculating <H> or <E> as was done in Chapter 2. Ideally we would like to calculate these quantities directly with no knowledge of the $\{\psi_n\}$, but this seems to be impossible.

CHAPTER FOUR

DISSIPATION IN STATISTICAL MECHANICS

4.1 Introduction

The system we are interested in describing is that of a particle, possibly subject to an harmonic oscillator potential, moving in a heat bath which exerts viscous forces on it. The system of particle + bath is open to the outside, and the particle is free to exchange energy with the bath.

The usual assumption (Buch and Denman, 1973) is that the energy of the oscillator is larger than the average energy of the bath so that the energy exchange is essentially one way - from particle to bath until equipartition is reached. This picture is of course incomplete, there being no indication of exactly where the energy is going to since we do not describe any sinks of energy in the bath.

The question of the thermodynamics of such systems has been studied by Haake (1973) using the Master equation approach. The method we shall adopt is that developed by Papadopoulos (1973, 1974), based on the work of Feynman and Vernon (1963).

In general the total density matrix $\hat{\rho}$ of an interacting system such as the above, is reduced to the density matrix of that part of the system whose properties are of interest by averaging over all unwanted coordinates. This is done by taking the trace over these coordinates. Since $\hat{\rho} = \exp(-\beta\hat{H})$, it is essentially a Hamiltonian approach to

the problem. Feynman and Vernon (1962) showed how to carry out the same procedure when the system can be described by means of Lagrangian functions for particle, interaction and bath. The unwanted coordinates are lumped together in an "influence functional" by carrying out path integrals over unwanted coordinates.

Such processes are barred to us by virtue of the fact that we begin with a single particle model where all the interaction effects are contained in λ (except of course the random forces which we have chosen to ignore).

Our first aim is to try to adapt the functional integral formalism of equilibrium statistical mechanics to include damping in the same way as was successfully done in the quantum theory. In equilibrium the density matrix of a system described by a quadratic Lagrangian is proportional to the exponential of the classical action functional analytically continued from real to imaginary time i.e. $\rho(x',x) \sim e^{-\bar{A}(x,\acute{x})/\hbar}$, where $\bar{A}(x',x)$ is the analytically continued action.

Incidentally, one can quite formally write the probability $P(x)$ for a given coordinate state as $P(x) \sim \exp-\frac{S(x)}{\kappa_B}$, where S is the entropy and κ_B is Boltzmann's constant. We also showed that our quadratic Lagrangian gives a quadratic action function, so that $\bar{A}$ is also quadratic. In the quasi-classical case, $S(x)$ is also quadratic in x (Landau and Lifschitz, 1959), so that $\bar{A}$ and S closely resemble each other. There is thus the suggestion of some basic connexion between

the action and entropy, these being the quantities which are central to the extremum principles of classical and statistical mechanics respectively.†

The basic characteristic of irreversible processes such as damping is that during the whole process the entropy of the universe should increase until a maximum value is attained when equilibrium is reached. Unfortunately, the definition of entropy out of equilibrium is not at all obvious (Meixner, 1969), especially since a clear splitting off of the system entropy from that of the environment is not always possible (Cox, 1955). The solution of the quantum DHO showed that there was a one to one relationship between states of the SHO and DHO. This means that from the point of view of information the entropy of the two systems will be the same*. The information theory definition of entropy is $S = -k \, \mathrm{Tr} \, \hat{\rho} \, \ell n \, \hat{\rho}$ ($\hat{\rho}$ being the density operator) and will be seen to give a time independent result. We shall try to obviate this difficulty by an alternative calculation of the entropy.

Below we shall recapitulate the path integral theory and then extend it in two different ways to find two possible density matrices.

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† de Broglie (1964) has discussed this point in detail in his monograph.

* Suggested to the author in private conversation with Dr. D. Ter Haar.

4.2 Resumé of Path Integral Theory of Equilibrium Statistical Mechanics

(1) If eigenvalues of the Hamiltonian of the system can be found such that

$$\hat{H}\phi_n(x) = E_n \phi_n(x),$$

one can write the density matrix in the canonical ensemble as

$$\rho(x';x) = \sum_n \phi_n(x')\, \phi_n^*(x)\, e^{-\beta E_n} \qquad (1)$$

where $\beta = \frac{1}{kT}$, T being the absolute temperature.

We have chosen the coordinate representation to facilitate comparison with equation (18), §3.4. If we set

$$\frac{i(t_b - t_a)}{\hbar} = \beta \qquad (2)$$

in this equation, we arrive back at equation (1) above. This is the same conclusion reached by comparison of the Schrödinger and Bloch equations.

(2) The replacement (2) is then given the status of a general rule: In equilibrium the analytic continuation of the propagator in coordinate representation is the density matrix (Abrikosov et al., 1965).

(3) Such a procedure is valid even when the energy eigenvalues do not exist or cannot be extracted analytically. This follows because like equation (18) §3.4, equation (2) above can be written as a path integral over a specific measure in which no mention is made of eigenvalues. The

path integration is over the imaginary time variable τ running from 0 to $\beta\hbar$:

$$\rho(x',x) = \int_x^{x'} \mathcal{D}x(\tau)\, \exp -\frac{1}{\hbar}\bar{A}(x',x,\beta\hbar) \tag{3}$$

with $\bar{A}$ as defined earlier.

For quadratic Lagrangian systems we then have

$$\rho_{equ.}(x',x) = \left\{\frac{i}{2\pi\hbar}\,\frac{\partial^2 A(x',x;-i\beta\hbar)}{\partial x'\partial x}\right\}^{\frac{1}{2}} \exp -\frac{A}{\hbar}(x',x;-i\beta\hbar) \tag{4}$$

where A is the classical action functional.

Since the eigenvalues of the DHO Hamiltonian could not be found, this procedure seems to offer the possibility of finding its density matrix with little difficulty.

(4) An elegant physical picture of the above process has been presented by Miller (1971) in a paper on the classical limit approximation.

Starting from the classical equation of motion, the change from real to imaginary time has the effect of reversing the sign of the potential V, so that the motion now takes place in a classically forbidden region. Thus to find $\rho(x',x)$ one calculates the propagator with $V \to -V$.

This procedure relies on the existence of a Lagrangian and action functional. We showed earlier how to modify the Lagrange formalism to include a particular kind of dissipation. It is to be hoped that a simple generalization of the analytic continuation will give us the required time-dependent density

matrix.

The assumption that the energy of DHO is greater than the average bath energy is equivalent to saying that the time-scale for smoothing out disturbances in the heat bath is much shorter than the damping time-scale, and consequently that the bath remains in thermal equilibrium at the temperature T. (See §2.5 and §4.6.)

For later comparison, we note here the results of the analytic continuation in the case of the free particle and the SHO.

Free particle

$$\rho(x',x) = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{1}{2}} \exp -\frac{m(x'-x)^2}{2\hbar^2\beta} \tag{5}$$

and

S.H.O.

$$\rho(x',x) = \left(\frac{m\omega_0}{2\pi\hbar \sinh\omega_0\beta\hbar}\right)^{\frac{1}{2}} \exp -\frac{m\omega_0}{2\hbar\sinh\omega_0\beta\hbar}\left\{(x^2+x'^2)\cosh\omega_0\beta\hbar - 2xx'\right\}. \tag{6}$$

Using Mehler's formula, equation (22) §3.4, it may directly be shown that, as required, the SHO density matrix is diagonal in the energy representation.

The partition function, Z, for the SHO is given by

$$Z = Tr\,\hat{\rho}$$

where $\hat{\rho}$ is the density operator. In the coordinate representation, the trace is given in general by

$$Z = \int_V dx\, \rho(x,x) , \tag{7}$$

where V indicates the domain of integration. For the SHO we have a trace on $(\infty, -\infty)$, so that

$$Z = \frac{1}{2 \sinh \omega_0 \beta \hbar/2} . \tag{8}$$

The free energy F, is defined by

$$F = -\frac{1}{\beta} \ln Z , \tag{9}$$

and the energy, E, by

$$E = -\frac{\partial}{\partial \beta} \ln Z . \tag{10}$$

The energy then takes the well-known value

$$E = \frac{\hbar \omega_0}{2} \coth \omega_0 \beta \hbar/2 . \tag{11}$$

The above definitions hold whenever H is time-independent. Having found F and E, we can find S from the relation

$$F = E - TS . \tag{12}$$

Hence S has the value

$$S = \frac{k_B \beta \hbar \omega_0}{2} \coth \omega_0 \beta \hbar/2 - k \ln \left(2 \sinh \omega_0 \beta \hbar/2\right) . \tag{13}$$

Alternatively, S may be calculated from

$$S = -k_B \, Tr\left(\hat{\rho}/Z\right) \ln\left(\hat{\rho}/Z\right) , \tag{14}$$

the information theory definition of entropy. Even if the energy representation of the density matrix is unknown, S can be evaluated from the above relation using e.g. $\rho(x',x)$.

The method is to write

$$\hat{\rho} = 1 - (1-\hat{\rho}),$$

and to use the McLaurin series for the logarithm,

$$\ln\{1-(1-\rho)\} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n} (1-\hat{\rho})^n .$$

Finally each term $(1-\hat{\rho})^n$ is expanded in powers of $\hat{\rho}$ using the Binomial theorem:

$$\ln\{1-(1-\rho)\} = \sum_{n=1}^{\infty}\sum_{m=0}^{n} \frac{(-1)^{n+m}}{n} C_m^n \hat{\rho}^m .$$

We then have

$$S = -\frac{k_B}{Z} \sum_{n=1}^{\infty}\sum_{m=0}^{n} (-1)^{n+m} \frac{1}{n} C_m^n \int_{-\infty}^{\infty} dx\, dx' \langle x|\hat{\rho}|x'\rangle\langle x'|\hat{\rho}^m|x\rangle + \\ + k \ln Z . \qquad (15)$$

The matrix element of $\hat{\rho}^m$ is then found (Appendix 2), and the summations carried out. The same result as equation (13) will be found.

We now proceed to find the DHO density matrix by analytic continuation.

4.3 Density Matrix by Analytic Continuation

The action for the DHO (and the LDP, if the motion commences not at t = o, but say at t = t") depends not only on the time difference, but also on the initial and final times themselves, so that it is not obvious how a replacement like equation (3) is to be made. This troublesome time dependence is confined to the exponential time factors accompanying the coordinates x and x'.

If we retain the metric idea, and employ the Ansatz of Miller, we can surmise as follows: the particle motion takes place in a certain geometry, fixed and immutable, but the potential acting on the particle is to be altered accordint to the replacement $t \to -i\tau$ in the equation of motion. Furthermore, the density matrix of equilibrium gives the probability of finding the particle in a particular state at the time t. Therefore, after modifying the propagator by the Ansatz, we obtain the density matrix in the limit $t_b = t_a$.

The substitution $t \to -i\tau$ in the equation of motion of the DHO gives

$$m\frac{d^2x}{d\tau^2} + i\lambda\frac{dx}{d\tau} - \omega_o^2 x = 0, \tag{16}$$

whence we find that the substitutions

$$\lambda \to -i\lambda$$

$$W^2 = \omega_o^2 - \frac{\lambda^2}{4m^2} \to -W^2 = \frac{\lambda^2}{4m^2} - \omega_o^2,$$

are to be made in the propagator. Then setting $t_b = t_a$,

we find*

$$\rho_t(x',x) = \left(\frac{mW}{2\pi\hbar \sinh W\beta\hbar}\right)^{\frac{1}{2}} \exp -\frac{mWe^{2\gamma t}}{2\hbar}\left[(x^2+x'^2)\frac{\cosh W\beta\hbar}{\sinh W\beta\hbar} - \right.$$

$$\left. -\frac{2x'x}{\sinh W\beta\hbar} - \frac{\gamma i}{W}(x^2-x'^2)\right]. \qquad (17)$$

We can now calculate the average values of quantities of interest for a damped oscillator at the constant temperature β, e.g. the averaged squared displacement $\langle x^2 \rangle$:

$$\langle x^2 \rangle = \frac{\int_{-\infty}^{\infty} x^2 \rho_t(x,x)\, d_t x}{\int_{-\infty}^{\infty} \rho_t(x,x)\, d_t x} \qquad (18)$$

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*We can obtain this result by a different method: recall the definition of our propagator;

$$K_{DHO}(x',t';x,t) = \sum_n e^{-iE_n(t'-t)} \phi_n(x'e^{\gamma t'}) \phi_n^*(xe^{\gamma t}).$$

At the temperature β, by analogy with the construction of the many body "temperature Greens functions" (Abrikosov.e.a, 1965) we assume

$$K^{\beta}_{DHO}(x',t';x,t) = \sum_n \frac{e^{-\beta W_n}}{Z} \cdot \phi_n(x'e^{\gamma t'}) \phi_n^*(xe^{\gamma t}) e^{-iE_n(t'-t)},$$

thus associating a canonical probability distribution with our wavefunctions. Then the density matrix is obtained by setting t = t', and performing the Mehler sum,

$$Z = \sum_n e^{-\beta W_n}, \quad W_n = W(n+\tfrac{1}{2}).$$

The same quantity as (17) is obtained.

The denominator of equation (18) will be termed the partition function, Z, even though we do not strictly have a set of eigenstates for our basic Hamiltonian. We have

$$Z = \frac{1}{2\sinh W\beta\hbar/2} , \tag{19}$$

which is the same as would be found in the case of an undamped oscillator of frequency W.

Now

$$\langle x^2 \rangle = \frac{e^{-2\gamma t}\hbar}{2mW} \coth W\beta\hbar/2 \tag{20}$$

and

$$\left\langle -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \right\rangle = e^{-2\gamma t}\left\{ -\frac{\hbar W}{4}\tanh W\beta\hbar/2 + \frac{\hbar W}{2}\coth W\beta\hbar - \right.$$

$$\left. -\left(\frac{\gamma}{2m}\right)^2 \frac{\hbar}{mW}\sinh W\beta\hbar \right\} , \tag{21}$$

for the averaged "kinetic energy". Multiplying (20) by $\frac{m\omega_o^2}{2}$, and adding to (21), we have an estimate of the total energy at temperature β,

$$E = e^{-2\gamma t}\frac{\hbar\omega_o^2}{2W}\coth W\beta\hbar/2 . \tag{22}$$

This agrees favourably with the values found in §2.4 for <E> and <H> in quantum theory at T = 0. The value E in the limit $\gamma \to 0$, i.e. $W \to \omega_o$, is exactly equal to the SHO value. The large time behavior of equation (17) will be discussed in the next section.

The free energy, F, is conventionally defined in

equilibrium by the expression

$$\hat{\rho} = e^{-\beta(\hat{H}-F)}, \tag{23}$$

whence $F = -\frac{1}{\beta}$ ℓn Z. We cannot apply this definition for two reasons: firstly equation (23) is strictly an equilibrium expression, assuming a canonical proability distribution, and we are clearly dealing with a non-equilibrium situation. Secondly, we do not have an operator (i.e. coordinate free) form for the density matrix. We only have equation (16), from which we have been unable to extract the quantity F.

As was pointed out in §4.1, if the entropy S, is taken as

$$\hat{S} = -k_B \mathrm{Tr}\left(\hat{\rho}/Z\right) \ln\left(\hat{\rho}/Z\right), \tag{24}$$

we shall find a result independent of time. What we have done in equation (24) is to take a formula which is supposedly valid both for reversible and irreversible processes, but does not take account of the "varying mass" (or metric) in the Lagrangian. To actually evaluate this expression we proceed as in the previous section, expanding the logarithm as a power series in $\rho(x',x)$. It is apparent from the asymmetry with respect to x',x of the imaginary exponent in equation (16) that there is no contribution to the entropy from this term since it cancels out exactly for all powers. Furthermore it is possible to make the transformation $Z = xe^{\gamma t}$ throughout, whence the calculation follows that for

a SHO of frequency W.

Therefore

$$S_{DHO} = k_B \ln Z + \frac{\hbar W}{2T} \coth \frac{\hbar W}{2k_B T} . \tag{25}$$

Now when $\frac{hW}{2k_B T} << 1$, i.e. when the time scale of the bath is much shorter than the oscillator decay time, equation (25) may be approximated by

$$S_{DHO} \approx k_B \left[\ln \left(\frac{k_B T}{\hbar W} \right) + 1 \right] , \tag{26}$$

and as W decreases for increasing λ (note that $\omega_o^2 > \gamma^2$), the entropy slowly increases. Damping leads to an increase of entropy.

It is important to note that the value obtained for the entropy and indeed any of the observables above does not depend on the identification of $e^{\lambda/m t}$ as a metric factor, since without this identification the modification of $\rho(x',x)$ leads to exactly the same integrations.

Although we have an entropy whose value is increased as compared with the undamped system, it, along with the values found for the velocity and position, is strictly time independent unless e.g. we resort to calculation of $\langle x^2 \rangle$ rather than $\langle x^2 \exp(2\gamma t) \rangle$ as above. Now, since our DHO and LDP equations of motion bear a close resemblance to the Langevin description of Brownian motion, and the functional integration is closely connected with diffusion processes, we expect a more complicated time evolution than the mere

$\exp(-2\gamma t)$ factors above. We shall now show how this may be accomplished.

4.4 Propagated Density Matrix

The path integral description of interacting systems at both zero and finite temperatures has been developed (Feynman and Vernon, 1963) especially in the case where the Lagrangian of the total system can be split up into the three parts of test particle, interaction and interaction bath. The formalism of such systems has been given the title of Influence Functional theory, since it is possible to write the influence of the interaction on the test particle solely in terms of test particle coordinates. This procedure is equivalent to the usual operation in statistical mechanics of taking the trace over unwanted co-ordinates.

Suppose $A(q(t))$ is the action of the test system q, $A_B(q(t))$ that of the bath, and $A_i(q(t), Q(t))$ that of the interaction. The probability of any event of the total system can be found from*

$$K = \iint \mathcal{D}q\, \mathcal{D}q'\, \mathcal{D}Q\, \mathcal{D}Q' \exp\frac{i}{\hbar}\Big[A(q) + A_i(q,Q) + A_B(Q) - A(q') - A_i(q';Q') - A_B(Q')\Big], \qquad (27)$$

and if one only wishes to measure the dependence on q, one

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* Feynman and Hibbs (1965) p. 344 - 351.

can write

$$K = \int\int \mathcal{D}q\, \mathcal{D}q'\, F[q,q']\, \exp\frac{i}{\hbar}\left[A(q) - A(q')\right], \quad (28)$$

where $F(q,q')$ is the influence functional.

The influence function due to a set of harmonic oscillators at finite temperature (β) is then given by

$$F[q(t), q(t')] = \int\int\int dQ\, dQ_1\, dQ_1'\, K(Q,t;Q_1,t_1)\, K^*(Q,t;Q_1',t_1) \cdot \sum_n e^{-\beta E_n} \phi_n(Q_1)\, \phi_n(Q_1'), \quad (29)$$

where $\phi_n(Q)$ is the wave function of the oscillator in the n^{th} state of energy E_n, and K is the kernel for the SHO including the interaction between each constituent of the bath and the test particle. Now the sum in equation (29) is exactly the coordinate representation of the SHO equilibrium density matrix given in §4.1, so that one can rewrite $F(q(t), q'(t))$:

$$F[q(t), q(t')] = \int dQ\, K(Q,t;Q_1,t_1)\, K^*(Q,t;Q_1',t_1)\, \rho(Q_1,Q_1')\, dQ_1\, dQ_1'. \quad (30)$$

This statement has general validity, not being restricted in any way only to a SHO. The only requirement is that $\{\phi_n\}$ should exist.

The integration over Q in equation (30) represents the condition that one is not interested in any properties of the Q system. We now remove this condition and allow

the final coordinate in the two kernels to be different. We denote this new quantity as

$$P(Q_2, Q_2'; t) = \iint dQ_1 dQ_1' K(Q_2, t; Q_1, t_1) K^*(Q_2', t; Q_1', t_1) \rho(Q_1, Q_1'). \tag{31}$$

It represents the propagated value of the initial conditions contained in $\rho(Q_1, Q_1')$. Papadopoulos (1973, 1974) has taken P to be the definition of the non-equilibrium density matrix. The correctness of this hypothesis is to be ascertained by the truth or otherwise of the predictions (31) makes. In equation (31) the initial wave functions are propagated by the propagator (including forces, damping or external fields), but the probability of each wave function at the temperature β remains constant and equal to its initial value, $\exp\{-\beta h\omega_0(n+\frac{1}{2})\}$. The temperature and time-dependence are thus not coupled, c.f. footnote on page 73.

For the interacting systems described by our Lagrangian theory, the 3 way splitting into bath, interaction and test particle is impossible, the averaging over internal parameters having already been done and embodied in the damping γ. The initial condition is that we release our oscillator of frequency ω_0 at time t_1 with the configuration determined by a canonical distribution $\exp-\{h\omega_0\beta(n+\frac{1}{2})\}$. Their condition at a later time is then given by the propagated value (31).

It must be emphasized that this construction does not

follow in a rigorous way from the theory of influence functionals, but is merely a working hypothesis based on the ideas of influence functional theory.

It is equally important to note that the propagators K are zero temperature propagators. All attempts on our part to generalize these to finite temperatures have been unsuccessful. We now proceed to evaluate $P(Q_2,Q_2',t)$ for an overdamped oscillator $W^2 = \gamma^2 - \omega_o^2$, as follows:

$$P(x,x',t) = \int_{-\infty}^{\infty}\int K(x,t;x,t_1)\, K^*(x',t;x_2,t_1)\, \rho_o(x_1,x_2)\, dt_{t_1}x_1\, d_{t_1}x_2 \tag{32}$$

$$= \left(\frac{mW}{2\pi\hbar \sinh Wt}\right)\left(\frac{m\omega_o}{2\pi\hbar \sinh \omega_o\beta\hbar}\right)^{\frac{1}{2}} \exp\frac{imW}{2\hbar}\left[\left(x^2e^{2\gamma t} - x'^2e^{2\gamma t}\right)\cdot\left(\frac{\cosh Wt}{\sinh Wt} - \frac{\gamma}{W}\right)\right]\cdot \int_{-\infty}^{\infty}\int dx_1\, dx_2 \exp -\left(Ax_1^2 + Bx_2^2 + Cx_1x_2 + Dx_1 + Ex_2\right) \tag{33}$$

where we have set $t_1 = 0$, and

$$A = \frac{m\omega_o \cosh \omega_o\beta\hbar}{2\hbar \sinh \omega_o\beta\hbar} - \frac{mWi \cosh Wt}{2\hbar \sinh Wt} - \frac{m\gamma i}{2\hbar}$$

$$B = \frac{m\omega_o \cosh \omega_o\beta\hbar}{2\hbar \sinh \omega_o\beta\hbar} + \frac{mWi \cosh Wt}{2\hbar \sinh Wt} + \frac{m\gamma i}{2\hbar}$$

$$C = \frac{-m\omega_o}{\hbar \sinh \omega_o\beta\hbar}$$

$$D = \frac{mWi\ xe^{\gamma t}}{\hbar \sinh Wt}$$

$$E = \frac{-mWi\ x' e^{\gamma t}}{\hbar \sinh Wt} .$$

To evaluate the double Gaussian integral, we first complete the squares for each variable in the argument i.e. transform the variables to shifted coordinates so that we have a purely quadratic form. Then the integration follows directly:

$$\int_{-\infty}^{\infty}\int dx_1 dx_2 \exp-(Ax_1^2+Bx_2^2+Cx_1x_2+Dx_1+Ex_2) = \frac{2\pi}{\sqrt{\Delta}} \exp -\frac{1}{\Delta}(CDE-AE^2-BD^2) \quad (34)$$

where

$$\Delta = 4AB-C^2 = \frac{m^2}{\hbar^2}\left[\omega_0^2 + W^2\left(\frac{\cosh Wt}{\sinh Wt}+\frac{\gamma}{W}\right)^2\right].$$

Then

$$\rho(x,x';t) = \left(\frac{mW}{2\pi\hbar \sinh Wt}\right)\left(\frac{m\omega_0}{2\pi\hbar \sinh \omega_0\beta\hbar}\right)^{\frac{1}{2}} \frac{2\pi}{\sqrt{\Delta}} \cdot$$

$$\cdot \exp -\frac{mW^2\omega_0 e^{2\gamma t}}{2\hbar\,\square \sinh\omega_0\beta\hbar \sinh Wt}\left\{\cosh(\omega_0\beta\hbar)\left[x^2+x'^2\right]-2xx'\right\} \cdot$$

$$\cdot \exp \frac{imWe^{2\gamma t}}{2\hbar}(x^2-x'^2)\left\{\left(\frac{\cosh Wt}{\sinh Wt}-\frac{\gamma}{W}\right)-\frac{W^2}{\square \sinh^2 Wt}\left(\frac{\cosh Wt}{\sinh Wt}+\frac{\gamma}{W}\right)\right\}, \quad (35)$$

with

$$\square = \frac{\hbar^2\Delta}{m^2} .$$

The trace of equation (35),

$$\mathcal{Z} = \int_{-\infty}^{\infty} d_L x \; P(x,x,t)$$

can be immediately calculated and is equal to that of a system of harmonic oscillators

$$\mathcal{Z} = \frac{1}{2 \sinh \omega_0 \beta\hbar/2} \quad . \tag{36}$$

Now allowing $\gamma \to 0$ in (35) reduces $P(x,x',t)$ to the exact density matrix of a SHO. Furthermore as $\omega_0 \to 0$ we find the equivalent function $P(x,x',t)$ for the LDP as we shall verify from first principles below. In addition, as pointed out earlier, the temperature and time remain uncorrelated, and the extra factor ($\square \sinh^2 Wt$) will be found to cancel exactly in the calculation of the observables.

The calculation of the information-theory entropy follows exactly as before, with the imaginary exponent cancelling out because of the asymmetry in x and x'. However, the value obtained here is that of an SHO with frequency ω_0, rather then the value W found earlier. This entropy is completely independent of the strength of damping.

We now calculate $\frac{m\omega_0^2}{2}\langle x^2\rangle$ and $\langle \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\rangle$, and after some tedious manipulation we find for the classical limit (taken for later convenience):

$$\frac{m\omega_0^2}{2}\langle x^2\rangle = \frac{k_B T e^{-2\gamma t}}{2}\left[\frac{\gamma}{W}\sinh 2Wt + \frac{\gamma^2}{W^2}\cosh 2Wt - \frac{\omega_0^2}{W^2}\right] \tag{37a}$$

and

$$-\frac{\hbar^2}{2m}\left\langle\frac{\partial^2}{\partial x^2}\right\rangle = \frac{k_B T e^{-2\gamma t}}{2}\left[\frac{-\gamma}{W}\sinh Wt + \frac{2\gamma^2}{W^2}\sinh^2 Wt + 1\right]. \tag{37b}$$

Taking the classical limit only alters the temperature-dependent factor in front of the square brackets. The general expression valid in the quantum regime has $kT = \frac{1}{\beta}$ replaced by $\coth\frac{\hbar\omega_0\beta}{2}$, with the same time evolution as above.

Both (37a) and (37b) hold for underdamped and critically damped motion where the relevant solution to the equation of motion is merely substituted.

We intimated earlier that there should be some connection between the above results and the theory of Brownian Motion. Chandrasekhar (1943) studied the classical Brownian Motion of a particle in a harmonic oscillator using a method which is essentially that of path integration.

Assuming that the random forces f(t) in the pertinent Langevin equation

$$m\ddot{x} + \lambda\dot{x} + kx = f(t) \tag{38}$$

have a Gaussian probability and are uncorrelated with one another at different times, and that the probability distributions tend to a Maxwell-Boltzmann distribution at the temperature T as $t \to \infty$, Chandrasekhar shows that a particle starting from x_0 at time zero with velocity u_0 is characterized at time t by

$$\langle x^2\rangle = \frac{k_B T}{m\omega_0^2}\left\{1 - e^{-2\gamma t}\left(\frac{\gamma}{W}\sinh 2Wt + \frac{\gamma^2}{W^2}\cosh 2Wt - \frac{\omega_0^2}{W^2}\right)\right\} + \langle x\rangle^2$$

(39)

$$\langle u^2\rangle = \frac{k_B T}{m}\left\{1 - e^{-2\gamma t}\left(\frac{\gamma}{W}\sinh 2Wt + \frac{2\gamma^2}{W^2}\sinh^2 Wt + 1\right)\right\} + \langle u\rangle^2 .$$

Our classical limit expressions (37) bear very close resemblance to these equations except for the presence of the equipartition terms and averages $\langle x\rangle^2$ and $\langle u\rangle^2$ which vanish in our case. However, as $t \to \infty$, equations (39) tend to the equipartition values, whereas ours do not. This is not surprising, since our formalism does not contain the random forces which are necessary to establish thermal equilibrium. In fact once we release our system at $t = t_1$, it moves in such a way that the motion gradually shrinks away, never actually reaching equilibrium.

What is surprising, is that notwithstanding our having commenced with dissimilar initial conditions viz. a canonical distribution in our case and a delta function in Chandrasekhar's, we have found essentially the same time evolution (apart from the sign). This is in part a consequence of the Langevin Ansatz, viz. that a splitting of systematic and random forces is permissible. On the other hand, the detailed evolution probably results from the stochastic aspect of functional integrals (Gel'fand and Yaglom, 1960) in that $K(x,t;x_1,t_1)$ is an integration over a Wiener process, and the solution of the Langevin equation is also such a Wiener process. In the limit $t \to \infty$, our density matrix tends to

a delta function located at the origin (c.f. comments in §2.4). Curiously we have as large time limit the Chandrasekhar starting condition, and correspondingly for the initial condition and Chandrasekhar's long time limit. In our case the energy of the particle decreases from the equipartition value, whereas in the other it increases to this value. For completeness we note

$$\langle E \rangle = e^{-2\delta t} k_B T \left\{ \frac{2\delta^2}{W^2} \sinh^2 Wt + I \right\}. \tag{40}$$

The above results for the DHO are entirely new.

The long time behavior of the density matrix found by analytic continuation viz. equation (17) is the same as above, tending to a delta function. Although the discussion in §4.6 applies to this matrix, also, we are mainly interested in the physics of the matrix (35), since it gives observables which show good agreement with the accepted theory of Brownian motion.

4.5 Density Matrix for the L.D.P.

Our discussion of the statistical mechanics has thus far mainly concentrated on the DHO. However the propagator method can be easily extended to the LDP. Instead of an initial distribution of undamped oscillators, we commence with an initial distribution of free particles at finite temperature and described by equation (4) at time t = o.

(This result can be obtained by allowing $\omega_o \to 0$ in the SHO matrix.) As before we need to evaluate a double Gaussian integral

$$P(x,x';t) = \left[\frac{\lambda}{(1-e^{-\lambda t/m})2\pi\hbar}\right]\{e^{-2\gamma t}\}\left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{1}{2}}\int_{-\infty}^{\infty}\int dx_1 dx_2 \cdot$$

$$\cdot \exp\frac{-i\lambda}{(1-e^{-\lambda t/m})}\left\{(x'-x_2)^2-(x-x_1)^2\right\}\exp\frac{-m}{2\hbar^2\beta}\{x_1-x_2\}^2 , \qquad (41)$$

where $\{e^{-\gamma t}\}$ is included if a metric interpretation is used.

As before we have

$$A = \frac{m}{2\hbar^2\beta} - \frac{i\lambda}{2\hbar(1-e^{-\lambda/m t})} = B^*$$

$$C = \frac{-m}{\hbar^2\beta}$$

$$D = \frac{i\lambda x'}{\hbar(1-e^{-\lambda/m t})}$$

$$E = \frac{-i\lambda x'}{\hbar(1-e^{-\lambda/m t})}$$

and $\Delta = \left(\frac{\lambda}{(1-e^{-\lambda/m t})\hbar}\right)^2$

then

$$P(x,x';t) = \{e^{-\gamma t}\}\left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{1}{2}}\exp\frac{-m}{2\hbar^2\beta}(x-x')^2. \qquad (42)$$

Equation (42) is also obtainable directly from equation (35) in the limit $\omega_o \to 0$.

The trace $\mathcal{Z}$ is simply

$$\mathcal{Z} = L \left(\frac{m}{2\pi\hbar^2\beta}\right)^{\frac{1}{2}} \tag{43}$$

where we use box normalization, side L, and (43) holds both with and without the metric idea. Apart from the irrelevant $e^{-\gamma t}$, (42) has the form of a free particle density matrix. The entropy is obviously then equal to the equilibrium value and is constant.

From §1.3 we have

$$\hat{H}_{LDP} = e^{-\lambda t/m} \frac{p^2}{2m} . \tag{44}$$

To find the average of this quantity, we need to find the average of $-\frac{\hbar^2}{2m} \langle \partial^2/\partial x^2 \rangle$. We find

$$\langle \hat{H} \rangle = e^{-\lambda t/m} \frac{k_B T}{2} , \tag{45}$$

and as $t \to \infty$, $\langle \hat{H} \rangle \to 0$ as in the DHO case. This agrees with the result in the quantum mechanics, $\frac{k_B T}{2}$ being the average energy of a thermalized free particle. From equations (42) and (15) we can again calculate the entropy, but as previously the result will be time-independent. In this case we find the free particle value both with and without the metric.

4.6 Entropy

It is clear that so far we have not found a satisfactory way of calculating the entropy for our irreversible system, since the entropy calculated for the density matrix, equation (35), is constant for all times, even though we have seen that this matrix contains sufficient detail to reproduce some of the features of the evolution in time of the Brownian motion, a process which is clearly irreversible.

In the calculation of the entropy we were always able to eliminate the time dependence of the integrand by making the transformation $x\exp(\gamma t) \rightarrow Z$. On the other hand, for a dissipating system such as ours we do not expect ensemble averages to show no time-dependence. In particular we are interested in the long time behavior of the density matrix given by equation (35).

We found earlier that the classical phase-space trajectory collapses into the origin, and that the quantum wave functions show a corresponding behavior in that

$$\lim_{t\to\infty} |\psi_n(x,t)|^2 \longrightarrow \delta(x).$$

In both these régimes there is a greater localization in space as time becomes indefinitely large.

Now consider the non-metrical* density matrix given by equation (35) with the additional pre-exponential factor $\exp(\gamma t)$. In an obvious notation, we can rewrite this

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* See footnote p. 40.

expression as

$$P(x,x';t) = \sqrt{\frac{L}{\pi}}\, exp - \left(L \cosh \omega_0 \beta\hbar \{x^2+x'^2\} - 2Lxy\right) \cdot$$

$$exp\, iM\{(x^2-x'^2)\} \cdot \tag{46}$$

L is a function of β and t; M is a function of t only. For the overdamped case it is obvious that as $t \to \infty$, $L \sim \exp 2(\gamma-W)t$ and $M \sim \exp(2\gamma t)$. Furthermore, the first exponent is a positive definite quadratic. It is easy to transform the coordinates (x,x') to values y,y') in which this quadratic assumes the diagonal form:

$$x = \frac{1}{\sqrt{2}}(y+y'), \quad x' = \frac{1}{\sqrt{2}}(y-y'). \tag{47}$$

Then under this rotation,

$$P(y,y';t) = \sqrt{\frac{L}{\pi}}\, exp - \{Ly^2(\cosh \omega_0 \beta\hbar - 1) + Ly'^2(\cosh \omega_0 \beta\hbar - 1)\} \cdot$$

$$exp\, 2iM\, yy' \cdot \tag{48}$$

Now since the limit of a product is equal to the product of the limits, we have as $t \to \infty$, $(L \to \infty)$,

$$P(x,x';t) = \delta(y)\,\delta(y') \lim_{t\to\infty} e^{2iMyy'} = \delta(x)\,\delta(x-x'). \tag{49}$$

Our infinite continuous matrix has only one entry, located at the origin, and it has infinite magnitude. This

agrees with the findings for the classical and quantal cases above. The same conclusion can be reached for the density matrix (17) obtained by analytic continuation. We see that in the limit $t \to \infty$, the transformation $x \exp(\gamma t) \to Z$ is not well defined for the density matrix. The mapping of the point at infinity is not unique.

Equation (35) refers to the overdamped case, but the argument above is applicable even to the underdamped case. There the value of M still goes as $\exp(2\gamma t)$ for all times, even at the zeros of the sine function. Furthermore the longtime behavior of $\frac{W'^2}{\sin^2 W't}$ □ is well-behaved, and the expression for M always has the same sign. We therefore have similar behavior to the above case, viz. collapse into the origin.

The same is true for the critically damped oscillator - we set $W = 0$ in equation (35), and will find identical behavior to that above.

Z, the trace of the density matrix is in the limit equal in value to the single entry of the matrix. We therefore have

$$\lim_{t \to \infty} P(x=0, x'=0; t) = 1.$$

The entropy is given by

$$S = -k_B 1 . \ln 1 = 0.$$

As necessary, the pure state reached as $t \to \infty$ has zero entropy. The entropy would thus appear to have decreased from the equilibrium value to zero. Unfortunately we

still do not have the behavior between these two cases.

To have a decreasing entropy associated with energy losses is not so strange however, since we are not asserting that the entropy consisting of that due to the oscillators + that of the reservoir defining the temperature is decreasing.* All that the above argument means is that when a particle is localized our information concerning it is the highest possible so that the entropy must be zero.

Unfortunately we cannot turn to the elementary concept of entropy as used by Clausius to explain the above, since the Clausius definition of entropy does not strictly apply during irreversible processes (Meixner, 1969), but rather makes a statement on the change of entropy between two equilibrium states A and B, where the changes $A \rightleftarrows B$ may or may not be reversible. Our initial state (with frequency ω_o, not W) is an equilibrium one by hypothesis, but the final state is approached only asymptotically and we therefore do not believe the Clausius statement is applicable. In

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* We wish to briefly discuss an alternative way of describing irreversible processes due to Cox (1955). In this approach the initial canonical distribution is perturbed not only by a systematic viscous force, but also by a time dependent contribution to the temperature. The Master equation is then set up and solved, and the entropy calculated from the information theory definition, and is found to be time dependent only if the temperature is allowed to vary in time. However even in this orthodox theory there are difficulties of interpretation. It appears that the entropy so calculated does not refer specifically to the damping system, but is in some way (Cox ibid, p. 37) a measure of the entropy of the system + environment. This environment is distinct from the heat bath, and is in addition in some unknown way responsible for the time variation of the reservoir temperature.

any event, even if it were applicable, the best we would obtain from it would be an inequality, which is of little use here.

What of the LDP? In essence the LDP motion and that of a critically damped DHO are the same, both motions being characterized solely by γ. However, from the LDP density matrix we cannot find the behavior of collapse into a pure state. The reason for this lies in the chosen initial conditions, and the way in which these determine the detailed mathematics through the action functional whose form depends critically on the initial conditions. The critically damped oscillator was set up with $x = x_o e^{-\lambda/m t}$: thus an ensemble of oscillators with different values x_o all have the same value of zero at large times. On the other hand we set up the LDP with $x - x_o = \frac{P_o}{m}(1-e^{-\lambda t/m})$, and for various x_o, P_o, these solutions tend to diverse values as $t \to \infty$.

4.7 General Conclusions

The above comments on the entropy associated with our simple model of dissipation conclude this thesis. We have shown in the statistical mechanics how a suitable Ansatz is made whereby we obtain a density matrix by the propagation of the initial conditions with a frictional propagator. This Ansatz has reasonable success in that contact can be made with the well established theory of Brownian Motion. The differences between the predictions based on this density

matrix and those of the Brownian motion are essentially due to the absence of explicit random forces in our theory, while the similar dynamical evolution arises from the similarity between the Brownian motion and path integration, which are both Wiener processes.

The entropy calculated directly by ensemble averaging is always constant in time when the transformation to co-moving coordinates is valid. However for long times when this transformation cannot be made, we find a different result to the ensemble average. We find a decrease in the entropy, which can be understood in the sense that our oscillators become more and more localized as time advances. The same conclusion can be drawn from the results of both the classical and quantum calculations.

We have laid out a complete description of the simple dissipation introduced by the inclusion of the exponential integrating factor in the simplest two Lagrangians, that of the free particle, and that of the harmonically bound particle. This quadratic Lagrangian approach is the simplest choice when one does not wish to attribute any fine detail to the bath. Having found the Lagrangian, one can discuss the quantum mechanics either via the action (Feynman path integration) or by solving the relevant Schrödinger equation (Hamiltonian method).

In the classical and quantal descriptions, the introduction of the notions of tensor calculus effected by the identification $g_{ij} = \delta_{ij} \exp(\frac{\lambda}{m}t)$, has no physical effect, but from a logical standpoint has proved quite useful.

Firstly we are able to discuss the canonical momentum without the embarassing time dependence, and secondly we only deal with real eigenvalues in the quantum case (the transformed Schrödinger equation has real eigenvalues). The one-to-one correspondence between DHO and SHO therefore involves a comparison of real frequencies, which is a desirable property. Thirdly our proposals for modifying the Miller Ansatz are reasonable and in agreement with an obvious generalization of the standard many-body Green's function to yield a density matrix at given time and temperature. At the very least, we note that the mathematical modifications necessitated by such an identification have been made in a self-consistent fashion.

No relation has been found between the entropy and the action: in the simple theory above, the entropy is time independent, whereas the action depends not only on the time difference but also on the starting time. Furthermore we do not have a completely satisfactory way of defining $\langle E \rangle$, $\hat{\rho}$ and S. There would seem to be no unambiguous way of analytically continuing the damped propagators to finite temperatures in the way that standard quantum many-body theory proceeds. The Feynman propagators are those of the full wave function, and not as in many-body theory those of a single excitation. As it is, we must stress that the entropy we have calculated refers to a subsystem, and not to the whole system of bath and particle.

Various applications of this Lagrangian approach to

damping are to be found in the literature. An application to tuned circuits is found in Stevens (1961); Papadopoulos (1973), on the other hand, concentrates on studying Brownian motion on a quantum level. Buch and Denman (1974) have used the LDP Hamiltonian to find the quantum mechanical electrical conductivity under an applied electric field.

APPENDIX 1

Calculation of the Normalization in Curved Spaces with $g_{ij} = g_{ij}(t)$

In this calculation we closely follow the method adopted by Feynman and Hibbs (1965). One can write any wavefunction as a superposition of earlier wavefunctions using the propagator as the kernel for such a summation i.e.

$$\psi(x',t') = \int_{-\infty}^{\infty} K(x',t';x,t)\,\psi(x,t)\,d_t x, \qquad (1)$$

where we integrate over the invariant volume element (one dimension) and x',x are taken as contravariant quantities. When t',t are very close together, the kernel reduces to

$$K(x',t';x,t) = \frac{1}{A}\exp\frac{i\epsilon}{\hbar}\mathcal{L}\left(\frac{x'-x}{\epsilon}, \frac{x'+x}{2}, \frac{2t+\epsilon}{2}\right). \qquad (2)$$

For the DHO the above Lagrangian is written as

$$\mathcal{L}(\dot{x},x;t) = e^{\frac{\lambda}{m}\left(\frac{2t+\epsilon}{2}\right)}\left\{\frac{1}{2}m\left(\frac{x'-x}{\epsilon}\right)^2 - \frac{1}{2}k\left(\frac{x'+x}{2}\right)^2\right\}. \qquad (3)$$

Now we write x' = x + η, expand (1) in ϵ, and by a stationary phase argument for η, obtain

$$\psi(x,t) = \frac{1}{A}\left(\frac{2\pi i\hbar\epsilon}{m}e^{-\lambda t/m}\right)^{\frac{1}{2}}\psi(x,t)\,e^{\lambda t/2m}.$$

The metric factors cancel, and in order for the equation to be the identity as $\epsilon \to 0$, we require

$$A = \left(\frac{2\pi i\hbar\epsilon}{m}\right)^{\frac{1}{2}}, \tag{4}$$

as is found in the case $g_{ij} = \delta_{ij}$, where the Lagrangian kinetic energy has a constant coefficient. The result for A above is general to <u>any</u> $g_{ij}(t)$.

APPENDIX 2

We have to calculate the integrals

$$I = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \, \langle x|\hat{\rho}|x'\rangle\langle x'|\hat{\rho}^m|x\rangle . \qquad (1)$$

There are two ways of doing this. The first based on work of Kac is due to Edwards and Lenard (1962).

Method of Edwards and Lenard

We can write out I as the following multiple integral by inserting complete sets of states.

$$\langle x'|\hat{\rho}^m|x\rangle = \int_{-\infty}^{\infty}\cdots\int dx_1 \cdots dx_{m-1}\, \rho(x',x_1)\rho(x_1,x_2)\cdots\rho(x_{m-1},x) . \qquad (2)$$

Now the right-hand side can be interpreted by means of the closure relation equation (2), §3.1, as being the density matrix $\rho(x',x;m\beta)$, since the "time" interval in each density matrix above is β.

Thus we have

$$\langle x'|\rho^m|x\rangle = \rho(x', x; m\beta) . \qquad (3)$$

The remaining integral is then carried out and the two sums evaluated.

Alternatively, if the above procedure were unknown, the Gaussian form of the SHO density matrix (indeed of any system whose action is a quadratic) can be utilized as follows:

$\langle x'|\rho^m|x\rangle$ is written out again, and use made of the general gaussian integral (c.f. §3.3).

Then

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \langle x|\hat{\rho}|x'\rangle\langle x'|\hat{\rho}^{m-1}|x\rangle = \frac{C^m(\pi)^{m/2}}{(\det A_{ik})^{1/2}} \qquad (4)$$

where $\rho(x';x) = C\exp-(\alpha x'^2 + \alpha x^2 - 2\beta x x')$

and A_{ik} are the elements of the mxm matrix $\underline{A}$

$$\underline{A} = \begin{pmatrix} 2\alpha & -\beta & & & -\beta \\ -\beta & 2\alpha & & & \\ & & \ddots & & \\ & & & 2\alpha & -\beta \\ -\beta & & & -\beta & 2\alpha \end{pmatrix}$$

A similar determinant arises in the study of chains of particles having only nearest neighbour interactions. To evaluate the determinant we require its eigenvalues. These are (Feynman, e.a. 1965)

$$E_n = 2\alpha - 2\beta\cos\frac{2n\pi}{m}$$

so that

$$\det A_{ik} = \prod_{n=0}^{m-1} 2\alpha - 2\beta \cos \frac{2n\pi}{m} .$$

Now inserting the values of α and β we find

$$\det A_{ik} = \left(\frac{2mw_o}{2\hbar \sinh w_o \beta \hbar}\right)^m \prod_{n=0}^{m-1} \left(\cosh w_o \beta \hbar - \cos \frac{2n\pi}{m}\right) \qquad (5)$$

and using equation 1.395 #2 of Gradshteyn and Rhyzik (1965), we find

$$\det A_{ik} = \left(\frac{mw_o}{\hbar \sinh w_o \beta \hbar}\right)^m \frac{\cosh (mw_o \beta \hbar) - 1}{2^{m-1}} . \qquad (6)$$

The procedure from this point on is the same as that earlier, viz. evaluation of the sums. The result is exactly the same as before.

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