Investigating the Statistical Mechanics of Quantum Mechanical Damped Simple Harmonic Oscillators

by

James Edward Morris

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Contents

Chapter 1

Introduction

Several quantum mechanical phenomena can be described in terms of simple harmonic oscillators modified by the inclusion of linear friction. For example, deep inelastic scattering and field-theoretic formulations of fundamental anyons can be so modelled. It has recently been shown [1] that squeezed light entering quantum optics can be statewise identified up to automorphisms with damped simple harmonic oscillators. An understanding of such oscillators is therefore of use.

The frictionally damped simple harmonic oscillator can be expressed in a Lagrangian formulation only with the addition of a second variable of motion. A suitable Lagrangian is known to be [3]

$$L = m\dot{x}\dot{y} + \frac{R}{2}(x\dot{y} - \dot{x}y) - kxy \tag{1.1}$$

where R characterizes the strength of the friction. Canonical momenta and a Hamiltonian can be obtained in the usual manner and canonical quantization carried out. Feshbach and Tikochinsky have shown [2] that the eigenvalues of the resulting Hamiltonian are

$$H = \hbar\Omega(n_A - n_B) \pm \frac{i\hbar R}{2m}(n_A + n_B + 1) \tag{1.2}$$

where $\Omega^2 \equiv \frac{k}{m} - \frac{R^2}{4m^2}$ and n_A and n_B range over the nonnegative integers. The complexity of the eigenvalues is expected, being characteristic of nonconservative systems, and causes no difficulties in nonstatistical questions.

Problems arise when an attempt is made to model the behavior of an ensemble of these oscillators. A first attempt follows the normal procedure, used for conservative systems (in which the Hamiltonian is equivalent to the energy), to calculate the partition function for a canonical formulation as

$$Z = \Sigma e^{-\beta H} \tag{1.3}$$

where H ranges over the Hamiltonian eigenvalues; such quantities as temperature, internal energy, and entropy are determined from the form of Z.

Two difficulties are immediately apparent. The first is that the real part of the Hamiltonian eigenvalues has no lower bound, as n_A can be held fixed while n_B ranges indefinitely upwards, and so the partition function sum diverges. The second is that even if some cutoff is made, Z is no longer positive definite, since $e^{-\beta H}$ can be negative for complex H (its reality is assured, since the sum includes the complex conjugate of each of its summands).

The problem is, simply, to find some suitable method of applying canonical statistics to such ensembles, and then to reach an understanding of any unusual features in the thus-calculated quantities — for instance, it appears possible that complexity will enter such things as the entropy, possibly indicating some sort of time evolution.

I shall give a set of criteria for a solution. I shall then go over several of the approaches we took, giving motivations and results of each. Finally, I shall present a solution in which the reasons for using Hamiltonian eigenvalues at all are examined and found wanting, motivating the use of energy eigenvalues instead.

Chapter 2

Criteria

An acceptable solution must yield approximately as much information about ensembles of the damped oscillators as normal methods do about ensembles of undamped oscillators. It must allow us to calculate thermodynamic quantities such as temperature, entropy, and energy. However, it is acceptable that it do so only with the aid of approximations.

In the $R = 0$ (no damping) case, a solution must yield the same results as those already known for the undamped situation. Further, we expect that the results for small R be close to these. More generally, the derived quantities should be continuous functions of R.

The latter criterion is only a fragment of a larger one, namely that the derived quantities must make sense. All differences between the damped and undamped cases must be explained. It is especially important that there be plausible physical and mathematical interpretations of any oddities that may appear in such quantities, such as complexity.

Finally, the derivation of the solution must itself be plausibly justifiable on both physical and mathematical grounds.

Chapter 3

Attempts

3.1 Separating the Hamiltonian

3.1.1 Motivation

We observe that the eigenvalues of the Hamiltonian can be rewritten as

$$H = (\hbar\Omega \pm \frac{i\hbar R}{2m})n_A - (\hbar\Omega \mp \frac{i\hbar R}{2m})n_B. \tag{3.1}$$

Since this is linear in n_A and n_B, it suggests that the Hamiltonian may also separate, as $H = H_A - H_B$. An appealing symmetry leads us to define

$$\alpha \equiv \Omega \pm \frac{iR}{2m} \equiv \omega e^{i\theta} \tag{3.2}$$

where

$$\theta \equiv \pm \arctan \frac{R}{2m\Omega} \tag{3.3}$$

so that we may write the decoupled eigenvalues as

$$H_A = \hbar\alpha(n_A + \frac{1}{2}), \qquad H_B = \hbar\alpha^*(n_B + \frac{1}{2}) \tag{3.4}$$

for each sign of θ, so that each looks like the spectrum for an undamped SHO, rotated in the complex plane, and the zero-point energies have appeared. Interpreting the Hamiltonian eigenvalues as the difference of two more normal spectra gives a reason for the lack of a zero-point value; there are two, which cancel.

While this does not logically imply that the Hamiltonian *operator* will separate into two parts, it makes it plausible. We therefore seek a transformation that will yield a Hamiltonian with no explicit coupling term. If we find such a Hamiltonian, we can be sure that we can treat the system as two separate systems.

3.1.2 Attempts

The obvious transformation is $u \equiv \frac{x+y}{\sqrt{2}}, v \equiv \frac{x-y}{\sqrt{2}}$ which suggests itself as a way to decouple the $p_x p_y$ and xy terms. This yields

$$L = \frac{m}{2}(\dot{u}^2 - \dot{v}^2) + \frac{R}{2}(\dot{u}v - u\dot{v}) - \frac{k}{2}(u^2 - v^2), \tag{3.5}$$

$$H = \frac{p_u^2}{2m} - \frac{p_v^2}{2m} + \frac{R}{2m}(up_v - vp_u) + \frac{m\Omega^2 u^2}{2} - \frac{m\Omega^2 v^2}{2} \tag{3.6}$$

which are decoupled for the $R = 0$ case only. In this case the system presents itself as the difference of two SHOs; letting $v \Rightarrow iv$, it becomes a sum. Although it was not expected to achieve separation, we then looked at the further "angular" transform $u = \rho cos\theta, v = \rho sin\theta$. This yields

$$L = \frac{m}{2}\dot{\rho}^2 + \frac{m\dot{\theta}^2 - iR\dot{\theta} - k}{2}\rho^2, \tag{3.7}$$

$$H = \frac{3p_\theta^2}{2m\rho^2} + \frac{p_\rho^2}{2m} + \frac{iRp_\theta}{2m} - \frac{m\Omega^2\rho^2}{2} \tag{3.8}$$

which bear the expected resemblance to the normal angular form of the two-dimensional SHO. While this form allows the separation $\psi(\rho, \theta) = F(\rho)e^{i\lambda\theta}$, the Hamiltonian does not separate into $H_\rho + H_\theta$.

It should be noted that any quantization undertaken after letting $v \Rightarrow iv$ is suspect, as the change in reality of variables necessarily corresponds to a change in which variables are observable and which nonphysical. In particular, the calculation of the eigenvalues of the number operators as the whole numbers depends on the creation and destruction operators being adjoint, so that $< \psi|N|\psi >$ has a positivity requirement; the loss of the reality of x and y destroys this. In fact, if quantization is carried out on the uv system after $v \Rightarrow iv$ (meaning that u and v are real, since they are being quantized, and that therefore x and y are complex and conjugate to each other), the eigenvalues of the number operator taken from x and y become the nonpositive integers. The eigenstates of the Hamiltonian therefore change; what previously formed the eigenstates are now unphysical. This may or may not be damaging, but it shows that care must be taken with such operations.

The form of the Hamiltonian eigenvalue spectrum leaves us still optimistic that separating the Hamiltonian into $H_A - H_B$ is possible. However, we discovered that no point transformation can accomplish this. Consider an arbitrary reversible point transformation $q_+ = q_+(x,y), q_- = q_-(x,y), x = x(q_+,q_-), y = y(q_+,q_-)$. The Lagrangian becomes

$$L = m(\tfrac{\partial x}{\partial q_+}\dot{q_+}+\tfrac{\partial x}{\partial q_-}\dot{q_-})(\tfrac{\partial y}{\partial q_+}\dot{q_+}+\tfrac{\partial y}{\partial q_-}\dot{q_-})+\frac{R}{2}(x(\tfrac{\partial y}{\partial q_+}\dot{q_+}+\tfrac{\partial y}{\partial q_-}\dot{q_-})-y(\tfrac{\partial x}{\partial q_+}\dot{q_+}+\tfrac{\partial x}{\partial q_-}\dot{q_-}))-kxy \tag{3.9}$$

from which we get

$$p_\pm \equiv \frac{\partial L}{\partial q_\pm} = 2m\tfrac{\partial x}{\partial q_\pm}\tfrac{\partial y}{\partial q_\pm}\dot{q_\pm} + \frac{R}{2}(x\tfrac{\partial y}{\partial q_\pm} - y\tfrac{\partial x}{\partial q_\pm}) \tag{3.10}$$

and

$$H = \frac{p_+^2}{4m}\tfrac{\partial q_+}{\partial x}\tfrac{\partial q_+}{\partial y}+\frac{R}{4m}(y\tfrac{\partial q_+}{\partial y}-x\tfrac{\partial q_+}{\partial x})p_+ +\frac{p_-^2}{4m}\tfrac{\partial q_-}{\partial x}\tfrac{\partial q_-}{\partial y}+\frac{R}{4m}(y\tfrac{\partial q_-}{\partial y}-x\tfrac{\partial q_-}{\partial x})p_- +m\Omega^2 xy. \tag{3.11}$$

Necessary and sufficient conditions for H to separate into $H_+ + H_-$ are therefore that $\frac{\partial q_\pm}{\partial x}\frac{\partial q_\pm}{\partial y}$ and $y\frac{\partial q_\pm}{\partial y} - x\frac{\partial q_\pm}{\partial x}$ are functions of $q_\pm$ only (keeping the signs consistent), and that xy be the sum of a function of q_+ only and a function of q_- only. In exact form, these conditions become

$$\frac{\partial y}{\partial q_\pm}\frac{\partial^2 x}{\partial q_+\partial q_-} + \frac{\partial x}{\partial q_\pm}\frac{\partial^2 y}{\partial q_+\partial q_-} = 0, \tag{3.12}$$

$$(x\frac{\partial^2 x}{\partial q_+\partial q_-} - \frac{\partial x}{\partial q_+}\frac{\partial x}{\partial q_-})(\frac{\partial y}{\partial q_\pm})^2 - (y\frac{\partial^2 y}{\partial q_+\partial q_-} - \frac{\partial y}{\partial q_+}\frac{\partial y}{\partial q_-})(\frac{\partial x}{\partial q_\pm})^2 = 0, \tag{3.13}$$

$$y\frac{\partial^2 x}{\partial q_+\partial q_-} + x\frac{\partial^2 y}{\partial q_+\partial q_-} = 0. \tag{3.14}$$

From eq.s 3.12 we see that since $\frac{\partial^2 x}{\partial q_+\partial q_-} = -\frac{\frac{\partial x}{\partial q_\pm}}{\frac{\partial y}{\partial q_\pm}}\frac{\partial^2 y}{\partial q_+\partial q_-}$ for both sign choices, either $\frac{\frac{\partial x}{\partial q_+}}{\frac{\partial y}{\partial q_+}} = \frac{\frac{\partial x}{\partial q_-}}{\frac{\partial y}{\partial q_-}}$ or $\frac{\partial^2 y}{\partial q_+\partial q_-} = \frac{\partial^2 x}{\partial q_+\partial q_-} = 0$. In the latter case eq.s 3.13 become

$$\frac{\partial y}{\partial q_\pm}\frac{\partial y}{\partial q_\mp}(\frac{\partial x}{\partial q_\pm})^2 - \frac{\partial x}{\partial q_\pm}\frac{\partial x}{\partial q_\mp}(\frac{\partial y}{\partial q_\pm})^2 = 0 \tag{3.15}$$

which we can divide through by $\frac{\partial y}{\partial q_\pm}\frac{\partial x}{\partial q_\pm}$ to show that

$$\frac{\partial x}{\partial q_+}\frac{\partial y}{\partial q_-} = \frac{\partial x}{\partial q_-}\frac{\partial y}{\partial q_+}. \tag{3.16}$$

Therefore we see that separation of the Hamiltonian requires that $\frac{\partial x}{\partial q_+}\frac{\partial y}{\partial q_-} = \frac{\partial x}{\partial q_-}\frac{\partial y}{\partial q_+}$. Since $\frac{\partial x}{\partial q_+}\frac{\partial y}{\partial q_-} + \frac{\partial x}{\partial q_-}\frac{\partial y}{\partial q_+}$ is identically zero, this requirement means that $\frac{\partial x}{\partial q_+}\frac{\partial y}{\partial q_-} = \frac{\partial x}{\partial q_-}\frac{\partial y}{\partial q_+} = 0$. This, in turn, means that either $\frac{\partial x}{\partial q_+} = \frac{\partial x}{\partial q_-} = 0$, in which case x is trivial; $\frac{\partial y}{\partial q_-} = \frac{\partial y}{\partial q_+} = 0$, in which case y is trivial; or $\frac{\partial x}{\partial q_\pm} = \frac{\partial y}{\partial q_\pm} = 0$ for one sign, in which case $q_\pm$ drops out of the equations for $x(q_+, q_-), y(q_+, q_-)$. Since any of these would make the transformation $x, y \Rightarrow q_+, q_-$ irreversible, we see that no point transform will achieve separation of the Hamiltonian.

3.2 Recoupling the Hamiltonian

3.2.1 Motivation

As noted above, the form of the Hamiltonian spectrum suggests that it is composed of two coupled parts. If we take this as given, even without explicitly separating the Hamiltonian operator, we may suppose that the minus sign between the parts is indicative only of the form of the coupling and is not important to the statistics of the system. If so, we can recouple the Hamiltonian as $H = H_A + H_B$, yielding values

$$H = \hbar\Omega(n_A + n_B + 1) \pm \frac{i\hbar R}{2m}(n_A - n_B) \tag{3.17}$$

The problem of the immediate divergence of Z is now solved, since $(n_A + n_B + 1)$ *does* have a lower limit, and the unbounded $(n_A - n_B)$ is now safely imaginary.

Continuing to use subsystems A and B, we see that Z is the product of Z_A and Z_B. Further, $Z_A = Z_B^*$ and so $Z = |Z_A|^2$. Reflecting that the variable y is fictitious, we may further suppose that this partition function is too large by a power of two, and therefore use $Z = |Z_A| = |Z_B|$ only. (This change is minor, being equivalent to halving the number of particles in the ensemble, and so not changing any dependencies.) It now appears that the effect of the damping, statistically, is to rotate the undamped spectrum in the complex plane, use the rotated values in the partition function, and then rotate back (not by the same amount) to the real axis. This has a certain intuitive appeal.

3.2.2 Discussion

The first quantity calculated from Z is the internal energy, $E = -\frac{d}{d\beta} lnZ$. We immediately encounter trouble: for certain combinations of the parameters, $E < 0$. Since the real part of the recoupled Hamiltonian is positive for each particle, this seems odd. An explanation is found in the fractional occupation numbers for the states k, $\frac{e^{-\beta H_k}}{Z}$. The problem is immediately apparent; while we have arranged for Z to be convergent, real, and positive, the numerator ranges over the complex plane. For H_k with imaginary parts of appropriate magnitude, the fractional occupation is negative; rarely is it purely real. Most k will have complex occupation numbers.

The meaning of the imaginary part of a complex occupation number could perhaps be sought in a Fourier transformation with time. However, no such option is readily available for the purely negative occupation numbers. This problem was left open-ended; the recoupling idea was found to be useful in several of our other attempts.

3.3 Restricting the Ensemble

3.3.1 Motivation

Because the y dimension is spurious, it seems reasonable to attempt to eliminate it before doing statistics. The possible evolutions in y-space are the time-reverse motions of x-space. In fact, the y variable could be eliminated from the Lagrangian formulation by relying directly on the action principle. Instead of using a monogenic Lagrangian as the integrand, we write x as $x(t)$ and y as $x(-t)$. This, however, does not lend itself to Hamiltonian reformulation. It may indicate that the x and y variables should not be considered as independent as they seem. One possible way to eliminate this dependence, in ensembles, is to require that a particle can be present in a state only if another particle is present in the time-reversed state, that is, the state with the conjugate eigenvalue. As this is simply a restriction on the initial conditions of the system, it is perfectly compatible with the Lagrange variational principle.

3.3.2 Results

With this pairing of particles with their time-reverses requirement, it seems reasonable to use the sums of the eigenvalues of the paired particles in the partition function, since the pairs are now the fundamental unit. The imaginary parts now simply vanish. Up to a few factors of 2, we are left with exactly the statistics of the undamped oscillator except that ω is replaced with Ω. We are now assured that, at least in the underdamped case, all thermodynamic variables will be as accessible and meaningful as in the undamped case. The overdamped and critically damped cases require further analysis, as some quantities take on strange values for the former and diverge for the latter. Our attention is focused on the underdamped case.

A slightly different path to this result takes the time-reverse symmetry as requiring that $n_A = n_B$. If this restriction is performed only after recoupling the Hamiltonian, the eigenvalues become, as above, those of the undamped oscillator with $\omega \Rightarrow \Omega$ with but a single unwanted factor of 2. (The previous restriction is the same as recoupling the Hamiltonian and then requiring that if (n_A, n_B) is present so is (n_B, n_A).)

3.3.3 Discussion

Elegant though this solution may be, it still has several problems. First, no way has been found to mathematically verify the assertions regarding time-reverse linkage with conjugate eigenvalues. Second, it is unclear that the proper weights for pairs of particles in the partition function are the sums of the particles' weights, even should the pairing be accomplished. Third, it is only somewhat physically plausible that the effect of the damping should be, statistically, to make the oscillators act as if they had smaller energy quanta. Further investigation may provide answers to these questions.

During the tail end of the research we encountered the preprint [4] in which the action for the damped SHO is calculated. Of interest to us are the final results of the real and imaginary parts of the action as

$$\mathcal{R}e\mathcal{A}[x, y] = \int_{t_i}^{t_f} dt\mathcal{L}, \tag{3.18}$$

$$\mathcal{L} = \mu\dot{x}\dot{y} - [V(x + \frac{1}{2}y) - V(x - \frac{1}{2}y)] + \frac{1}{2}[xF_y^{ret} + yF_x^{adv}], \tag{3.19}$$

$$\mathcal{I}m\mathcal{A}[x, y] = \frac{1}{2\hbar}\int_{t_i}^{t_f}\int_{t_i}^{t_f} dtdsN(t - s)y(t)y(s) \tag{3.20}$$

([4], eq. 30). In particular, the authors note that "The classical constraint $y = 0$ occurs because nonzero y yields an 'unlikely process' in view of the large imaginary part of the action (in the classical '$\hbar \Rightarrow 0$' limit) implicit in [the above equations]" ([4] p10). While this restriction does not directly obtain in the quantum level, any restriction that *is* imposed on the quantum ensemble must be, when the ensemble is taken to the classical $\hbar \Rightarrow 0$ limit, compatible with this $y = 0$ restriction. This should be kept in mind in any further exploration of this approach.

3.4 Studying Time Evolution

It was thought that knowledge of the exact time evolution of the Heisenberg operators might be useful in inspiring an interpretation of the system.

As stated in [2], the metric of the system must be altered so that time-reverse replaces adjoint in order to achieve normalizability. We therefore have the Schrödinger equations

$$i\hbar\frac{d|\psi(t)>}{dt} = H\psi(t), \qquad i\hbar\frac{d<\psi^T|}{dt} =<\psi^T|H^T \tag{3.21}$$

with which we can derive the Heisenberg equation of motion by examining the expectation value of an operator with no explicit time dependance in the usual fashion.

Having thus justified use of the usual Heisenberg equation of motion, we find the fundamental operators to evolve as

$$\dot{A} = \frac{1}{i\hbar}[A,H] = -i\Omega A + \frac{R}{2m}B^\dagger, \qquad \dot{B} = \frac{1}{i\hbar}[B,H] = i\Omega B + \frac{R}{2m}A^\dagger. \tag{3.22}$$

These coupled equations are easily solved to yield

$$A = (A_0 cosh\frac{Rt}{2m} + B_0^\dagger sinh\frac{Rt}{2m})e^{-i\Omega t}, \qquad B = (B_0 cosh\frac{Rt}{2m} + A_0^\dagger sinh\frac{Rt}{2m})e^{i\Omega t}, \tag{3.23}$$

from which we directly verify that the CCR $[A,B] = 0$ and $[A,A^\dagger] = [B,B^\dagger] = 1$ hold true at all time t. Backtracking to the original creation and destruction operators for x, p_x and y, p_y via the definitions $A = \frac{a+b}{\sqrt{2}}, B = \frac{a-b}{\sqrt{2}}$ yields

$$a = (a_0 cosh\frac{Rt}{2m} + a_0^\dagger sinh\frac{Rt}{2m})cos\Omega t - i(b_0 cosh\frac{Rt}{2m} - b_0^\dagger sinh\frac{Rt}{2m})sin\Omega t, \tag{3.24}$$

$$b = (b_0 cosh\frac{Rt}{2m} - b_0^\dagger sinh\frac{Rt}{2m})cos\Omega t - i(a_0 cosh\frac{Rt}{2m} + a_0^\dagger sinh\frac{Rt}{2m})sin\Omega t \tag{3.25}$$

which we substitute into $a = \frac{1}{\sqrt{2\hbar\Omega}}(\frac{p_x}{\sqrt{m}} - i\sqrt{m}\Omega x)$, $b = \frac{1}{\sqrt{2\hbar\Omega}}(\frac{p_y}{\sqrt{m}} - i\sqrt{m}\Omega y)$ to obtain our final results

$$x(t) = (x(0)cos\Omega t + \frac{1}{m\Omega}p_y(0)sin\Omega t)e^{-\frac{Rt}{2m}} \tag{3.26}$$

$$p_x(t) = (p_x(0)cos\Omega t - m\Omega y(0)sin\Omega t)e^{\frac{Rt}{2m}} \tag{3.27}$$

$$y(t) = (y(0)cos\Omega t + \frac{1}{m\Omega}p_x(0)sin\Omega t)e^{\frac{Rt}{2m}} \tag{3.28}$$

$$p_y(t) = (p_y(0)cos\Omega t - m\Omega x(0)sin\Omega t)e^{-\frac{Rt}{2m}} \tag{3.29}$$

which have reasonable forms given the nature of this system. This information proved useful in subsequent calculations.

3.5 Studying Correlations

The correlation functions were defined as

$$corr(\Theta) = \frac{<\psi|\Theta(0)\Theta(t)|\psi> - <\psi|\Theta(0)|\psi><\psi|\Theta(t)|\psi>}{<\psi|\Theta^2(0)|\psi>} \tag{3.30}$$

where $|\psi>$ is a stationary state, so that for the normal formalism of the undamped simple harmonic oscillator we have the usual

$$corr(p) = cos\omega t + \frac{isin\omega t}{2n+1}. \tag{3.31}$$

Using the equations of motion given above, the correlations become

$$corr(p_x) = e^{\frac{Rt}{2m}}cos\Omega t, \quad corr(p_y) = e^{-\frac{Rt}{2m}}cos\Omega t, \qquad corr(\vec{p}) = 2cosh\frac{Rt}{2m}cos\Omega t. \tag{3.32}$$

The only apparent characteristic of interest of these equations is that while as $R \Rightarrow 0$ they become the real part of the usual undamped correlation, they continue to lack any imaginary part. This is somewhat intriguing, especially since the interpretation of imaginary quantities as Fourier-transformed time evolution would require the complexity to be present only in the damped case rather than only in the undamped case, rather than the reverse.

It is quite possible that the imaginary part is simply an artifact of the Lagrangian form and has no physical significance. It is more likely to be related to the zero-point energy, especially since in the classical limit $n \Rightarrow \infty$ it vanishes; if this is the case then its lack is probably due to the zero-point contributions of the two decoupled systems cancelling in the difference system.

Chapter 4

Solution: Discarding the Hamiltonian

4.1 Motivation

Examination of [2] reveals a small error in terminology: the Hamiltonian is identified with the energy. While this identification is of course valid in most (i.e. conservative) systems, it fails for nonconservative systems such as the damped SHO. In fact, looking more closely, we realize that since the Lagrangian was not derived as $T-V$ but simply as an expression that gives the desired equation of motion, there is no reason to believe the derived Hamiltonian will have anything to do with the energy. Indeed, even for the $R = 0$ case the eigenvalue spectra of the Hamiltonian and the energy differ. Restricting the states to those annihilated by B, as suggested in [2] for recovery of the normal case, the Hamiltonian eigenvalues are $\hbar\omega n$. These lack the zero-point energy even though we have eliminated the B system.

This, in turn, leads to an examination of the role of the Hamiltonian eigenvalues in statistical mechanics. Textbooks on the subject use the terms "Hamiltonian" and "energy" interchangeably, since they are identical for the systems these books are concerned with, leaving doubt as to what aspect of the Hamiltonian makes it relevant. That is, is it that it governs the time evolution, or that it is the energy?

Correct time evolution is given by an infinite number of Hamiltonians. (Everything in this paragraph holds true for corresponding Lagrangians.) To be crude, if H produces correct evolution, so does $H' \equiv c_1 H + c_2, c_1, c_2 \in C$. While the eigenstates of any such Hamiltonian are, of course, the same, the eigenvalues differ. Further, introduction of spurious variables can alter the spectrum even more; for instance, use of the two-variable Hamiltonian removes both the zero-point energy and the lower bound for the undamped SHO. If the partition sum is to use the eigenvalue spectrum of a time-evolution operator, it must be possible to uniquely specify which such operator. Otherwise, two identical systems in equilibrium with each other could be mathematically described with different time-evolution operators, yielding different partition sums, yielding different values of thermodynamic quantities, contradicting the explicitly physical fact of their equilibrium. That is, the math cannot give two physical values. In addition, some Hamiltonians cause the calculations to blow up. To give a simple example, if the Hamiltonian $H_0 \equiv \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}$ for the (undamped) SHO is replaced with $H' \equiv -\frac{p^2}{2m} - \frac{m\omega^2 x^2}{2} = -H_0$, the eigenvalues become $-\hbar\omega(n+\frac{1}{2})$. These values cause the partition sum to diverge. Since H_0 and H' are indistinguishably good time-evolution operators, we have trouble reasoning *a priori* why only the former's eigenvalues should be used in the partition sum.

This leads us to consider use of the energy. For normal (conservative system) thermodynamics, there is no difference. (For that matter, classical thermodynamics *always* speaks of energy, rather than of time evolution.) In these systems, the energy can be seen as specifying one of the time-evolution operators uniquely (i.e. the one that is identical with it). Damped systems such as ours will usually have energy spectra different from all Hamiltonian spectra. Since the energy operator is still uniquely determined, we do not have the multiplicity problem that plagued us earlier. Further, it makes sense physically that states should be weighted by something with physical significance, i.e. the eigenvalues of energy, rather than something with none, i.e. the eigenvalues of time evolution. (The time-evolution *operator* is of course tremendously relevant physically, but its eigenvalues seem useless except when they are energy.)

4.2 Results

What are the results of this proposal? The energy operator is unchanged by the presence of a frictional force and remains $\mathcal{E} = \frac{p_x^2}{2m} + \frac{kx^2}{2}$. Since the CCR $[x, p_x] = i\hbar$ holds, we can (as done in [2]) form the usual creation and destruction operators $a^\dagger, a$ with $[a, a^\dagger] = 1$. This is sufficient to show that the eigenvalues of $\mathcal{E}$ are $\hbar\omega(n + \frac{1}{2})$, as usual.

This means that, when we use the energy values in the partition sum, we get exactly the statistical mechanics of the undamped oscillator. This holds whether the system is underdamped, critically damped, or overdamped. Such a solution certainly makes subsequent math simple; but does it make sense physically?

4.3 Discussion

The use of the partition sum means that we are dealing with a canonical ensemble. Although there are multiple ways to approach the canonical ensemble, to make the identification $\beta = \frac{1}{k_b T}$ and thereby give the math involved physical significance it is always necessary to model the system as coupled to a heat bath. In our case, we may hope that the sink into which the oscillators' energy flows forms the bath, but it does not matter; if and only if there is such a bath, the quantities calculated from the partition function have physical and not merely mathematical meaning. What this is telling us, then, seems to be that the damping is countered by the presence of the heat bath for the oscillators to absorb energy from (or emit it to). They maintain the same equilibrium distribution as undamped oscillators would; the ensemble is continuously losing energy to friction and gaining it back from the bath.

In this context it is important to distinguish between the energy eigenvalues and eigenstates being constant and being stationary. Since $[\mathcal{E}, H] \neq 0$ for nonzero damping, the energy eigenstates will not be stationary. Thus, a ket in one of these states at time t will not have the same energy eigenvalue at time $t + \Delta t$ (it is unlikely to be in an energy eigenstate at all). However, as $\mathcal{E}$ does not explicitly depend on time, its eigenstates and eigenvalues are constant. This means there is no time-dependence difficulty in putting the eigenvalue spectrum into the partition sum. The oscillators (in isolation) make their way through the eigenstates, which themselves are unchanged. With the bath, apparently, the oscillators are continuously restored at $t + dt$ to whatever combination of energy eigenstates they occupied at t. The nonstationary nature of the energy eigenstates would only be a problem if we considered a microcanonical ensemble; in this case time-dependence at all stages of calculation seems unavoidable.

4.4 Confidence

The above logic shows fairly convincingly that time-evolution operator eigenvalues are unfit candidates for the partition sum spectrum, and that energy eigenvalues should be substituted. It is certainly not a proof, however. Several objections have come up and been countered with varying degrees of surety.

First, it is *not* to be thought that the eigenvalues of the above $\mathcal{E}$ can be used for an arbitrarily modified harmonic oscillator system. As noted earlier, it is only because both the potential and the kinetic energy of the damped system are identical with those of the regular system that this can be done. If one were to modify a harmonic oscillator with some potential, the form of the energy would change and the new energy operator would have to be used. It is only elements such as friction that are dropped.

Second, it has been thought that the decaying harmonic oscillator might have the ability to experience canonical statistics even in the absence of an external heat bath due to the presence of both dissipative and regenerative terms. That is, the energy lost in the x dimension is gained in or made up for by that in the y dimension. Essentially, the heat bath is internalized. One of the advantages of restricting the ensemble is that it seems to indicate such an elegant equilibrium mechanism. Since the x and y equations of motion are the same up to the sign of R, whenever $x = y$ and $\dot{x} = \dot{y}$, $dE_x = -dE_y$. If the energy gained each instant in the y motion is immediately transferred to the x motion they can "cancel" each other's frictions and continue to do so forever. The method of using energy eigenvalues in the partition sum does not require that any such thing is the case.

Nonetheless, it is quite possible that it implies that something of the sort is occurring. In fact, if we remove any external heat bath and assert that the system still has canonical thermodynamics we are forcing such a relationship to be present, though only on a larger scale. That is, if *all* the x-motions together lose dE and *all* the y-motions together gain dE then equilibrium can be maintained by multiple transfers whether or not the individual dEs can be paired up. Further, it may be the case that the equilibrium distribution given by the partition sum using energy eigenvalues *does* yield a situation in which x and y motions only occur in pairs, indicating that such a mechanism is quite likely. Insofar as the elegance of the pairing makes its presence probable at all, this is probable; and insofar as it does not, its lack is not a problem.

Thirdly, the use of the heat bath, whether internal or external, to feed energy into the system is by no means exceptional. Any normal thermodynamic system reaches equilibrium via interactions, described by a small Hamiltonian which is always omitted from the system's written Hamiltonian, among the particles and between them and the walls. During this process the bath will either contribute energy to or take energy from the ensemble, generally in large amounts. Further, the bath continues to "push" the ensemble back into equilibrium with energy additions and subtractions as the ensemble continuously fluctuates. The statement that the damped oscillator has a constant equilibrium distribution simply means that the bath is doing this in a more regular fashion than usual, since the ensemble is always "fluctuating" (that is, decaying) in the same direction. There is no reason to doubt that this is a legitimate function of a heat bath.

In conclusion, while this solution is not rigorously proven, it satisfies our criteria and there are no known overriding objections to it.

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