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STEADY STATES OF HARMONIC OSCILLATOR CHAINS AND SHORTCOMINGS OF HARMONIC HEAT BATHS †

Max Tegmark

and

Leehwa Yeh

Department of Physics, University of California,
Berkeley, California 94720
Email: max@physics.berkeley.edu, yehl@csa.lbl.gov

ABSTRACT

We study properties of steady states (states with time-independent density operators) of systems of coupled harmonic oscillators. Formulas are derived showing how adiabatic change of the Hamiltonian transforms one steady state into another. It is shown that for infinite systems, sudden change of the Hamiltonian also tends to produce steady states, after a transition period of oscillations. These naturally arising steady states are compared to the maximum-entropy state (the thermal state) and are seen not to coincide in general. The approach to equilibrium of subsystems consisting of n coupled harmonic oscillators has been widely studied, but only in the simple case where $n = 1$. The power of our results is that they can be applied to more complex subsustems, where $n > 1$. It is shown that the use of coupled harmonic oscillators as heat baths models is fraught with some problems that do not appear in the simple $n = 1$ case. Specifically, the thermal states that are though to be achievable through hard-sphere collisions with heat-bath particles can generally *not* be achieved with harmonic coupling to the heat-bath particles, except approximately when the coupling is weak.

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I. INTRODUCTION

Quantum systems with quadratic Hamiltonians have been studied extensively. One reason for this is that they are just about the only quantum systems whose time evolution can be found analytically. Hence they have provided useful and tractable models in a wide range of fields, including statistical mechanics, quantum optics and solid state physics.

In this paper, we derive some useful formulas for the subset of such systems known as harmonic chains. These may be pictured as a chain of coupled harmonic oscillators where the coupling between any two oscillators depends only on the distance between them. We derive the most general steady states of coupled harmonic oscillators, and then study how adiabatic and sudden changes of the Hamiltonian convert one such steady state into another.

The main motivation for studying harmonic chains has been the pursuit of a dynamical basis for equilibrium statistical mechanics. In short, we frequently assume that the density matrix of a system is $\rho \propto e^{-H/kT}$, *i.e.* the thermal state corresponding to a temperature T, and it would be rather embarrassing if we had no completely solvable heat bath model that explicitly evolved systems into such states. An excellent summary of the early developments is given by Huerta and Robertson (see [1] and references therein). The main idea is to study the time evolution of the mean values and correlations of some small subset of the oscillators, called the *system*, by taking a partial trace over the rest of the oscillators, called the *heat bath*. The goal is to show that the system will exhibit standard thermodynamic features such as Brownian motion and approach to thermal equilibrium.

Numerous models have been developed that show such features, and we will give only a brief overview here. The dynamics of an infinite, one-dimensional chain of oscillators bound only to their nearest neighbors was solved in 1914 by Schrödinger [2]. Klein and Prigogine [3] used these results to show that suitable initial conditions for the heat bath led to equipartition of energy in the system. Hemmer [4] studied the same model in more detail and found that the heat bath could produce Brownian motion of the system. Results for more general quadratic Hamiltonians have since been derived by numerous authors $[5-11]$. An up-to-date overview of the models is given by Ford, Lewis and O'Connell (see [12] and references therein), who summarize six successful models and show that they are all unitarily equivalent. Most of the recent literature on the subject has focused on reduced descriptions of a single oscillator in the chain such as a Langevin or Fokker-Planck equation.

Thus the approach to equilibrium of subsystems consisting of n coupled harmonic oscillators has been widely studied, but only in the special case where $n = 1$. This is rather unfortunate, since as we shall see, some interesting complications can arise when $n > 1$. We will study subsystems consisting of an arbitrary number of oscillators, including the seldom mentioned case where the mean values of the heat bath oscillators are non-zero. We do this using a model involving cyclic matrices, similar to that of [5]. As will be seen below, the great advantage of this model is that subsystems with large n can be treated with the same ease as the $n = 1$ case, since we need not distinguish beetween the system and the heat bath *a priori*.

This paper is organized as follows: In section II, we establish some notation and derive the most general steady state of coupled harmonic oscillators. In section III, we review some useful properties of cyclic matrices. In sections IV, V and VI, we study how adiabatic and sudden changes of the Hamiltonian transform one steady state into another. Finally, in sections VII and VIII we compare these naturally arising steady states with thermal states and discuss some shortcomings of coupled harmonic oscillators as heat bath models. A rigorous convergence proof for the sudden change case is given in Appendix A.

II. THE GENERAL STEADY STATE

In this section, we establish some notation and derive the covariance matrix of the most general time-independent state of coupled harmonic oscillators of equal mass.

As our quantum system, let us take $2N+1$ coupled harmonic oscillators of equal mass, labelled $-N, ..., -1, 0, 1, ..., N$. Denoting a point in the $2(2N+1)$-dimensional phase space by

$$\mathbf{z} = \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix} \tag{1}$$

and the corresponding operators by

$$\hat{\mathbf{z}} = \begin{pmatrix} \hat{\mathbf{q}} \\ \hat{\mathbf{p}} \end{pmatrix}, \tag{2}$$

we can write the Hamiltonian as

$$\hat{H} = \frac{1}{2m}\hat{\mathbf{p}}^T\hat{\mathbf{p}} + \frac{m\omega_0^2}{2}\hat{\mathbf{q}}^T A\hat{\mathbf{q}}, \tag{3}$$

where the time-dependent matrix A is symmetric and positive definite. Throughout this paper, we will use units where $m=\omega_0=1$. The number of oscillators can be either finite or infinite. Let us define the mean vector μ and the covariance matrix C by

$$\begin{cases} \mu & \equiv \langle\hat{\mathbf{z}}\rangle, \\ C & \equiv \begin{pmatrix} \langle\hat{\mathbf{q}}\hat{\mathbf{q}}^T\rangle & \frac{1}{2}\langle\hat{\mathbf{q}}\hat{\mathbf{p}}^T + \hat{\mathbf{p}}\hat{\mathbf{q}}^T\rangle \\ \frac{1}{2}\langle\hat{\mathbf{q}}\hat{\mathbf{p}}^T + \hat{\mathbf{p}}\hat{\mathbf{q}}^T\rangle & \langle\hat{\mathbf{p}}\hat{\mathbf{p}}^T\rangle \end{pmatrix} - \mu\mu^T. \end{cases} \tag{4}$$

(The symmetric ordering is necessary since $\hat{\mathbf{q}}$ and $\hat{\mathbf{p}}$ do not commute.) It is well-known that since $\hat{H}$ is quadratic, the time evolution of μ and C is identical in classical and quantum statistical mechanics and is given by

$$\begin{cases} \mu(t) & = U(t)\mu(0), \\ C(t) & = U(t)C(0)U(t)^T, \end{cases} \tag{5}$$

where the time-evolution matrix is defined by

$$\begin{cases} \frac{d}{dt}U = \begin{pmatrix} 0 & I \\ -A(t) & 0 \end{pmatrix} U, \\ U(0) = I. \end{cases} \tag{6}$$

In the special case where the matrix A is independent of t, this equation can be integrated, yielding †

$$U(t) = \exp\left[\int_0^t \begin{pmatrix} 0 & I \\ -A & 0 \end{pmatrix} d\tau\right] = \begin{pmatrix} \cos A^{1/2}t & A^{-1/2}\sin A^{1/2}t \\ -A^{1/2}\sin A^{1/2}t & \cos A^{1/2}t \end{pmatrix}. \tag{8}$$

† Here and throughout this paper, the action of a function on a symmetric matrix is defined as the corresponding real-valued function acting on its eigenvalues: Since all symmetric matrices A can be diagonalized as

$$A = R\Lambda R^T,$$

where R is orthogonal and $\Lambda = \operatorname{diag}\{d_i\}$ is diagonal and real, we can extend any mapping f on the real line to symmetric matrices by defining

$$f(R\operatorname{diag}\{d_i\}R^T) \equiv R\operatorname{diag}\{f(d_i)\}R^T. \tag{7}$$

It is easy to see that this definition is consistent with power series expansions whenever the latter converge. For example,

$$\cos A^{1/2} = \sum_{n=0}^{\infty}\frac{(-1)^n}{(2n)!}A^n.$$

One useful feature of μ and C is that if the phase-space distribution (the Wigner distribution [13]) is Gaussian, then they determine the state completely. For all the steady states considered below, this will indeed be the case. (Such Gaussian states in quantum optics are often referred to as multimode thermal squeezed coherent states, but we will refer to them as Gaussian for brevity.) For a good review of Wigner distributions, see [14], [15] and references therein.

μ and C are also very useful for studying subsystems, as we will do in sections VII and VIII. Rather than having to take cumbersome partial traces of the density operator, the means and internal correlations of any subsystem can simply be read off as subsets of the entries in μ and C. If the state of the total system is Gaussian, so is the state of the subsystem, which means that the latter is uniquely determined by these subsets.

By a *steady state* of a time-independent Hamiltonian, we mean a state whose density operator (or equivalently its Wigner function) is independent of time. The most general steady state is clearly a statistical mixture of energy eigenstates, *i.e.* a density operator of the form

$$\hat{\rho} = \sum w_n |E_n\rangle\langle E_n|, \tag{9}$$

where $w_n \geq 0$ and $\sum w_n = 1$. In terms of the Wigner function, this becomes

$$W(\mathbf{q},\mathbf{p}) = \sum w_n W_n(\mathbf{q},\mathbf{p}). \tag{10}$$

Since the energy eigenstates W_n are cumbersome products of Laguerre polynomials, this expression does not shed much light on the physical nature of steady states. Fortunately, we can obtain a simple and useful result for their covariance matrices: By differentiating Eq. (5) with respect to t using Eq. (8), it is readily shown that the mean vector and the covariance matrix will remain constant over time if and only if they are of the form

$$\begin{cases} \mu &= 0, \\ C &= \begin{pmatrix} D & 0 \\ 0 & AD \end{pmatrix}, \end{cases} \tag{11}$$

where D is a symmetric, positive definite matrix that commutes with A, and A is independent of time. We will discuss the case $\mu \neq 0$ in Section VIII. Note, however, that a covariance matrix of the above form will remain constant over time regardless of the value of μ.

In section IV, we will see how adiabatic change transforms one such steady state into another. In section V, we will see that these steady states are a form of attractors, in that quite general states tend to converge towards them as $t \to \infty$. In section VI, we will study a one-parameter subset of steady states, the thermal states, and compare them with the states arising for adiabatic and sudden change.

III. CYCLIC MATRICES

In many parts of this paper, we assume that the potential matrix A is *cyclic*, which means that we can write $A_{ij} = a_{|i-j|}$ and interpret the system as a chain of harmonic oscillators where the coupling between any two oscillators depends only on the separation between them. For finite N, we will for computational simplicity identify $N+i$ with $-N-1+i$ and picture a ring of oscillators rather than an array with two ends (thus $A_{ij} = A_{kl}$ if $i-j = k-l \mod (2N+1)$). Using (7), we can write any function of a (cyclic or non-cyclic) matrix A as

$$f(A)_{mn} = \sum_{k=-N}^{N} R_{mk} R_{nk} f(\lambda_k^2). \tag{12}$$

Cyclic matrices have the great advantage that they all commute. This is because they can all be diagonalized by the same matrix R, an orthogonal version of the discrete Fourier matrix. Physically, this means that plane waves form a complete set of solutions. Ford, Kac and Mazur [5] (hereafter referred to as FKM) show that if A is symmetric, positive-definite, cyclic and infinite-dimensional, then Eq. (12) reduces to

$$f(A)_{mn} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta f\left[\lambda^2(\theta)\right] \cos(m-n)\theta, \tag{13}$$

where the spectral function $\lambda^2(\theta)$ is the function whose Fourier coefficients are row zero of A. The spectral function can be interpreted as a dispersion relationship, λ being the frequency of a wave with wave number θ. Note that $f(A)$ is cyclic as well, *i.e.* its components depend only on the distance to the diagonal.

A cyclic potential frequently discussed in the literature is the *nearest neighbor potential*, the case where each mass is coupled only to a fixed spring and to its nearest neighbor:

$$\hat{H} = \sum_{k=-N}^{N} \left[\frac{1}{2}\hat{p}_k^2 + \frac{1}{2}\hat{q}_k^2 + \frac{\gamma^2}{2}\left(\hat{q}_{i+1} - \hat{q}_i\right)^2\right], \tag{14}$$

i.e. $A_{kk} = 1 + 2\gamma^2$, $A_{k,k\pm 1} = -\gamma^2$ and all other elements of A vanish. For this special case, the spectral function is

$$\lambda^2(\theta) = 1 + 4\gamma^2 \sin^2 \frac{\theta}{2}. \tag{15}$$

IV. ADIABATIC CHANGE

In this section we will study the time evolution of C during an adiabatic change of the Hamiltonian of a steady state.

For generic time-dependent cyclic Hamiltonians, the time-evolution operator $U(t)$ depends on the entire history $A(\tau)$, $0 \leq \tau \leq t$, according to Eq. (6). For the case where A changes extremely slowly relative to the eigenfrequencies, this simplifies so that $U(t)$ depends only on the values of A at $\tau = 0$ and $\tau = t$, and is independent of A at intermediate times. According to a well-known result, the time evolution of a single harmonic oscillator ($N = 0$) where the frequency ω changes adiabatically is given by [16]

$$U(t) = \begin{pmatrix} \omega(t)^{-1/2} & 0 \\ 0 & \omega(t)^{1/2} \end{pmatrix} \begin{pmatrix} \cos\theta(t) & \sin\theta(t) \\ -\sin\theta(t) & \cos\theta(t) \end{pmatrix} \begin{pmatrix} \omega(0)^{1/2} & 0 \\ 0 & \omega(0)^{-1/2} \end{pmatrix}, \tag{16}$$

where

$$\theta(t) \equiv \int_0^t \omega(\tau) d\tau. \tag{17}$$

We are interested in the case of arbitrary N. Since we are assuming that the matrices $A(t)$ are cyclic for all t, they can all be diagonalized by the same time-independent matrix R,

$$A(t) = R^T \operatorname{diag}\{\omega_i(t)^2\} R,$$

where the eigenfrequencies ω_i also change adiabatically. Hence we can apply (16) to each mode separately, which after employing (7) yields

$$U(t) = \begin{pmatrix} A(t)^{-1/4} & 0 \\ 0 & A(t)^{1/4} \end{pmatrix} \begin{pmatrix} \cos\Theta(t) & \sin\Theta(t) \\ -\sin\Theta(t) & \cos\Theta(t) \end{pmatrix} \begin{pmatrix} A(0)^{1/4} & 0 \\ 0 & A(0)^{-1/4} \end{pmatrix}, \tag{18}$$

where

$$\Theta(t) \equiv \int_0^t A(\tau)^{1/2} d\tau. \tag{19}$$

If our system is in a cyclic steady state initially, *i.e.* if $C(0)$ is cyclic, then $D(0)$ is cyclic and commutes with all the above matrices, so substituting (18) into (5) yields

$$C(t) = \begin{pmatrix} D(t) & 0 \\ 0 & A(t)D(t) \end{pmatrix}, \tag{20}$$

where

$$D(t) = \left[A(0)A(t)^{-1}\right]^{1/2} D(0). \tag{21}$$

Note that the quantity $A(t)D(t)^2$ is an *adiabatic invariant*, *i.e.* stays constant over time. We see that adiabatic change forms an Abelian transformation group on the set of all steady states, and that any given steady state can be transformed into exactly those steady states that have the same adiabatic invariant.

V. SUDDEN CHANGE FOR INFINITE SYSTEMS

In this section we will study the time evolution of C after a sudden change in the Hamiltonian of a steady state. We will mainly be interested in the following question: Does $C(t)$ keep oscillating forever, or does the state converge towards a new steady state as $t \to \infty$?

If the system is in a steady state

$$C(t) = \begin{pmatrix} D_0 & 0 \\ 0 & A_0 D_0 \end{pmatrix} \tag{22}$$

for $t < 0$ and the potential matrix in the Hamiltonian (3) changes abruptly from A_0 to a new constant value A at $t = 0$, then the time evolution for $t > 0$ will be given by (5) and (8). Let us temporarily choose the simple initial conditions $A_0 = D_0 = I$, and return to the general case later. For this choice, $C(0) = I$, so that Eq. (5) gives $C(t) = U(t)U(t)^T$, *i.e.*

$$C(t) = \begin{pmatrix} \cos^2\left[A^{1/2}t\right] + A^{-1}\sin^2\left[A^{1/2}t\right] & \left[A^{-1/2} - A^{1/2}\right]\sin\left[A^{1/2}t\right]\cos\left[A^{1/2}t\right] \\ \left[A^{-1/2} - A^{1/2}\right]\sin\left[A^{1/2}t\right]\cos\left[A^{1/2}t\right] & \cos^2\left[A^{1/2}t\right] + A\sin^2\left[A^{1/2}t\right] \end{pmatrix}. \tag{23}$$

We can separate this $C(t)$ into a time-independent part and an oscillating part with zero time average by writing $C(t) = C_1 + C_2(t)$, where

$$\begin{cases} C_1 & = \frac{1}{2}\begin{pmatrix} I + A^{-1} & 0 \\ 0 & I + A \end{pmatrix}, \\ C_2(t) & = \frac{1}{2}\begin{pmatrix} \left[I - A^{-1}\right]\cos\left[2A^{1/2}t\right] & \left[A^{-1/2} - A^{1/2}\right]\sin\left[2A^{1/2}t\right] \\ \left[A^{-1/2} - A^{1/2}\right]\sin\left[2A^{1/2}t\right] & \left[I - A\right]\cos\left[2A^{1/2}t\right] \end{pmatrix}. \end{cases} \tag{24}$$

In Appendix A, we show that for a generic cyclic infinite-dimensional symmetric positive definite matrix A, $C_2(t) \to 0$ as $t \to \infty$, so that $C(t)$ roughly speaking evolves as follows:

$$\begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \to \begin{pmatrix} \text{Time}-\text{dep.} \\ \text{mess} \end{pmatrix} \to \begin{pmatrix} \frac{1+A^{-1}}{2} & 0 \\ 0 & \frac{1+A}{2} \end{pmatrix} \quad \text{as } t \to \infty. \tag{25}$$

These results are readily generalized to arbitrary cyclic initial conditions at $t = 0$:

$$\begin{pmatrix} X & Z \\ Z & Y \end{pmatrix} \to \begin{pmatrix} D & 0 \\ 0 & AD \end{pmatrix} \quad \text{as } t \to \infty, \tag{26}$$

where

$$D = \frac{1}{2}\left[X + A^{-1}Y\right]. \tag{27}$$

If the initial state is the steady state (22), this reduces to

$$D = \frac{1}{2}\left[I + A_0 A^{-1}\right] D_0. \tag{28}$$

The fact that all matrices are cyclic is crucial, since it means that they can all be simultaneously diagonalized and hence all commute.

Note that whereas adiabatic change formed a transformation group on the set of steady states, sudden change (and subsequently waiting until the oscillations have died down) does not. The steady state reached through a sequence of two sudden changes, one after the other, can in general not be achieved with a single sudden change. This is obvious from the fact that no more than half of the energy can be lost in single sudden change.

A second difference from the adiabatic case is that sudden changes in general have no inverse, *i.e.* cannot be undone. If the potential is suddenly changed from A_0 to A and then, after the oscillations have died down, back to A_0, the net result is

$$D \mapsto \frac{1}{4}\left[2I + A_0^{-1}A + A_0 A^{-1}\right] D. \tag{29}$$

This steady state has a greater energy than the initial one for any $A \neq A_0$.

VI. SUDDEN CHANGE FOR LARGE BUT FINITE SYSTEMS

The result $C_2(t) \to 0$ as $t \to \infty$ does not hold for finite N. Indeed, for finite N, the components of $C_2(t)$ must return to their initial values an infinite number of times, the typical time between such recurrences being the Poincaré recurrence time. How can this be reconciled with the results of the previous section? An excellent discussion of these matters is given by Mazur and Montroll [6] for some special cases. Here we will limit ourselves to an informal heuristic discussion, whose aim is to give a qualitative feeling for the non-cyclic case and the $N \to \infty$ limit.

Applying Eq. (12) to the components of the various terms in $C_2(t)$, the function $f(\lambda^2)$ always contains a trigonometric factor that oscillates increasingly rapidly with respect to λ^2 as $t \to \infty$. Suppose for a moment that the product $R_{mk}R_{nk}$ varies smoothly with k and that the spectrum λ_k^2 is not too degenerate. Then for very large t, all phase coherence between different terms in the sum is lost and we can for all practical purposes replace the arguments of the trigonometric functions by random variables ϕ_i that are uniformly distributed on the interval $[0, 2\pi]$. Using $\langle \cos\phi_i \rangle = 0$ and $\langle \cos\phi_i \cos\phi_k \rangle = \frac{1}{2}\delta_{ik}$, this means that if we let t be a random variable uniformly distributed on the interval $[-T, T]$ for some large enough T, then the expectation value and variance of a typical term like

$$X(t) \equiv A\cos\left[2A^{1/2}t\right] \tag{30}$$

is approximately given by

$$\langle X(t)_{mn} \rangle = \langle \sum_{k=-N}^{N} R_{mk}R_{nk}\lambda_k^2 \cos(2\lambda_k t) \rangle = \sum_{k=-N}^{N} R_{mk}R_{nk}\lambda_k^2 \langle \cos\phi_k \rangle = 0, \tag{31}$$

$$\langle X(t)_{mn}^2 \rangle = \sum_{k=-N}^{N}\sum_{l=-N}^{N} R_{mk}R_{nk}R_{ml}R_{nl}\lambda_k^2\lambda_l^2 \langle \cos\phi_k \cos\phi_l \rangle = \frac{1}{2}\sum_{k=-N}^{N} \left(R_{mk}R_{nk}\lambda_k^2\right)^2. \tag{32}$$

Since the typical element of a generic $N \times N$ orthogonal matrix R is of order $N^{-1/2}$, the sum above will be of order $N \times N^{-2}$, which yields a standard deviation of order $N^{-1/2}$. Thus for large but finite systems, we expect the elements of $C_2(t)$ to evolve as follows:

(i) During an initial transition period whose duration is of the order of the dynamical time scale ω_0^{-1}, they decay from their initial values of order unity to values of order $N^{-1/2}$.

(ii) After that, they oscillate around zero with an oscillation amplitude of order $N^{-1/2}$.

(iii) Since their time evolution is almost periodic, they must return to values of order unity an infinite number of times. This happens approximately once every Poincaré recurrence time. However, as shown by Mazur and Montroll, the Poincaré time scale is generally enormous compared to the dynamical time scale, since it tends to grow exponentially with N for systems of this type.

VII. IMPLICATIONS FOR HEAT BATH MODELS

In this section we will discuss thermal states, and compare them to the stationary states arising from adiabatic and sudden change. It will be seen that the latter two are in general not thermal.

Thermal states

The energy of a steady state is

$$E = \langle H \rangle = \frac{1}{2}\mathrm{tr}\begin{pmatrix} A & 0 \\ 0 & I \end{pmatrix}\begin{pmatrix} D & 0 \\ 0 & AD \end{pmatrix} = \mathrm{tr}\, AD. \tag{33}$$

Given a Hamiltonian and a fixed energy, the *thermal state* is the state that has the maximum entropy consistent with this energy. The Wigner function of a thermal state is Gaussian. FKM show that a thermal state of temperature T is the steady state given by

$$\begin{cases} \mu &= 0 \\ C &= \frac{1}{2}\begin{pmatrix} A^{-1/2}\coth\beta A^{1/2} & 0 \\ 0 & A^{1/2}\coth\beta A^{1/2} \end{pmatrix} \end{cases}, \tag{34}$$

where we have defined $\beta \equiv \frac{\hbar\omega_0}{2kT}$. In the classical limit $\beta \ll 1$, this reduces to

$$C = \frac{1}{2\beta}\begin{pmatrix} A^{-1} & 0 \\ 0 & I \end{pmatrix}, \tag{35}$$

whereas $T = 0$ yields the ground state

$$C = \frac{1}{2}\begin{pmatrix} A^{-1/2} & 0 \\ 0 & A^{1/2} \end{pmatrix}. \tag{36}$$

Heat bath models

According to the standard interpretation, a system will be in a thermal state if it has been exposed to an ideal heat bath long enough to reach thermal equilibrium. (After this the heat bath can be removed if the system is kept isolated, since the thermal state is a steady state.) Numerous attempts have been made to model ideal heat baths by infinite systems of coupled harmonic oscillators. We will now use the results we have derived for adiabatic and sudden change to illustrate some shortcomings of such models, and clarify what they can and can not do.

Typically, the time evolution of some small subset of oscillators, called the *system*, is studied by taking a partial trace over (*i.e.* ignoring) the rest of the oscillators, called the *heat bath*. A goal of all such pursuits has been to devise interaction Hamiltonians $A(t)$ such that the state of the subsystem becomes thermal.

Our use of μ and C has the advantage that we need not distinguish between system and heat bath *a priori*: if we decide to view some subset of oscillators as the system, then their means and internal correlations are simply given as subsets of the entries in μ and C.

We can summarize our previous results for steady states as follows:

$$\begin{cases} D \mapsto \left(A_0 A^{-1}\right)^{1/2} D & \text{in adiabatic case,} \\ D \mapsto \frac{1}{2}\left[I + A_0 A^{-1}\right] D & \text{in sudden case,} \\ D = \frac{1}{2}A^{-1/2}\coth\beta A^{1/2} & \text{in thermal case.} \end{cases} \tag{37}$$

From this it readily follows that we can transform an arbitrary steady state given by A_0 and D_0 into a thermal state with an arbitrary temperature T by adiabatically changing A_0 into

$$A \equiv \left[\frac{1}{\beta}\coth^{-1}\left(2A_0^{1/2}D_0\right)\right]^2. \tag{38}$$

However, we are not interested in such "fine-tuned" models, where $A(t)$ is chosen to depend on the initial data D_0. Rather, we are looking for a fairly robust heat bath model, where one single interaction potential can thermalize fairly general initial states.

Initially uncoupled oscillators

As a simple example, let us choose the initial state to be the thermal state at some temperature T_0 for a Hamiltonian given by $A_0 = I$. Since this corresponds to uncoupled oscillators, this state is simply a direct product of single-oscillator states: $\mu = 0$ and $C = \frac{1}{2}\coth\beta_0 I$, where $\beta_0 \equiv \frac{\hbar\omega_0}{2kT_0}$. Now let a cyclic interaction potential A be switched on, either adiabatically or suddenly. After a while (after the switch-on is complete in the adiabatic case or after the oscillations have died down in the sudden case), we can compare the resulting steady states with the thermal state:

$$C = \begin{cases} C_a = \frac{1}{2}\begin{pmatrix} A^{-1/2} & 0 \\ 0 & A^{1/2} \end{pmatrix}\coth\beta_0 & \text{after adiabatic change,} \\ C_s = \frac{1}{2}\begin{pmatrix} \frac{I+A^{-1}}{2} & 0 \\ 0 & \frac{I+A}{2} \end{pmatrix}\coth\beta_0 & \text{as } t\to\infty \text{ after sudden change,} \\ C_t = \frac{1}{2}\begin{pmatrix} A^{-1/2}\coth\beta A^{1/2} & 0 \\ 0 & A^{1/2}\coth\beta A^{1/2} \end{pmatrix} & \text{for a thermal state.} \end{cases} \tag{39}$$

We see that these three covariance matrices are in general all different. In particular, the final states in the adiabatic and sudden cases are not thermal. Although there is no reason to expect the total correlation matrices to be thermal, one might hope that certain submatrices of C_a or C_s should be thermal, in the sense that they equal the corresponding submatrices of C_t — at least if C_t is allowed to refer to a different temperature, *i.e.* allowing $T \neq T_0$. In other words, one might hope that certain subsystems would approach the state that they would have if the total system were thermal †. It should be fairly obvious that this is not the case for generic A. The nearest-neighbor coupling is a simple counterexample. For this simple case, we can evaluate the momentum correlations explicitly in the limit $\gamma \gg 1$, $kT \gg \hbar\omega_0$:

$$\langle\hat{\mathbf{p}}_m\hat{\mathbf{p}}_n\rangle \approx \begin{cases} \left(\frac{\gamma\coth\beta_0}{2\pi}\right)\frac{1}{1-4(m-n)^2} & \text{after adiabatic change,} \\ \left(\frac{\coth\beta_0}{2}\right)\left[(1+\gamma^2)\delta_{m,n} - \frac{\gamma^2}{2}(\delta_{m,n-1}+\delta_{m,n+1})\right] & \text{after sudden change,} \\ \frac{1}{2\beta}\delta_{m,n} & \text{in thermal case.} \end{cases} \tag{40}$$

(The adiabatic result has been derived using Eq. (13) and $\gamma \gg 1$, the sudden result is exact and the thermal result is only valid for $kT \gg \hbar\omega_0$.) We see that the qualitative behavior is quite different in all three cases: In the adiabatic case, weak long-range correlations exist. In the sudden case, correlation exist only between nearest neighbors. In the high-temperature thermal case, there are no correlations at all.

For $|m-n| \ll \gamma$, the integral (13) for position correlations is completely dominated by the region around $\theta = \gamma$, and we obtain

$$\langle\hat{\mathbf{q}}_m\hat{\mathbf{q}}_n\rangle \approx \begin{cases} \frac{\ln(2\pi\gamma)}{2\pi\gamma} & \text{after adiabatic change,} \\ \frac{1}{4}\delta_{m,n} + \frac{1}{8\gamma} & \text{after sudden change,} \\ \frac{1}{4\gamma\beta} & \text{in thermal case.} \end{cases} \tag{41}$$

Note that for the adiabatic and thermal cases, this is independent of m and n , which physically means that oscillators with separation $|m-n| \ll \gamma$ move as one rigid unit, having their positions almost perfectly correlated.

† This is perhaps the only reasonable definition of what to mean by a subsystem becoming thermalized. Recall that we have only defined thermality of a system *relative to some Hamiltonian*. Thus if a subsystem in some sense becomes thermal, the question is: Relative to which Hamiltonian? It would be naive to expect the answer to be the Hamiltonian describing only the forces within the subsystem, since when a subsystem is coupled to its surrounding, the Hamiltonian that governs it by definition involves parts outside of the subsystem.

The simple 2×2 submatrices corresponding to a single oscillator are all diagonal, just as they are for the thermal state of a single oscillator. Since they contain only two non-zero elements, they are indeed identical to the thermal state of a single oscillator with some temperature T and coupling $\omega_{eff} \neq \omega$, or identical to the 2×2 submatrices of C_t with some temperature T and coupling $\gamma_{eff} \neq \gamma$. In this limited sense, both adiabatic and sudden change can be said to thermalize $n = 1$ subsystems. For subsystems with n oscillators, C_a, C_s and C_t each have $n(n+1)$ different non-zero elements in the submatrix, so we see that the above-mentioned match by adjusting the two parameters T and γ_{eff} was just a fortuitous coincidence that worked when $n = 1$.

Another popular choice of initial conditions in the literature has been a thermal state with some coupling $A_0 \neq I$. Also this case can be readily treated with the above formalism, and generally fails to yield thermal states for $n > 1$ subsystems.

Does this mean that cyclic quadratic Hamiltonians are totally incapable of acting as heat baths for $n > 1$, or is there some simple limit in which subsystems can be thermalized? One frequently discussed limit is that of weak coupling.

The weak coupling limit

In the case of infinitesimally weak coupling, say $A = I + \epsilon F$, Equations (39) reduce to

$$C = \begin{cases} \begin{pmatrix} I - \frac{\epsilon}{2}F & 0 \\ 0 & I + \frac{\epsilon}{2}F \end{pmatrix} \frac{\coth \beta_0}{2} & \text{after adiabatic change,} \\ \begin{pmatrix} I - \frac{\epsilon}{2}F & 0 \\ 0 & I + \frac{\epsilon}{2}F \end{pmatrix} \frac{\coth \beta_0}{2} & \text{as } t \to \infty \text{ after sudden change,} \\ \begin{pmatrix} I - [1+a]\frac{\epsilon}{2}F & 0 \\ 0 & I + [1-a]\frac{\epsilon}{2}F \end{pmatrix} \frac{\coth \beta}{2} & \text{for a thermal state,} \end{cases} \tag{42}$$

where

$$a \equiv \frac{2\beta}{\sinh 2\beta}. \tag{43}$$

Thus we see that for infinitesimally weak coupling, the sudden case coincides with the adiabatic case, but that the resulting state is generally still not thermal. It should come as no surprise that the sudden case coincides with the adiabatic case in this limit, since a sudden infinitesimal change is in a sense adiabatic. We see that there are only two cases when the resulting state is thermal:

The first is if F is a multiple of I, which gives $T \neq T_0$ and corresponds to the trivial case of the oscillators remaining uncoupled.

The second is when $a = 0$, which implies $T = T_0 = 0$. This simply reflects the fact that adiabatic change changes the ground state into the new ground state. Note that this is a pure quantum phenomenon, since $a \to 1 \neq 0$ as $\hbar \to 0$.

The sense in which harmonic heat baths work

Although the above results for the weak-coupling limit showed that subsystems did not become thermal, they did indeed become almost thermal, the difference being terms of order ϵ. This is not very impressive at all, in view of the fact that the initial state was also almost thermal. However, a general feature of infinite harmonic chains is that the final state after sudden change remains the same even if the initial states of a finite number of oscillators is changed. This follows directly from the fact that all components of $U(t)$ approach zero as $t \to \infty$. This means that a sudden change will result in the same almost thermal state even if some subsystem starts out in a completely different, quite non-thermal state. It is in this sense that the many harmonic heat bath models in the literature can transform a subsystem into an approximately thermal state.

Unfortunately, the interesting case where the system has internal couplings stronger than those of the heat bath cannot be treated with the formulas derived in this paper, since the matrix A would not be cyclic. It would appear, however, that the strength of the coupling between the system and the heat bath must be carefully balanced for such a heat bath model to work. If the coupling is so strong that it is comparable to the couplings within the system, then the final state of the system will probably deviate considerably from the thermal state. If, on the other hand, the coupling is too weak, then the relaxation time, the time scale over which the system approaches the thermal state, will be unreasonably long.

VIII. THE INDEPENDENCE OF DISPLACEMENT AND DISPERSION

In this section, we will discuss how the previous results for sudden change are modified in the case of non-zero means, *i.e.* when $\mu \neq 0$. It will be seen that the fact that μ and C evolve independently of each other makes systems with $\mu \neq 0$ totally unable to produce thermal states.

We can generalize (3) to arbitrary quadratic Hamiltonians by writing

$$H = \hat{\mathbf{z}}^T B \hat{\mathbf{z}} = \mathrm{tr}\, B \hat{\mathbf{z}} \hat{\mathbf{z}}^T, \tag{44}$$

where B is any symmetric matrix. This covers both cases where the different particles have different masses and cases where the potential is not positive definite.

$$\langle H \rangle = \mathrm{tr}\, B \langle \mathbf{z}\mathbf{z}^T \rangle = \mathrm{tr}\, B\mu\mu^T + \mathrm{tr}\, BC = E_1 + E_2, \tag{45}$$

say, where we will call $E_1 \equiv \mathrm{tr}\, B\mu\mu^T$ the *displacement energy* and and $E_2 \equiv \mathrm{tr}\, BC$ the *dispersion energy.* (To be precise, the second equal sign is valid only if the two off-diagonal $n \times n$ submatrices of B are symmetric and thus identical — otherwise the non-commutativity of $\hat{\mathbf{q}}$ and $\hat{\mathbf{p}}$ gives rise to an uninteresting extra additive constant.) We see from (5) that μ and C evolve completely independently of each other. By formally setting either μ or C equal to zero, (5) thus shows that the displacement energy and the dispersion energy are *separately* conserved, independently of one another. Hence displacement energy can never be used to increase dispersion and entropy. This is in stark contrast to an approach to the thermal state, where the resulting equilibrium entropy for subsystems is the maximum allowed by the total available energy. This difference between the thermal state and the actual state as $t \to \infty$ is illustrated in Figure 1. The Gaussian Wigner distribution in the phase-space of a single oscillator is shown by the contour at which it has dropped to half its maximum value, a circle. Recall that the entropy of the oscillator depends on the area of the circle, whereas the energy depends on the average distance to the origin. Thus the circle symbolizing the equilibrium state has the maximum area consistent with the available energy. The actual state has the same energy but much less entropy.

Thus oscillator systems which are able to evolve a state with non-zero means into something resembling the thermal state cannot have purely quadratic Hamiltonians, but must contain some non-linear couplings.

IX. CONCLUDING REMARKS

We have studied steady states of coupled harmonic oscillators, and how adiabatic and sudden changes in a cyclic potential transform one steady state into another. Our main conclusions are as follows:

(i) Adiabatic change can transform a given steady state into any other steady state, subject to the constraint that the adiabatic invariant AD^2 is conserved.

(ii) After a sudden change, the covariance matrix undergoes an oscillatory phase, after which it generally converges to a new steady state. This asymptotic behavior depends crucially on how degenerate the spectrum of A is. Generic sudden changes are not reversible, and a sequence of sudden changes, where the final and initial potentials A are the same, leads to a net increase in energy.

(iii) The states resulting from adiabatic and sudden changes are in general not thermal states, not even if we restrict our attention to subsystems. We conclude that harmonic heat bath models can lead to approximately thermal subsystems only under the following conditions:

1) The coupling between the system and the heat bath is weak.

2) $\mu = 0$, *i.e.* the expectation values of the displacements and momenta of the oscillators vanish.

We summarise the state of affairs for heat bath models as follows: It is frequently assumed that the density matrix of a system is $\rho \propto e^{-H/kT}$, *i.e.* the thermal state corresponding to a temperature T. Unfortunately, no completely solvable heat bath model has ever been found that explicitly evolves multiparticle ($n > 1$) systems into such states. The problem appears to arise when the coupling between the system particles and individual heat bath particles is so strong that it is comparable to the couplings within the system. Thus approximately thermal states can be created only when the when the system particles are very weakly coupled to the bath particles. If this is the case, the system particles must be coupled to very many heat path particles to avoid the approach to equilibrium taking an unreasonably long time. Only in the limit when a typical system particle becomes infinitesimally coupled to infinitely many bath particles (such as in the limit of the FKM model [5] or the IO model [12], both dealing with the $n = 1$ case) is the limiting state exactly thermal. Thus we may expect nature to be full of approximately thermal states, but devoid of exactly thermal states.

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APPENDIX A

In this appendix, we will discuss the circumstances under which $C_2(t) \to 0$ as $t \to \infty$.

Applying Eq. (12) to the components of the various terms in $C_2(t)$, the function $f(\lambda^2)$ always contains a trigonometric factor that oscillates increasingly rapidly with respect to λ^2 as $t \to \infty$. In Section VI, we gave a qualitative discussion of how this causes $C_2(t)$ to approach zero for general symmetric positive definite A with non-degenerate spectra, as well as what happens when N is large but finite. Here we will give a rigorous treatment for the special case when A is infinite-dimensional and cyclic.

The behavior of $C_2(t)$ depends crucially on how degenerate the spectrum of A is. Since all cyclic Hamiltonians are invariant under parity, they all have the degeneracy

$$\omega(-\theta) = \omega(\theta), \tag{46}$$

where we have defined the frequency $\omega \equiv |\lambda|$. If this is the *only* degeneracy, *i.e.* if $\omega(\theta)$ is invertible for $\theta \geq 0$, and if in addition $\omega(\theta)$ is differentiable, then we can change variables in Eq. (13) and obtain

$$f(A)_{mn} = 2\int_{\omega_{min}}^{\omega_{max}} f(\omega^2) g(\omega) \cos\left[(m-n)\theta(\omega)\right] d\omega. \tag{47}$$

Here we have introduced the *spectral density function* $g(w)$, defined so that $g(\omega)d\omega$ is the fraction of the frequencies that lie in the interval $[\omega, \omega + d\omega]$. Note that

$$g(\omega) = \frac{1}{2\pi}\frac{d\theta}{d\omega} \tag{48}$$

if $\theta(\omega)$ is single-valued and invertible, but that $g(\omega)$ is well-defined as a distribution for *any* spectrum $\omega(\theta)$. For the case of nearest-neighbor coupling,

$$g(\omega) = \begin{cases} \frac{1}{\pi}\frac{\omega}{\sqrt{(\omega^2-1)(4\gamma^2+1-\omega^2)}} & \text{if } 1 \leq |\omega| \leq 1+4\gamma^2, \\ 0 & \text{otherwise.} \end{cases} \tag{49}$$

We wish to examine the various terms in $C_2(t)$. Let us define

$$a_n \equiv f(A)_{m,m+n} \tag{50}$$

and choose the function to be

$$f(A) = \cos(A^{1/2}t). \tag{51}$$

Eq. (47) now yields

$$a_n(t) = 2\int_{\omega_{min}}^{\omega_{max}} \cos(\omega t) g(\omega) \cos\left[n\theta(\omega)\right] d\omega. \tag{52}$$

By extending the functions g and θ to the entire real line by $g(-\omega) \equiv g(\omega)$, $\theta(-\omega) \equiv \theta(\omega)$, and $g(\omega) = 0$ unless $\omega_{min} \leq |\omega| \leq \omega_{max}$, we see that this can be written as a Fourier transform:

$$a_n(t) = \hat{u}_n(t), \tag{53}$$

where

$$u_n(\omega) \equiv g(\omega)\cos\left[n\theta(\omega)\right]. \tag{54}$$

According to Riemann-Lebesgue's Lemma,

$$\hat{u}_n(t) \to 0 \quad \text{as} \quad |t| \to \infty \tag{55}$$

if $u_n(\omega)$ is an integrable function. Since the latter is trivially satisfied for all n (indeed $\int_{-\infty}^{\infty} u_n(\omega)d\omega = 2\pi\delta_{0n}$), this implies that †

$$\cos(A^{1/2}t) \to 0 \quad \text{as} \quad t \to \infty. \tag{56}$$

In an almost identical fashion it is readily shown that $\sin(A^{1/2}t) \to 0$ as $t \to \infty$. By multiplying these results by various constant matrices, it follows that all terms in $C_2(t)$ approach zero. In summary, we have shown that all components of $C_2(t) \to 0$ as $t \to \infty$ for any symmetric, positive definite, cyclic, infinite-dimensional A if its spectral function $\lambda^2(\theta)$ is invertible and differentiable for $\theta > 0$.

It is straightforward to generalize this result in a number of ways:

* If $\lambda^2(\theta)$ is differentiable but not invertible because it turns around a finite number of times, then the same result is obtained by integrating over each monotonic segment separately.
* If A is merely non-negative definite, then $A^{-1/2}$ and A^{-1} are undefined. However, the result still holds for the momentum-momentum part of the covariance matrix.

Roughly speaking, the key result $C_2(t) \to 0$ as $t \to \infty$ fails if the spectrum is too degenerate. An easy way to appreciate this is to study the diagonal terms of the matrix $\cos(A^{1/2}t)$, which simply equal

$$a_0(t) = \hat{g}(t). \tag{57}$$

For uncoupled oscillators, we have $A \propto I$ and the spectrum is totally degenerate, *i.e.* the spectral density $g(\omega) = \delta(\omega - \omega_0) + \delta(\omega + \omega_0)$ and $a_0(t) \propto \cos\omega_0 t$ for all t. By Riemann-Lebesgue's Lemma, $a_0(t) \to 0$ as $t \to \infty$ if the spectral density is an integrable function, not if it is merely a tempered distribution such as δ. Furthermore, from partial integration of the Fourier integral, we know that if the spectral density is a k times differentiable function, then $a_n(t)$ approaches zero faster than t^{-k}.

† The convergence is not necessarily uniform, *i.e.* although $\cos(A^{1/2}t)_{mn} \to 0$ for any fixed m and n, we do not always have $\sup_{m,n} \cos(A^{1/2}t)_{mn} \to 0$. A more careful analysis shows that uniform convergence is obtained if the spectral function λ is analytic on the entire interval $[-\pi, \pi]$ and in addition is nonlinear.

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