Adiabatic propagation of distributions: Exactly solvable models

J. K. Percus^{1,2} and L. Šamaj^{1,*}

¹Courant Institute of Mathematical Sciences, New York University, 251 Mercer Street, New York, New York 10012

²Physics Department, New York University, New York, New York 10003

(Received 26 April 1995; revised manuscript received 21 August 1995)

We study the analytical structure of corrections to perfect adiabatic evolution associated with an ensemble of classical ergodic Hamiltonians with specific correlation properties, distributed at inital time, e.g., over a single energy shell. In particular, we aim to check the prediction of the multiple-time-scale method concerning the structure of energy moments that measure the extent of violation of an ergodic adiabatic invariant when the slowness parameter is small but finite. Solving exactly for the evolution of the phase space density, we find the explicit form of the energy moments for an infinite one-dimensional system of harmonic oscillators with time-decaying couplings. A comparison with the multiple-time-scale method shows its restricted applicability to a marginal limit of a vanishing slow time scale.

PACS number(s): 05.45. + b, 03.20. + i

I. INTRODUCTION

Complex systems ordinarily proceed on multiple time scales. Prototypically, one distinguishes between fast motions, and slow motions that serve as the environment for the former. The fast variables are thus subject to adiabatic time-varying forces, and a perennial problem in the ensemble format that we will adhere to is that of describing the resulting quasistatic propagation of the fast variable distribution.

The general adiabatic process is defined as follows: We assume that the time evolution of a dynamical system is governed by a time-dependent Hamiltonian of the scaling form $H(\mathbf{z},t) = h(\mathbf{z},\tau)$, where z denotes a point in phase space (it will be mostly omitted as a functional argument), and $\tau = \epsilon t$ defines, besides a fast time scale over which t changes by order unity, a slow time scale determined by the dimensionless slowness parameter ϵ . For an ideal adiabatic process, t is regarded as arbitrarily large $(t \to \infty), \epsilon$ arbitrarily small $(\epsilon \rightarrow 0)$, maintaining the finite value of τ . The corresponding time evolution is, in principle, now well understood for ergodic systems, due to the existence of specific adiabatic invariants [1,2]. For a process which is not perfectly adiabatic, the slow time scale τ is still considered to be finite, while the slowness parameter ϵ is small but finite, and one attempts to find the ϵ expansion of adiabatic invariants. The analytic character of the leading-order ϵ corrections, which remains a puzzle in many aspects, then tells us about the "goodness" of these invariants when applied to a realistic time-dependent process where ϵ is never negligibly small.

It turns out that the treatment of ϵ corrections to the

pa tion stem is scaling phase ment), first phase ment), first phich t the call adisplant and is still ter ϵ is parameter with the call and is still ter ϵ is parameter of these parameter of these parameter of these parameters.

perfectly adiabatic evolution depends very much on the fast time t asymptotics of correlations among dynamical variables induced by the instantaneous (or frozen) Hamiltonian $h(\mathbf{z},\tau)$, with τ fixed. For simple classical Hamiltonians with few degrees of freedom and underlying correlations as superpositions of terms purely oscillating in time, the leading-order corrections to adiabatic invariants exhibit an exponentially fast decay to zero of type $O(e^{-c/\epsilon}), c > 0$ in the adiabatic limit $\epsilon \to 0$ [1]. For dissipative classical Hamiltonians with underlying correlations decaying to zero at asymptotically large times, an attempt to account systematically for corrections to adiabatic trajectories in lower orders of ϵ has been made generally in the ensemble format within the so-called multiple-time-scale (MTS) method (see, e.g., [3]), applied first by Ott [2] and developed subsequently by many authors [4-7] up to an elegant form [8] which resolves a technical discrepancy of the different approaches. The final result is rather surprising and predicts, under certain consistency requirements, the leading order correction to adiabatic invariants to be of the form $O(\epsilon)$. This indicates an unexpected relevance of corrections to the ideal adiabaticity for such systems, and modifies our traditional point of view to the subject. The present work deals with the latter class of adiabatic processes, and since the MTS approach is our main reference we will recapitulate it briefly.

The MTS perturbation analysis [3] is a method for solving ordinary differential equations, time dependent by virtue of a small parameter, as a perturbative series in this parameter. Its essential feature is the extension of the number of independent time variables—a well-behaved solution of physical interest is then determined uniquely by removing, order by order in the perturbation parameter, any time secularities. In particular, for an ensemble of adiabatic Hamiltonians $H(\mathbf{z},t)=h(\mathbf{z},\tau)$, the phase space density at time t of $O(\epsilon^{-1})$ is written in the familiar two-time form $\rho(t,\tau)$ [2,4–8], so that the dynamical Liouville equation $\partial \rho/\partial t + \{\rho,h(\tau)\}=0$ appears in-

^{*}On leave from the Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia.

stead as

$$\frac{\partial \rho}{\partial t} + \epsilon \frac{\partial \rho}{\partial \tau} + \{\rho, h(\tau)\} = 0. \tag{1.1}$$

If ρ is expanded in ϵ as

$$\rho(t,\tau) = \rho_0(\tau) + \epsilon \rho_1(t,\tau) + \epsilon^2 \rho_2(t,\tau) + \cdots , \qquad (1.2)$$

and (1.1) is regarded as an identity in ϵ , we then have

$$\{\rho_0(\tau), h(\tau)\} = 0$$
, (1.3a)

$$\frac{\partial}{\partial t}\rho_{1}(t,\tau) + \{\rho_{1}(t,\tau), h(\tau)\} = -\frac{\partial}{\partial \tau}\rho_{0}(\tau) , \qquad (1.3b)$$

$$\frac{\partial}{\partial t} \rho_2(t,\tau) + \{\rho_2(t,\tau), h(\tau)\} = -\frac{\partial}{\partial \tau} \rho_1(t,\tau) , \qquad (1.3c)$$

and so on, to which one can append the initial condition $\rho(0,0)=\rho_0$, expanded as

$$\rho_0(0) = \rho_0$$
, $\rho_1(0,0) = 0$, $\rho_2(0,0) = 0$,... (1.4)

The first major assumption is that $h(\tau)$ is ergodic, so that, at fixed τ , it is the only regular constant of the motion. The first equation (1.3a) then tells us that

$$\rho_0(\tau) = f_0(h(\tau), \tau) \tag{1.5}$$

for some function f_0 , and the first of (1.4) that the decomposition is consistent only if the initial ρ_0 is a function of h(0),

$$\rho_0 = f_0(h(0), 0) . \tag{1.6}$$

The explicit form of f_0 follows from the requirement that all terms in the next-order relation (1.3b), which grow secularly with time, must be removed:

$$f_0(E,\tau) = g(\Omega(E,\tau)) , \qquad (1.7)$$

where

$$\Omega(E,\tau) = \int d\mathbf{z} \, \theta(E - h(\mathbf{z},\tau)) \tag{1.8}$$

 $[\theta(x)]$ stands for the unit step function] is the volume in phase space enclosed by the energy shell E of $h(z,\tau)$, and the function g is given by the initial condition (1.6),

$$f_0(E,0) = g(\Omega(E,0))$$
 (1.9)

In this paper, we will concentrate on the special case in which the initial phase space density ρ_0 is distributed uniformly over a single energy shell, and hence

$$f_0(E,0) = \delta(E - E_0) / \Sigma(E,0)$$
, (1.10a)

with the normalization constant

$$\Sigma(E,0) = \int d\mathbf{z} \, \delta(E - h(\mathbf{z},0)) \ . \tag{1.10b}$$

The solution of (1.7)–(1.9) then reads

$$f_0(E,\tau) = \delta(E - \mathcal{E}(\tau)) / \Sigma(E,\tau) , \qquad (1.11a)$$

$$\Sigma(E,\tau) = \int d\mathbf{z} \, \delta(E - h(\mathbf{z},\tau)) , \qquad (1.11b)$$

where $\mathscr{E}(\tau)$ is given by

$$\Omega(\mathcal{E}(\tau), \tau) = \Omega(E_0, 0) , \qquad (1.12)$$

i.e., the system ensemble remains distributed over the single energy shell $\mathcal{E}(\tau)$, evolving in accordance with the adiabatic invariance of the volume in phase space enclosed by the instantaneous energy shell.

In a higher order of the decomposition scheme, the formal solution of (1.3b) for $\rho_1(t,\tau)$ can be written in the form [8]

$$\rho_{1}(\mathbf{z},t,\tau) = -\frac{\partial f_{0}}{\partial E}(h,\tau) \int_{0}^{t} dt' \left[\frac{\partial h}{\partial \tau}(\mathbf{Z},\tau) - u(h,\tau) \right] + f_{1}(h,\tau) . \tag{1.13}$$

Here, $Z=Z(z,t,t',\tau)$ is the point in phase space reached by starting at z at time t and then evolving a trajectory backward in time to t', under the frozen (i.e., timeindependent or, equivalently, with τ fixed) Hamiltonian $h(\tau)$,

$$u(E,\tau) = \langle \partial h / \partial \tau \rangle_{E,\tau} , \qquad (1.14)$$

where

$$\langle \cdots \rangle_{E,\tau} = \frac{1}{\sum (E,\tau)} \int d\mathbf{z} \, \delta(E - h(\mathbf{z},\tau))(\cdots)$$

denotes the phase space average over the energy shell E of $h(\mathbf{z},\tau)$, and f_1 is arbitrary apart from initial conditions $f_1(E,0)=0$. The removal of secularities at $O(\epsilon^2)$, Eq. (1.3c), then specifies $f_1(E,\tau)$ via the partial differential equation

$$\frac{\partial}{\partial \tau} (\Sigma f_1) + \frac{\partial}{\partial E} (u \Sigma f_1) - \frac{1}{2} \frac{\partial}{\partial E} \left[\Sigma G_2 \frac{\partial f_0}{\partial E} \right] = 0 . \quad (1.15)$$

Here

$$G_2(E,\tau) = \int_{-\infty}^{+\infty} ds \ C(s) \ ,$$
 (1.16)

and $C(E, \tau; s)$ is an autocorrelation function

$$C(s) = \left\langle \left[\frac{\partial h}{\partial \tau} - u \right] \mathcal{O}_{\tau}(s) \left[\frac{\partial h}{\partial \tau} - u \right] \right\rangle_{E,\tau}, \qquad (1.17)$$

where $\mathcal{O}_{\tau}(s)$ stands for a time evolution operator, evolving point z for a time s under the frozen Hamiltonian $h(\tau)$. The vanishing of C(s) for asymptotically large time s (an inherent property of real physical systems with energy dissipation) and the convergence of integral G_2 are further major assumptions ensuring the consistency of the two-time-scale scheme. For the ensemble of interest, with initial phase space density distributed uniformly over a single energy shell [(1.10a) and (1.10b)] and the corresponding pure adiabatic solution [(1.11) and (1.12)], the extent of the violation of the adiabatic Ω invariance when the slowness parameter ϵ is finite is usually measured by the energy moments

$$M_n(t) = \int d\mathbf{z} \rho(\mathbf{z}, t, \tau) [h(\mathbf{z}, \tau) - \mathcal{E}(\tau)]^n , \qquad (1.18)$$

which are also adiabatic invariants equal to zero in the limit $\epsilon \rightarrow 0$. It can be shown [8] that in expansion of the

total ρ up to the first order in ϵ , only term $\epsilon f_1(h,\tau)$ contributes to the integrals (1.18) in such a way that the first two moments M_1 and M_2 scale like ϵ while all higher-order moments M_n scale like $\epsilon^{\nu_n}(\nu_n \ge 2)$ for t of order $O(\epsilon^{-1})$.

The leading ϵ -order structure of the moments $\{M_n(t)\}$ is the most important finding of the MTS. The result $M_1, M_2 \sim \epsilon$ shows that the adiabatic invariants are violated substantially when ϵ is finite and, after some algebra, implies an evolution equation of the Fokker-Planck type for the distribution of energies, widely discussed in the literature [6-8]. The main aim of this work is to check, by solving exactly a family of adiabatic time-dependent Hamiltonians fulfilling all consistency requirements of the MTS scheme, whether the MTS prediction as to the leading-order ϵ correction to the adiabatic invariants $\{M_n(t)\}\$ is correct. The motivation comes from the fact that the MTS decomposition, with a partially analytical structure assumed ad hoc, lacks the control over contributions produced by higher-order terms of the formal ϵ expansion: their resummation can modify fundamentally the analytic form of the leading-order ϵ term, or at least change its proportionality prefactor. Under such circumstances, exactly solvable situations serve us as benchmarks for analytic developments, but these are few and far between. In this paper, we recall such a system of ancient vintage, show that it generalizes quite easily to many-particle systems, and apply this to an adiabatic change of the coupling of a simple but in many ways nontrivial system. This will allow us to point out potential difficulties in current treatments of adiabatic processes. In particular, we find that the MTS result is correct only in the marginal limit $\tau \rightarrow 0$. In the slow-time-scale region of physical interest τ finite, the leading-order terms of the ϵ expansion of the adiabatic invariants scale like ϵ , as predicted by the MTS method, but the proportionality prefactors are renormalized with respect to their MTS estimates. That is, while the MTS theory implies that $M_1, M_2 \sim \epsilon$ and all higher-order moments M_n scale like ϵ^{ν_n} ($\nu_n \ge 2$), the exact result reveals that all moments are of order $O(\epsilon)$: they couple successively into pairs $\{M_{2n-1}, M_{2n}\}$ according to the prefactors of the same slow-time-scale order $O(\tau^{2n-1})$. The hierarchical structure of the energy moments observed is suggested to be a more general feature of adiabatic processes.

The paper is organized as follows. In Sec. II, we introduce both quantum and classical versions of the Hamiltonian with a specific type of adiabatic time dependence,

$$H(\mathbf{z},t) = \sum_{j} \frac{p_j^2}{2} + \frac{1}{1 + 2\epsilon t} v \left\{ \left\{ \frac{x_j}{\sqrt{1 + 2\epsilon t}} \right\} \right\}. \quad (1.19)$$

Using explicit unitary (or canonical) time-dependent transformations of dynamical variables we show that, for an arbitrary interparticle potential v, the time evolution of the corresponding phase space density ρ is expressible in terms of ρ_0 associated with a stationary Hamiltonian $H_0(\mathbf{z}) = \sum_j (p_j^2 - \epsilon^2 x_j^2)/2 + v(\{x_j\})$.

In Sec. III, we apply this mapping to a onedimensional (1D) system of harmonic oscillators with coupling decaying in time,

$$H(\mathbf{z},t) = \sum_{j=0}^{N} \frac{p_j^2}{2} + \frac{1}{2} \left[\frac{\lambda}{1 + 2\epsilon t} \right]^2 \sum_{j=0}^{N} (x_j - x_{j+1})^2 ,$$
(1.20)

where $x_{N+1}=x_0$ is assumed. The system can be interpreted as a set of particles $\{j\}$, coupled consecutively according to their indices by harmonic strings (with the last Nth particle coupled to the zeroth one). The particle coordinates $\{x_j\}$ range from $-\infty$ to ∞ , and they can cross with each other. The Hamiltonian (1.20) is invariant with respect to the uniform shift in particle coordinates $x_j \rightarrow x_j + \text{const.}$, which implies, within the normal-mode analysis, the existence of a zero-frequency mode with the associated momentum as a constant of motion. To ensure the ergodicity, we project out the zero-frequency momentum by choosing suitable initial conditions and solve exactly for the evolution of the phase space density with the aid of the formalism of Sec. II.

In the mostly technical Sec. IV, we use this exact solution to compute a generating function for the energy moments (1.18). We concentrate especially on the limit of infinite number of particles $N \to \infty$ because, as is known in lattice dynamics (see, e.g., [9]), only in this limit can the system fall into the category of interest treatable by the MTS method [i.e., time correlations of dynamical variables induced by the adiabatic Hamiltonian (1.20) frozen at given $\tau = \epsilon t$ decay to zero at asymptotically large time]. The exact solution for the moment generating function is found in an implicit form.

In the concluding Sec. V, we determine the leading order of the true ϵ expansion of the energy moments. The result reveals an interesting hierarchical structure for the moments. Comparison with the prediction of the MTS is made, and the observed similarities and discrepancies are discussed.

II. SOLVABLE FAMILY OF ADIABATIC HAMILTONIANS

If one consults tables of solvable ordinary differential equations generalizing nontrivial ones of Newtonian type to time-dependent forces, one of rather general form (Kamke [10]) stands out. This is

$$\ddot{x} = t^{-3/2} f(x t^{-1/2}) \tag{2.1}$$

for arbitrary f, which yields to an energylike integral for the combination $xt^{-1/2}$. The scaling form of this equation suggests that its solvability is not restricted to one degree of freedom. Indeed, it is one of a vast array of solvable time-dependent systems produced by time-dependent canonical (unitary) transformations. For our present purposes, the obvious scaling extensions of (2.1) will suffice. They relate solvable dynamics for time-independent Hamiltonians to those with model time dependence; the former is implicitly solvable for one degree of freedom, but only in special cases for a many-body system.

There is no difficulty in extending dynamics to statisti-

cal dynamics, and we shall do so. We presuppose the solvable system

$$H_0 = \frac{1}{2}p^2 + v(x) - \frac{1}{2}\epsilon^2 x^2$$
, (2.2)

where x denotes all particle coordinates and p all momenta, in the sense that we are also given a density matrix $\rho_0(x,p,t)$ that belongs to it:

$$\frac{\partial}{\partial t} \rho_0(x, p, t) + \{ \rho_0(x, p, t), H_0 \} = 0 , \qquad (2.3)$$

where $\{\ ,\ \}$ denotes the Poisson bracket for a classical system or $(1/i\hbar)[\ ,\]$ for a quantum system. The purpose of setting aside the term $-\epsilon^2x^2/2$ is that it cancels under the canonical (unitary) transformation $x\to x, p\to p-\epsilon x$, which converts (2.3) to

$$\frac{\partial}{\partial t} \rho_0(x, p - \epsilon x, t) + \{\rho_0(x, p - \epsilon x, t), H_1\} = 0 , \quad (2.4a)$$

where $(a \cdot b \text{ signifies scalar product})$

$$H_1 = \frac{1}{2}p^2 - \frac{\epsilon}{2}(x \cdot p + p \cdot x) + v(x) . \qquad (2.4b)$$

It is convenient to change the time scale, rewriting (2.4)

as

$$(1+2\epsilon t)\frac{\partial}{\partial t}\rho_{0}\left[x,p-\epsilon x,\frac{1}{2\epsilon}\ln(1+2\epsilon t)\right] + \left\{\rho_{0}\left[x,p-\epsilon x,\frac{1}{2\epsilon}\ln(1+2\epsilon t)\right],H_{1}\right\} = 0, \qquad (2.5)$$

and then follow with the time-dependent canonical transformation $x \rightarrow x/(1+2\epsilon t)^{1/2}$, $p \rightarrow p(1+2\epsilon t)^{1/2}$. Since

$$[\partial/\partial t - \frac{1}{2}\epsilon/(1+2\epsilon t)\{x \cdot p + p \cdot x, \}]p(1+2\epsilon t)^{1/2} = 0$$

and

$$\left[\frac{\partial}{\partial t} - \frac{1}{2}\epsilon/(1 + 2\epsilon t)\left\{x \cdot p + p \cdot x, \right\}\right] x/(1 + 2\epsilon t)^{1/2} = 0,$$

(2.5) is transformed to

$$\left[(1+2\epsilon t)\frac{\partial}{\partial t} - \frac{1}{2}\epsilon \{x \cdot p + p \cdot x, \} \right] \rho(x,p,t) + \{\rho(x,p,t), H_1(t)\} = 0, \quad (2.6)$$

where $\{a, \}b \equiv \{a,b\},\$

$$\rho(x,p,t) = \rho_0 \left[x / (1 + 2\epsilon t)^{1/2}, p(1 + 2\epsilon t)^{1/2} - \epsilon x / (1 + 2\epsilon t)^{1/2}, \frac{1}{2\epsilon} \ln(1 + 2\epsilon t) \right],$$

$$H_1(t) = \frac{1}{2} (1 + 2\epsilon t) p^2 - \frac{\epsilon}{2} (x \cdot p + p \cdot x) + v \left[x / (1 + 2\epsilon t)^{1/2} \right],$$

and hence to our final expression

$$\frac{\partial}{\partial t}\rho(x,p,t) + \{\rho(x,p,t), H(t)\} = 0, \qquad (2.7a)$$

with

$$H(t) = \frac{1}{2}p^2 + (1 + 2\epsilon t)^{-1}v[x/(1 + 2\epsilon t)^{1/2}]. \tag{2.7b}$$

 ϵ sets the scale of the time-dependent potential in H(t), and plays the role of the adiabatic slowness parameter.

It is the dynamics (2.7) that we want to analyze. We must supply an initial condition $\rho(x,p,0) = \rho(x,p)$, or, according to (2.6),

$$\rho_0(x,p,0) = \rho(x,p+\epsilon x) \tag{2.8}$$

seen as initial condition for (2.3). In general, (2.8) will produce a transient in the development of (2.3). However, if $\rho_0(x,p,0)=f(H_0)$, then $\rho_0(x,p,t)=f(H_0)$ as well and a smoothly scaled behavior results: if

$$\rho(x,p,0) = f(H_0(x,p-\epsilon x)), \qquad (2.9)$$

then

$$\rho(x,p,t) = f(H_0(x/(1+2\epsilon t)^{1/2}, p(1+2\epsilon t)^{1/2} - \epsilon x/(1+2\epsilon t)^{1/2})).$$

Nonetheless, most studies have been with ergodic initial condition

$$\rho(x,p) = f(H(0)) \tag{2.10a}$$

or

$$\rho_0(x,p,0) = f(\frac{1}{2}(p+\epsilon x)^2 + v(x))$$

$$= f(H_0 + (\epsilon/2)(x \cdot p + p \cdot x) + \epsilon^2 x^2), \qquad (2.10b)$$

and so for comparison purposes, we adopt (2.10). In symbolic form, from elementary mechanics, (2.10b) thus implies the solution for (2.3):

$$\begin{split} \rho_0(x,p,t) = & f \left[H_0(x,p) + \frac{\epsilon}{2} [x_0(x,p,t) \cdot p_0(x,p,t) \\ & + p_0(x,p,t) \cdot x_0(x,p,t)] + \epsilon^2 x_0^2(x,p,t) \right] \,, \end{split}$$

where the initial value $x_0(x,p,t)$ satisfies an evolution equation "backward" in time

$$\left[\frac{\partial}{\partial t} + \{, H_0(x, p)\}\right] x_0(x, p, t) = 0$$
 (2.12a)

with initial condition

$$x_0(x,p,0) = x$$
, (2.12b)

and similarly for $p_0(x, p, t)$. Consequently,

$$\rho(x,p,t) = f\left[H_0(x',p') + \frac{\epsilon}{2} \left[x_0(x',p',t') \cdot p_0(x',p',t') + p_0(x',p',t') \cdot x_0(x',p',t')\right] + \epsilon^2 x_0^2(x',p',t')\right], \tag{2.13a}$$

with

$$x' = x/(1+2\epsilon t)^{1/2},$$

$$p' = p(1+2\epsilon t)^{1/2} - \epsilon x/(1+2\epsilon t)^{1/2},$$

$$t' = \frac{1}{2\epsilon} \ln(1+2\epsilon t).$$
(2.13b)

To summarize, the phase space density $\rho(x,p,t)$, associated with the Hamiltonian H(t) (2.7b) and fulfilling the initial condition (2.10a), is given by (2.13), where the time evolution of initial values of dynamical variables (x_0,p_0) , considered as functions of the final (x,p) and time t, is determined by the stationary Hamiltonian H_0 (2.2) via (2.12).

III. MODEL ADIABATIC SYSTEM OF HARMONICAL OSCILLATORS

To document explicitly the analytical structure of an adiabatic evolution, we will concentrate on the case (1.20) of 1D harmonic strings. The time dependence of the coupling $\lambda/(1+2\epsilon t)$ in (1.20) does not prevent application of the ordinary normal-mode technique in phase space. That is, the canonical transformation of coordinates and momenta

$$x_j(t) = \sum_{\alpha=0}^{N} \Delta_{j\alpha} x_{\alpha}(t) \quad \text{or} \quad x_{\alpha}(t) = \sum_{j=0}^{N} \Delta_{j\alpha} x_j(t) , \qquad (3.1a)$$

$$p_j(t) = \sum_{\alpha=0}^{N} \Delta_{j\alpha} p_{\alpha}(t) \quad \text{or} \quad p_{\alpha}(t) = \sum_{j=0}^{N} \Delta_{j\alpha} p_j(t) , \qquad (3.1b)$$

with

$$\Delta_{j\alpha} = \frac{1}{\sqrt{N+1}} \left[\cos \left[\frac{2\pi}{N+1} \alpha j \right] + \sin \left[\frac{2\pi}{N+1} \alpha j \right] \right]$$
(3.2)

satisfying the orthonormality conditions

$$\sum_{\alpha=0}^{N} \Delta_{j\alpha} \Delta_{k\alpha} = \delta_{jk} , \quad \sum_{j=0}^{N} \Delta_{j\alpha} \Delta_{j\beta} = \delta_{\alpha\beta} ,$$

enables one to map the original Hamiltonian (1.20) onto the one of N+1 independent oscillators with time-dependent frequencies

$$\widetilde{H} = \frac{1}{2} \sum_{\alpha=0}^{N} p_{\alpha}^{2} + \frac{1}{2} \sum_{\alpha=0}^{N} \left[\frac{\omega_{\alpha}}{1 + 2\epsilon t} \right]^{2} x_{\alpha}^{2} , \qquad (3.3a)$$

$$\omega_{\alpha} = 2\lambda \sin \left[\frac{\pi}{N+1} \alpha \right], \quad \alpha = 0, 1, \dots, N.$$
 (3.3b)

In what follows, in order to simplify the notation, we set $\lambda = \frac{1}{2}$. The corresponding equations of motion

$$\frac{\partial x_{\alpha}}{\partial t} = \frac{\partial \widetilde{H}}{\partial p_{\alpha}} = p_{\alpha} , \qquad (3.4a)$$

$$\frac{\partial p_{\alpha}}{\partial t} = -\frac{\partial \tilde{H}}{\partial x_{\alpha}} = -\left[\frac{\omega_{\alpha}}{1 + 2\epsilon t}\right]^{2} x_{\alpha} \tag{3.4b}$$

result in

$$\frac{\partial^2 x_{\alpha}}{\partial t^2} = -\left[\frac{\omega_{\alpha}}{1 + 2\epsilon t}\right]^2 x_{\alpha} . \tag{3.5}$$

The zero-frequency mode $\omega_0 = 0$, corresponding to the center-of-mass coordinate $x_0/\sqrt{N+1}$, is special from the point of view of the adiabatic process—because p_0 is the constant of motion, it breaks up the ergodicity. Therefore, we will project it out by choosing suitable initial conditions: we first divide the Hamiltonian \tilde{H} into two parts:

$$\widetilde{H} = \frac{p_0^2}{2} + \mathcal{H}(\mathbf{x}, \mathbf{p}, t) , \qquad (3.6a)$$

$$\mathcal{H}(\mathbf{x},\mathbf{p},t) = \frac{1}{2} \sum_{\alpha=1}^{N} p_{\alpha}^{2} + \frac{1}{2} \sum_{\alpha=1}^{N} \left[\frac{\omega_{\alpha}}{1 + 2\epsilon t} \right]^{2} x_{\alpha}^{2} , \quad (3.6b)$$

then consider the initial condition

$$\tilde{\rho}(x_0,p_0;\mathbf{x},\mathbf{p};t=0) = f(\mathcal{H}(\mathbf{x},\mathbf{p},0))g(x_0,p_0)$$

with arbitrary $g(x_0,p_0)$ normalized to unity, and finally study the time evolution of

$$\rho(\mathbf{x}, \mathbf{p}, t) = \int dx_0 dp_0 \widetilde{\rho}(x_0, p_0; \mathbf{x}, \mathbf{p}; t)$$

associated with the Hamiltonian $\mathcal{H}(\mathbf{x},\mathbf{p},t)$ and subject to the initial condition

$$\rho(\mathbf{x}, \mathbf{p}, 0) = f \left[\sum_{\alpha=1}^{N} (p_{\alpha}^{2} + \omega_{\alpha}^{2} x_{\alpha}^{2})/2 \right]. \tag{3.7}$$

The stationary Hamiltonian \mathcal{H}_0 , associated with \mathcal{H} (3.6b) in the sense explained in Sec. II, reads

$$\mathcal{H}_0(\mathbf{x}, \mathbf{p}) = \frac{1}{2} \sum_{\alpha=1}^{N} p_{\alpha}^2 + \frac{1}{2} \sum_{\alpha=1}^{N} (\omega_{\alpha}^2 - \epsilon^2) x_{\alpha}^2 . \tag{3.8}$$

The corresponding set of independent harmonic oscillators splits into two subsets: those with $\omega_{\alpha} < \epsilon$ exhibit imaginary frequencies and the initial t=0 values of canonical variables $\{x_{\alpha 0}, p_{\alpha 0}\}$ are given as functions of $\{x_{\alpha}, p_{\alpha}, t\}$ by

$$x_{\alpha 0} = x_{\alpha} \cosh(t \sqrt{\epsilon^2 - \omega_{\alpha}^2}) - \frac{p_{\alpha}}{\sqrt{\epsilon^2 - \omega_{\alpha}^2}} \sinh(t \sqrt{\epsilon^2 - \omega_{\alpha}^2}), \qquad (3.9a)$$

$$p_{\alpha 0} = p_{\alpha} \cosh(t \sqrt{\epsilon^2 - \omega_{\alpha}^2})$$

$$-x_{\alpha} \sqrt{\epsilon^2 - \omega_{\alpha}^2} \sinh(t \sqrt{\epsilon^2 - \omega_{\alpha}^2}), \qquad (3.9b)$$

while those characterized by $\omega_{\alpha} \ge \epsilon$ and ordinary real frequencies yield

$$x_{\alpha 0} = x_{\alpha} \cos(t \sqrt{\omega_{\alpha}^{2} - \epsilon^{2}})$$

$$- \frac{p_{\alpha}}{\sqrt{\omega_{\alpha}^{2} - \epsilon^{2}}} \sin(t \sqrt{\omega_{\alpha}^{2} - \epsilon^{2}}), \qquad (3.10a)$$

$$p_{\alpha 0} = p_{\alpha} \cos(t \sqrt{\omega_{\alpha}^{2} - \epsilon^{2}}) + x_{\alpha} \sqrt{\omega_{\alpha}^{2} - \epsilon^{2}} \sin(t \sqrt{\omega_{\alpha}^{2} - \epsilon^{2}}) . \tag{3.10b}$$

Using formulas (2.13a) and (2.13b), the resulting phase space density then takes the form

$$\rho(\mathbf{x},\mathbf{p},t) = f\left[\sum_{\alpha=1}^{N} \left[A_{\alpha}(t)x_{\alpha}^{2} + B_{\alpha}(t)p_{\alpha}^{2} + C_{\alpha}(t)x_{\alpha}p_{\alpha}\right]\right],$$

where

$$A_{\alpha}(t) = \frac{\omega_{\alpha}^{2}}{2(1+2\epsilon t)} \left[1 + \frac{2\epsilon \sinh\phi_{\alpha}\cosh\phi_{\alpha}}{\sqrt{\epsilon^{2} - \omega_{\alpha}^{2}}} + \frac{2\epsilon^{2}\sinh^{2}\phi_{\alpha}}{\epsilon^{2} - \omega_{\alpha}^{2}} \right], \qquad (3.12a)$$

$$B_{\alpha}(t) = \frac{1 + 2\epsilon t}{2} \left[1 - \frac{2\epsilon \sinh\phi_{\alpha}\cosh\phi_{\alpha}}{\sqrt{\epsilon^2 - \omega_{\alpha}^2}} + \frac{2\epsilon^2 \sinh^2\phi_{\alpha}}{\epsilon^2 - \omega_{\alpha}^2} \right],$$

(3.12b)

$$C_{\alpha}(t) = -\frac{2\epsilon\omega_{\alpha}^{2}\sinh^{2}\phi_{\alpha}}{\epsilon^{2} - \omega_{\alpha}^{2}}, \qquad (3.12c)$$

$$\phi_{\alpha} = \frac{\sqrt{\epsilon^2 - \omega_{\alpha}^2}}{2\epsilon} \ln(1 + 2\epsilon t)$$
 (3.12d)

for $\omega_{\alpha} < \epsilon$, and

$$A_{\alpha}(t) = \frac{\omega_{\alpha}^{2}}{2(1+2\epsilon t)} \left[1 + \frac{2\epsilon \sin\phi_{\alpha}\cos\phi_{\alpha}}{\sqrt{\omega_{\alpha}^{2} - \epsilon^{2}}} + \frac{2\epsilon^{2}\sin^{2}\phi_{\alpha}}{\omega_{\alpha}^{2} - \epsilon^{2}} \right],$$
(3.13a)

$$B_{\alpha}(t) = \frac{1 + 2\epsilon t}{2} \left[1 - \frac{2\epsilon \sin\phi_{\alpha}\cos\phi_{\alpha}}{\sqrt{\omega_{\alpha}^{2} - \epsilon^{2}}} + \frac{2\epsilon^{2}\sin^{2}\phi_{\alpha}}{\omega_{\alpha}^{2} - \epsilon^{2}} \right],$$
(3.13b)

$$C_{\alpha}(t) = -\frac{2\epsilon\omega_{\alpha}^{2}\sin^{2}\phi_{\alpha}}{\omega_{\alpha}^{2} - \epsilon^{2}}, \qquad (3.13c)$$

$$\phi_{\alpha} = \frac{\sqrt{\omega_{\alpha}^2 - \epsilon^2}}{2\epsilon} \ln(1 + 2\epsilon t)$$
 (3.13d)

for $\omega_{\alpha} \ge \epsilon$. Note that coefficients A_{α} , B_{α} , and C_{α} are constrained by a useful algebraic relation

$$4A_{\alpha}(t)B_{\alpha}(t) - C_{\alpha}^{2}(t) = \omega_{\alpha}^{2}. \qquad (3.14)$$

For the case of interest in which the system ensemble at initial time is distributed uniformly over a single energy shell, rescaled by N in order to adapt the formalism to the thermodynamic limit, we have

$$f(E) = \frac{1}{\Sigma(E_0)} \delta(NE_0 - E) . \tag{3.15}$$

The normalization constant

$$\Sigma(E_0) = \int \prod_{\alpha=1}^{N} dx_{\alpha} dp_{\alpha} \delta \left[NE_0 - \sum_{\alpha=1}^{N} (p_{\alpha}^2 + \omega_{\alpha}^2 x_{\alpha}^2)/2 \right]$$
(3.16)

is obtained, after some algebra, in the form

$$\Sigma(E_0) = \frac{(2\pi)^N (NE_0)^{N-1}}{(N-1)! \prod_{\alpha=1}^N \omega_{\alpha}} . \tag{3.16'}$$

Finally, the phase space density reads

$$\rho(\mathbf{x}, \mathbf{p}, t) = \frac{1}{\Sigma(E_0)} \delta \left[NE_0 - \sum_{\alpha=1}^{N} \left[A_{\alpha}(t) x_{\alpha}^2 + B_{\alpha}(t) p_{\alpha}^2 + C_{\alpha}(t) x_{\alpha} p_{\alpha} \right] \right], \quad (3.17)$$

where the normalization constant is found to be time independent.

IV. ANALYTICAL STRUCTURE OF CORRECTIONS TO THE IDEAL ADIABATICITY

For $\epsilon t = \tau$ fixed and in the limit $\epsilon \rightarrow 0$, (3.17) reduces to

$$\rho_0(\mathbf{x}, \mathbf{p}, t) = \frac{1}{\Sigma(E_0)} \delta(NE_0 - (1 + 2\tau)h(\mathbf{x}, \mathbf{p}, \tau)) , \qquad (4.1a)$$

where

$$h(\mathbf{x}, \mathbf{p}, \tau) = \frac{1}{2} \sum_{\alpha=1}^{N} p_{\alpha}^{2} + \frac{1}{2} \sum_{\alpha=1}^{N} \left[\frac{\omega_{\alpha}}{1 + 2\tau} \right]^{2} x_{\alpha}^{2}$$
 (4.1b)

is the "adiabatic transcription" of our Hamiltonian (3.6b). This agrees with the general formula (1.11a) and (1.11b) and, since $\Omega(NE,\tau) \sim (NE)^N (1+2\tau)^N$, with the prescription (1.12) for calculating the slow-time-scale dependence of the single energy shell $\mathcal{E}(\tau) = NE_0/(1+2\tau)$ over which the system ensemble is distributed under ideal adiabaticity conditions. It also agrees with the well-known adiabatic invariance of the action variables. The counterparts of energy moments (1.18), measuring the adiabatic invariance of Ω when ϵ is finite, read

$$M_n(t) = \int d\mathbf{x} d\mathbf{p} \, \rho(\mathbf{x}, \mathbf{p}, t) \left[h(\mathbf{x}, \mathbf{p}, \tau) - \frac{NE_0}{1 + 2\tau} \right]^n \tag{4.2}$$

(for tactical reasons, we do not rescale the expression in square brackets by N).

To clarify the general analytical structure of the moments, we will first study in detail the lowest-order moment $M_1(t)$. It is readily obtained in the explicit form

$$M_1(t) = \frac{2NE_0}{1 + 2\tau} \frac{1}{N} \sum_{\alpha=1}^{N} v_{\alpha} , \qquad (4.3)$$

with

$$v_{\alpha} = \begin{cases} \frac{\epsilon^{2}}{\epsilon^{2} - \omega_{\alpha}^{2}} \sinh^{2} \left[\frac{\sqrt{\epsilon^{2} - \omega_{\alpha}^{2}}}{2\epsilon} \ln(1 + 2\tau) \right] & \text{for } \omega_{\alpha} < \epsilon \\ \frac{\epsilon^{2}}{\omega_{\alpha}^{2} - \epsilon^{2}} \sin^{2} \left[\frac{\sqrt{\omega_{\alpha}^{2} - \epsilon^{2}}}{2\epsilon} \ln(1 + 2\tau) \right] & \text{for } \omega_{\alpha} \ge \epsilon \end{cases}$$
 (4.4a)

For finite N, M_1 is a singular function of ϵ with a nontrivial leading term, as was expected: the time correlations of dynamical variables corresponding to instantaneous Hamiltonian (3.6b) with ϵt fixed do not decay to zero at asymptotically large times, which evokes an inconsistency even on the first level of the MTS scheme. In the limit $N \to \infty$, i.e., in the regime with energy dissipation, (4.3) and (4.4) can be rewritten as

$$M_1(t) = \frac{2NE_0}{1 + 2\tau} (I_1 + I_2) , \qquad (4.5a)$$

where

$$I_1 = \int_0^{\arcsin\epsilon} \frac{d\psi}{\pi/2} v_{\psi} , \quad I_2 = \int_{\arcsin\epsilon}^{\pi/2} \frac{d\psi}{\pi/2} v_{\psi} ,$$
 (4.5b)

and v_{ψ} is the continuous counterpart of v_{α} :

$$v_{\psi} = \begin{cases} \frac{\epsilon^{2}}{\epsilon^{2} - \sin^{2}\psi} \sinh^{2}\left[\frac{\sqrt{\epsilon^{2} - \sin^{2}\psi}}{2\epsilon} \ln(1+2\tau)\right] & \text{for } \psi < \arcsin\epsilon \\ \frac{\epsilon^{2}}{\sin^{2}\psi - \epsilon^{2}} \sin^{2}\left[\frac{\sqrt{\sin^{2}\psi - \epsilon^{2}}}{2\epsilon} \ln(1+2\tau)\right] & \text{for } \psi > \arcsin\epsilon \end{cases}$$

$$(4.6a)$$

Substituting $\phi = \arccos \sqrt{1 - \sin^2 \psi / \epsilon^2}$ in integral I_1 , we obtain

$$I_{1} = \int_{0}^{\pi/2} \frac{d\phi}{\pi/2} \frac{\mu}{\cos\phi\sqrt{1 + \mu^{2}\cos^{2}\phi}} \sinh^{2}\left[\frac{\cos\phi}{2}\ln(1 + 2\tau)\right] , \qquad (4.7)$$

with $\mu = \epsilon/\sqrt{1-\epsilon^2}$. Taylor expansion of the square root in powers of μ^2 then provides a convergent series expansion of I_1 around $\mu = 0$ and hence $\epsilon = 0$:

$$I_1 = \sum_{n=0}^{\infty} (-1)^n \frac{(2n)!}{2^{2n} (n!)^2} \mu^{2n+1} \int_0^{\pi/2} \frac{d\phi}{\pi/2} \cos^{2n-1}\phi \sinh^2 \left[\frac{\cos\phi}{2} \ln(1+2\tau) \right] . \tag{4.8}$$

The <u>analytical</u> properties of integral I_2 near $\epsilon = 0$ pose a more complicated problem. The substitution $x = \sqrt{\sin^2 \psi / \epsilon^2 - 1}$ yields

$$I_2 = \frac{\mu}{\pi/2} \widetilde{I}_2(\mu) , \qquad (4.9a)$$

$$\widetilde{I}_{2}(\mu) = \int_{0}^{1/\mu} \frac{dx}{x\sqrt{1+x^{2}\sqrt{1-\mu^{2}x^{2}}}} \sin^{2}\left[\frac{x}{2}\ln(1+2\tau)\right]. \tag{4.9b}$$

To deduce the value of $\lim_{\mu\to 0} \widetilde{I}_2(\mu)$, let us first split the integral $\int_0^{1/\mu}$ into two parts $\int_0^{1/\mu^{\delta}} + \int_{1/\mu^{\delta}}^{1/\mu} = \widetilde{I}_2^{(1)} + \widetilde{I}_2^{(2)}$ where $0 \le \delta \le 1$. The lower and upper bounds of the first integral part $\widetilde{I}_2^{(1)}$ are given by

$$\int_{0}^{1/\mu^{\delta}} \frac{dx}{x\sqrt{1+x^{2}}} \sin^{2}\left[\frac{x}{2}\ln(1+2\tau)\right] \leq \widetilde{I}_{2}^{(1)}(\mu) \leq \frac{1}{\sqrt{1-\mu^{2(1-\delta)}}} \int_{0}^{1/\mu^{\delta}} \frac{dx}{x\sqrt{1+x^{2}}} \sin^{2}\left[\frac{x}{2}\ln(1+2\tau)\right]. \tag{4.10}$$

Since

$$\int_{1/\mu^{\delta}}^{1/\mu} \frac{x \, dx}{\sqrt{1-\mu^{2}x^{2}}} = \frac{\sqrt{1-\mu^{2(1-\delta)}}}{\mu^{2}} ,$$

the second integral part $\tilde{I}_2^{(2)}$ is bounded as follows:

$$\mu \left[\frac{1 - \mu^{2(1-\delta)}}{1 + \mu^{2}} \right]^{1/2} \min_{1/\mu^{\delta} \le x \le 1/\mu} \sin^{2} \left[\frac{x}{2} \ln(1+2\tau) \right] \\ \le \widetilde{I}_{2}^{(2)}(\mu) \le \mu^{3\delta-2} \left[\frac{1 - \mu^{2(1-\delta)}}{1 + \mu^{2\delta}} \right]^{1/2} \max_{1/\mu^{\delta} \le x \le 1/\mu} \sin^{2} \left[\frac{x}{2} \ln(1+2\tau) \right] . \tag{4.11}$$

By combining (4.10) and (4.11) we see that, for $\frac{2}{3} < \delta < 1$, the lower and upper bounds of $\tilde{I}_2(0)$ coincide, and one obtains

$$\widetilde{I}_{2}(0) = \int_{0}^{\infty} \frac{dx}{x\sqrt{1+x^{2}}} \sin^{2}\left[\frac{x}{2}\ln(1+2\tau)\right]. \tag{4.12}$$

To specify the character of higher-order terms of the μ expansion, let us suppose that $\tilde{I}_2(\mu)$ is analytic around $\mu = 0$, i.e.,

$$\widetilde{I}_{2}(\mu) = \widetilde{I}_{2}(0) + \mu \frac{\partial \widetilde{I}_{2}(\mu)}{\partial \mu} \bigg|_{\mu=0} + \cdots , \qquad (4.13)$$

where

$$\frac{\partial \tilde{I}_{2}(\mu)}{\partial \mu} = -\frac{1}{\mu} \int_{0}^{1/\mu} \frac{dx}{\sqrt{1 - \mu^{2} x^{2}}} \frac{\partial}{\partial x} \left[\frac{\sin^{2}[x \ln(1 + 2\tau)/2]}{\sqrt{1 + x^{2}}} \right]. \tag{4.14}$$

Using the procedure applied to the calculation of $\tilde{I}_2(0)$, the expression on the right-hand side of (4.14) can be shown to include terms of the form $\sin[\ln(1+2\tau)/2\mu]$ oscillating increasingly rapidly in the limit $\mu \to 0$, which is evidence of singular behavior. We therefore conclude that the first moment exhibits a singular expansion around $\epsilon = 0$, but with the leading term $\sim \epsilon$:

$$M_{1}(t) = \frac{2NE_{0}}{1+2\tau} \left\{ \frac{\epsilon}{\pi/2} \left[\int_{0}^{\pi/2} \frac{d\phi}{\cos\phi} \sinh^{2}\left[\frac{\cos\phi}{2} \ln(1+2\tau) \right] + \int_{0}^{\infty} \frac{dx}{x\sqrt{1+x^{2}}} \sin^{2}\left[\frac{x}{2} \ln(1+2\tau) \right] \right] + (\text{singular } \epsilon \text{ terms of order} > \epsilon) \right\}.$$

$$(4.15)$$

In order to reveal the analytical structure of all moments $\{M_n(t)\}_{n=1}^{\infty}$, we introduce the generating function

$$M(y) = \int \prod_{\alpha=1}^{N} dx_{\alpha} dp_{\alpha} \rho(\mathbf{x}, \mathbf{p}, t) \exp \left\{ -y \left[h(\mathbf{x}, \mathbf{p}, \tau) - \frac{NE_0}{1 + 2\tau} \right] \right\}, \tag{4.16}$$

which produces moments according to

$$M_n(t) = (-1)^n \frac{\partial^n M(y)}{\partial y^n} \bigg|_{y=0} . \tag{4.17}$$

Expressing the δ function in ρ [see (3.17)] via

$$\delta(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \exp[(ik + c_1)x],$$

with arbitrary $c_1 > 0$, we have

$$M(y) = \exp\left[\frac{NE_0 y}{1+2\tau}\right] \frac{(N-1)! \prod_{\alpha=1}^{N} \omega_{\alpha}}{(2\pi)^N (NE_0)^{N-1}} \times \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{(ik+c_1)NE_0} \prod_{\alpha=1}^{N} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx_{\alpha} dp_{\alpha} \exp\left[-\frac{1}{2}(x_{\alpha}, p_{\alpha}) \mathbf{V}_{\alpha}(x_{\alpha}, p_{\alpha})^T\right]$$

$$(4.18a)$$

where the 2×2 matrix V_{α} is given by

$$\mathbf{V}_{\alpha} = \begin{bmatrix} 2A_{\alpha}(ik+c_{1}) + y \left[\frac{\omega_{\alpha}}{1+2\tau}\right]^{2} & C_{\alpha}(ik+c_{1}) \\ C_{\alpha}(ik+c_{1}) & 2B_{\alpha}(ik+c_{1}) + y \end{bmatrix}. \tag{4.18b}$$

Its determinant reads

$$\det \mathbf{V}_{\alpha} = \left[\frac{y \,\omega_{\alpha}}{1 + 2\tau} \right]^{2} \left\{ 1 + 2(1 + 2v_{\alpha}) \left[\frac{(ik + c_{1})(1 + 2\tau)}{y} \right] + \left[\frac{(ik + c_{1})(1 + 2\tau)}{y} \right]^{2} \right\}, \tag{4.19}$$

where v_{α} is defined by (4.4). Let us assume that c_1 is sufficiently large to ensure the convergence of Gaussian integrals in (4.18a), i.e., the real parts of the two eigenvalues are positive for every \mathbf{V}_{α} . Performing the integrations over all (x_{α}, p_{α}) , and using the substitutions

$$k \to l = k(1+2\tau)/y$$
, $c_1 \to c_2 = c_1(1+2\tau)/y$,
 $y \to \overline{y} = yE_0/(1+2\tau)$,

one obtains

$$M(\bar{y}) = e^{N\bar{y}} \frac{(N-1)!}{N^{N-1}(i\bar{y})^{N-1}} \times \int_{-\infty}^{\infty} \frac{dl}{2\pi i} e^{(il+c_2)N\bar{y}} \times \prod_{\alpha=1}^{N} \frac{1}{\sqrt{(l-il_{\alpha}^{+})(l-il_{\alpha}^{-})}}, \qquad (4.20a)$$

$$l_{\alpha}^{\pm} = 1 + c_2 + 2v_{\alpha} \pm 2\sqrt{v_{\alpha}(1 + v_{\alpha})}$$
 (4.20b)

Without any loss of generality, we will restrict ourselves to the case N even. Taking advantage of the symmetry in frequencies

$$v_{\alpha} = v_{N+1-\alpha} \ (\alpha = 1, \ldots, N/2)$$
,

and using the substitutions

$$l \to z = (il + c_2 + 1)\overline{y}$$
, $c_2 \to c_3 = (c_2 + 1)\overline{y}$,

we finally arrive at

$$M(\bar{y}) = \frac{(N-1)!}{N^{N-1}} \int_{c_3 - i\infty}^{c_3 + i\infty} \frac{dz}{2\pi i} e^{Nz} \prod_{\alpha=1}^{N/2} \frac{1}{(z + z_{\alpha}^+)(z + z_{\alpha}^-)},$$

(4.21-)

$$z_{\alpha}^{\pm} = 2\overline{y} \left[v_{\alpha} \pm \sqrt{v_{\alpha} (1 + v_{\alpha})} \right]. \tag{4.21b}$$

For the case of interest, $N \rightarrow \infty$, (4.21) can be rewritten as follows:

$$M(\bar{y}) = \frac{(N-1)!}{N^{N-1}} \int_{c_3 - i\infty}^{c_3 + i\infty} \frac{dz}{2\pi i} \exp[N\Phi(z)] , \qquad (4.22)$$

where

$$\Phi(z) = z - \frac{1}{2} \int_0^{\pi/2} \frac{d\psi}{\pi/2} \ln[(z + z_{\psi}^+)(z + z_{\psi}^-)], \quad (4.23a)$$

$$z_{\psi}^{\pm} = 2\overline{y}[v_{\psi} \pm \sqrt{v_{\psi}(1+v_{\psi})}],$$
 (4.23b)

and v_{ψ} is given by (4.6). Let z^* be the extreme point of $\Phi(z)$: $\partial \Phi(z)/\partial z\big|_{z=z^*}=0$ or, more explicitly,

$$1 - \frac{1}{2} \int_0^{\pi/2} \frac{d\psi}{\pi/2} \left[\frac{1}{z^* + z_{\psi}^+} + \frac{1}{z^* + z_{\psi}^-} \right] = 0 . \quad (4.24)$$

Since $\partial^2 \Phi(z)/\partial z^2 > 0$ everywhere, z^* is the only minimum point of $\Phi(z)$. Let us choose $c_3 = z^*$. Consequently, along the integration path in (4.22), $\Phi(z)$ attains its maximum at $z = z^*$, and in the limit $N \to \infty$ we find

$$M(\bar{y}) \sim \exp\{N[\Phi(z^*) - 1]\}$$
 (4.25)

This relation, together with the definition of $\Phi(z)$, z_{ψ}^{\pm} (4.23) and the implicit equation for z^* (4.24), represent a closed-form solution for the generating function of moments

It is simple to deduce systematically from Eq. (4.24) the y expansion of z^* around y = 0,

$$z^*(y) = 1 - \frac{2E_0 y}{1 + 2\tau} \int_0^{\pi/2} \frac{d\psi}{\pi/2} v_{\psi} + \left[\frac{2E_0 y}{1 + 2\tau} \right]^2 \left[\int_0^{\pi/2} \frac{d\psi}{\pi/2} v_{\psi} (1 + 2v_{\psi}) - \left[\int_0^{\pi/2} \frac{d\psi}{\pi/2} v_{\psi} \right]^2 \right] + O(y^3) . \tag{4.26}$$

The moments, generated according to (4.17), are then available explicitly: in the lowest n=1 order $M_1(t)$, (4.5) is reproduced,

$$M_2(t) = \left[\frac{2E_0}{1+2\tau}\right]^2 \left[N(N-1)\left[\int_0^{\pi/2} \frac{d\psi}{\pi/2} v_{\psi}\right]^2 + N\int_0^{\pi/2} \frac{d\psi}{\pi/2} v_{\psi}(1+2v_{\psi})\right], \tag{4.27}$$

and so on.

As has been indicated above, our primary interest is directed toward the calculation of the leading term of the moment (generating function) expansion in the slowness parameter ϵ . To simplify the notation, we set $E_0/(1+2\tau)$ equal to unity—this combination enters into the expression for M_n only in the *n*th power as the proportionality prefactor. Let us rewrite (4.23) as

$$\Phi(z) = z - \ln z - \frac{1}{2}(I_1 + I_2) , \qquad (4.28)$$

where

$$I_1 = \int_0^{\arcsin \epsilon} \frac{d\psi}{\pi/2} \ln[1 + 4yz^{-1}(1 - yz^{-1})v_{\psi}], \qquad (4.29a)$$

$$I_2 = \int_{\arcsin \epsilon}^{\pi/2} \frac{d\psi}{\pi/2} \ln[1 + 4yz^{-1}(1 - yz^{-1})v_{\psi}] . \tag{4.29b}$$

Using the analysis of the analytical structure of integrals I_1, I_2 around $\epsilon = 0$ analogous to that presented previously for $M_1(t)$, it is easy to show that

$$I_{1} \sim \frac{\epsilon}{\pi/2} \int_{0}^{\pi/2} d\phi \cos\phi \ln\left\{1 + \frac{4yz^{-1}(1 - yz^{-1})}{\cos^{2}\phi} \sinh^{2}\left[\frac{\cos\phi}{2}\ln(1 + 2\tau)\right]\right\},$$
(4.30a)

$$I_{2} \sim \frac{\epsilon}{\pi/2} \int_{0}^{\infty} \frac{dx \, x}{\sqrt{1+x^{2}}} \ln \left\{ 1 + \frac{4yz^{-1}(1-yz^{-1})}{x^{2}} \sin^{2} \left[\frac{x}{2} \ln(1+2\tau) \right] \right\}. \tag{4.30b}$$

Since $z^* \sim 1$ in the limit $\epsilon \rightarrow 0$, and $z^* - \ln z^* = 1 + O(\epsilon^2)$, we finally obtain

$$M(y) \sim 1 - \frac{N\epsilon}{\pi} \left[\int_0^{\pi/2} d\phi \cos\phi \ln\left\{ 1 + 4y(1-y) \frac{1}{\cos^2\phi} \sinh^2\left[\frac{\cos\phi}{2} \ln(1+2\tau) \right] \right\}$$

$$+ \int_0^{\infty} \frac{dx \, x}{\sqrt{1+x^2}} \ln\left\{ 1 + 4y(1-y) \frac{1}{x^2} \sin^2\left[\frac{x}{2} \ln(1+2\tau) \right] \right\}$$

$$+ (\operatorname{singular} \epsilon \text{ terms of order} > \epsilon) . \tag{4.31}$$

V. COMPARISON WITH THE MTS APPROACH AND DISCUSSION

Let us now study the propagation of the microcanonical ensemble governed by our adiabatic Hamiltonian (4.1b), within the MTS method explained in Sec. I. The adiabatic normalization constant (1.11b) and the auxiliary quantity $u(E,\tau)$, defined by (1.14), are readily obtained in the form

$$\Sigma(E,\tau) = \frac{(2\pi)^N}{(N-1)!} \prod_{\alpha=1}^N \omega_{\alpha} E^{N-1} (1+2\tau)^N , \qquad (5.1)$$

$$u(E,\tau) = -\frac{2E}{1+2\tau} \ . \tag{5.2}$$

Since

$$\begin{split} \frac{\partial h}{\partial \tau} - u &= \frac{2E}{1 + 2\tau} - \sum_{\alpha = 1}^{N} \frac{2\omega_{\alpha}^{2} x_{\alpha}^{2}}{(1 + 2\tau)^{3}} , \\ \mathcal{O}_{\tau}(s) \left[\frac{\partial h}{\partial \tau} - u \right] &= \frac{2E}{1 + 2\tau} - \sum_{\alpha = 1}^{N} \frac{2\omega_{\alpha}^{2}}{(1 + 2\tau)^{3}} \left[x_{\alpha} \cos \left[\frac{\omega_{\alpha} s}{1 + 2\tau} \right] + \frac{p_{\alpha}}{\omega_{\alpha}} (1 + 2\tau) \sin \left[\frac{\omega_{\alpha} s}{1 + 2\tau} \right] \right]^{2} , \end{split}$$

then after some algebra, the autocorrelation function (1.17) becomes

$$C(s) = \left[\frac{2E}{1+2\tau}\right]^2 \frac{1}{(N+1)N} \sum_{\alpha=1}^{N} \cos\left[\frac{2\omega_{\alpha}s}{1+2\tau}\right]. \tag{5.3}$$

For finite N, C(s) is a superposition of oscillating terms which does not tend to zero for asymptotically large s. On the other hand, in the limit $N \rightarrow \infty$ we have

$$C(s) = \left[\frac{2E}{1+2\tau}\right]^2 \frac{1}{N+1} J_0 \left[\frac{2s}{1+2\tau}\right], \tag{5.4}$$

where

$$J_0(z) = \int_{-\pi}^{\pi} \frac{d\psi}{2\pi} e^{iz \sin\psi} = \int_{0}^{\pi} \frac{d\psi}{\pi} \cos(z \sin\psi)$$
 (5.5)

is the ordinary Bessel function. Owing to $\int_0^\infty dz \, J_0(z) = 1$ [11], the key correlation integral (1.16) converges as is needed,

$$G_2(E,\tau) = \frac{4E^2}{1+2\tau} \frac{1}{N+1} . \tag{5.6}$$

As concerns the components of the ϵ expansion (1.2) of the phase space density ρ , the lowest-order ρ_0 has already been obtained in (4.1a) and, with respect to (1.5), one has

$$f_0(E,\tau) = \frac{(N-1)! \prod_{\alpha=1}^{N} \omega_{\alpha}}{(2\pi)^{N} (NE_0)^{N-1}} \delta(NE_0 - (1+2\tau)E) . \tag{5.7}$$

The unknown part of ρ_1 (1.13), f_1 , satisfies a PDE of type (1.15), which is written, after the substitution

$$f_1(E,\tau) = \frac{(N-1)! \prod_{\alpha=1}^{N} \omega_{\alpha}}{(2\pi)^N (NE_0)^{N-1}} \widetilde{f}_1(E,\tau) , \qquad (5.8)$$

as follows:

$$(1+2\tau)\frac{\partial \tilde{f}_{1}}{\partial \tau} - 2E\frac{\partial \tilde{f}_{1}}{\partial E}$$

$$= \frac{2}{N+1}E^{2}(1+2\tau)^{2}\delta''(NE_{0} - (1+2\tau)E)$$

$$-2E(1+2\tau)\delta'(NE_{0} - (1+2\tau)E) . \tag{5.9}$$

This PDE can be solved by using the method of characteristics:

$$\widetilde{f}_{1}(E,\tau) = \ln(1+2\tau) \left\{ \frac{1}{N+1} E^{2} (1+2\tau)^{2} \delta''(NE_{0} - (1+2\tau)E) - E(1+2\tau)\delta'(NE_{0} - (1+2\tau)E) \right\}, \tag{5.10}$$

so that

$$f_{1}(E,\tau) = \frac{(N-1)! \prod_{\alpha=1}^{N} \omega_{\alpha}}{(2\pi)^{N} (NE_{0})^{N-1}} \ln(1+2\tau) \left[\frac{1}{N+1} \frac{\partial^{2}}{\partial E_{0}^{2}} \left\{ \left[\frac{E(1+2\tau)}{N} \right]^{2} \delta(NE_{0} - (1+2\tau)E) \right\} - \frac{\partial}{\partial E_{0}} \left\{ \left[\frac{E(1+2\tau)}{N} \right] \delta(NE_{0} - (1+2\tau)E) \right\} \right].$$
 (5.11)

As explained in Sec. I, the term $\epsilon f_1(h,\tau)$ in ρ is the only one which contributes to the generating function of moments $\{M_n(t)\}$:

$$M(y) = 1 + \epsilon \int d\mathbf{z} \, f_1(h,\tau) \exp\left\{ y \left[\frac{N\overline{E}_0}{1 + 2\tau} - h(\mathbf{z},\tau) \right] \right\} \Big|_{\overline{E}_0 = E_0}$$

$$= 1 + \frac{\epsilon \ln(1 + 2\tau)}{E_0^{N-1}} \left[\frac{1}{N+1} \frac{\partial^2}{\partial E_0^2} \left\{ E_0^{N+1} \exp\left[\frac{yN}{1 + 2\tau} (\overline{E}_0 - E_0) \right] \right\} \right]$$

$$- \frac{\partial}{\partial E_0} \left\{ E_0^N \exp\left[\frac{yN}{1 + 2\tau} (\overline{E}_0 - E_0) \right] \right\} \Big|_{\overline{E}_0 = E_0}. \tag{5.12}$$

Finally, in units of $E_0/(1+2\tau)=1$, we find the relation

$$M(v) = 1 - N\epsilon v (1 - v) \ln(1 + 2\tau)$$
 (5.13)

possessing the symmetry $y \rightarrow 1-y$ of the exact leading order of the generating function (4.31). Only the first two moments are nonzero in the leading ϵ order,

$$M_1 = N\epsilon \ln(1+2\tau) , \qquad (5.14a)$$

$$M_2 = 2N\epsilon \ln(1+2\tau) , \qquad (5.14b)$$

as generally holds with the MTS method.

To make contact with the exact result, let us expand M(y), (4.31) for a given power of y, in $\ln(1+2\tau)$, and consider the leading-order term (obviously analogous to the leading-order term of the τ expansion):

$$M(y) = 1 - \frac{2N\epsilon}{\pi} \left\{ \sum_{n=1}^{\infty} \left[y^{2n-1} - \frac{1}{n} y^{2n} \right] \right\}$$

$$\times [\ln(1+2\tau)]^{2n-1}$$

$$\times \int_0^\infty dx \frac{\sin^{2n}x}{x^{2n}} + \cdots \bigg\} . \qquad (5.15)$$

Note that only the second integral in (4.31) contributes to (5.15), and that the expansion in $ln(1+2\tau)$ is singular. Form (5.15), one finds

$$M_{2n-1} = N\epsilon \left\{ (2n-1)! [\ln(1+2\tau)]^{2n-1} \frac{2}{\pi} \right.$$

$$\times \int_{0}^{\infty} dx \frac{\sin^{2n}x}{x^{2n}} + \cdots \right\}, \qquad (5.16a)$$

$$M_{2n} = N\epsilon \left\{ 2(2n-1)! [\ln(1+2\tau)]^{2n-1} \frac{2}{\pi} \right.$$

$$\times \int_{0}^{\infty} dx \frac{\sin^{2n}x}{x^{2n}} + \cdots \right\}, \qquad (5.16b)$$

for $n=1,2,\ldots$. Taking into account the equality $\int_0^\infty dx \sin^2 x/x^2 = \pi/2$ and comparing (5.16a) and (5.16b) for n=1 with (5.14a) and (5.14b), we observe that the MTS scheme at the assumed level produces the exact result in the leading order of $\ln(1+2\tau)$, i.e., its validity (in the leading order of ϵ) is restricted to very small values of slow time scale τ . As τ increase, higher moments become relevant: they constitute an interesting hierarchy of pairs $\{M_{2n-1}, M_{2n}\}$ with prefactors to ϵ of the same order $O(\tau^{2n-1})$.

In conclusion, expansions in ϵ of the energy moments $\{M_n(t)\}\$ (1.81), which measure the deviation from the ideal adiabaticity, exhibits, for our exactly solvable example of adiabatic evolution, the leading-order terms $\sim \epsilon$ as predicted by the MTS method; i.e., possible resummations of higher-order singular terms have no fundamental effects. On the other hand, the proportionality factor of the leading-order terms is renormalized with respect to the MTS estimate. While the MTS theory based on the of the formal expansions $\rho(t,\tau) = \rho_0(\tau) + \epsilon \rho_1(t,\tau)$ implies that $M_1, M_2 \sim \epsilon$ and all higher-order moments M_n scale like e^{ν_n} $(\nu_n \ge 2)$, the exact result reveals that all moments are of order $O(\epsilon)$: they couple into pairs $\{M_{2n-1}, M_{2n}\}$ with the prefactors of the same slow-time-scale order $O(\tau^{2n-1})$, and the MTS method is adequate only in the marginal limit $\tau \to 0$. The MTS theory with $\rho_1(t,\tau)$ included picks out the lowest couple of the hierarchy, $\{M_1,M_2\}$, of the order $O(\tau)$ for $h(\mathbf{z},\tau)$ analytic at $\tau=0$, as can be shown from (1.15) with initial condition $f_1(E,0)=0$, for an arbitrary ergodic adiabatic evolution which satisfies consistency requirements. We therefore suggest that the hierarchical structure of the moments observed here is a more general feature of adiabatic processes. The failure of the MTS approach to predict correctly the prefactor of the leading ϵ term is intuitively connected with an inconsistency on a higher level of the scheme.

We do not consider our solvable model to be exceptional, and expect similar phenomena for a large class of systems. It must be stressed that this class is characterized by the decay of transients (physically, because their energy is sent out to infinity), and so it is only the slowly varying component, mirroring the applied adiabatic forces, that remains to be analyzed in detail. The reader can readily verify that if we were to have used only a finite set of oscillators, there would have remained as well a quasisinusoidal variation which induces a completely different type of correction term. In any case, the worked-out example shows that the MTS method has to be developed further in higher orders to obtain relevant information abut the character of nonanalyticity around $\epsilon = 0$ as well as possible additional more strict consistency requirements. The practical relaxation of such a program is, however, far from simple.

ACKNOWLEDGMENTS

This work was supported in part by grants from the National Aeronautics and Space Administration, and the National Science Foundation.

^[1] V. I. Arnold, Dynamical Systems III (Springer-Verlag, Berlin, 1988), Chap. 5.

^[2] E. Ott, Phys. Rev. Lett. 42, 1628 (1979).

^[3] R. C. Davidson, Methods in Nonlinear Plasma Theory (Academic, New York, 1972), Sec. 1.3.

^[4] R. Brown, E. Ott, and C. Grebogi, Phys. Rev. Lett. 59, 1173 (1987).

^[5] R. Brown, E. Ott, and C. Grebogi, J. Stat. Phys. 49, 511 (1987).

^[6] M. Wilkinson, J. Phys. A 23, 3603 (1990).

^[7] C. Jarzynski, Phys. Rev. A 46, 7498 (1992).

^[8] C. Jarzynski, Phys. Rev. Lett. 71, 839 (1993).

^[9] A. A. Maradudin, E. W. Montroll, G. W. Weiss, and I. P. Ipatova, Theory of lattice Dynamics in the Harmonic Approximation, 2nd ed. (Academic, New York, 1971).

^[10] E. Kamke, Differential Gleichungen, 3rd ed. (Chelsea, New York, 1959).

^[11] I. S. Gradsteyn and I. M. Ryzhik, *Table of Integrals*, Series, and Products, 5th ed. (Academic, San Diego, 1994).