

Classical dynamics of the quantum harmonic chain

Todd A. Brun*

Institute for Theoretical Physics, University of California, Santa Barbara, California 93106-4030

James B. Hartle†

Department of Physics, University of California, Santa Barbara, California 93106-9530

(Received 21 May 1999; published 11 November 1999)

The origin of classical predictability is investigated for the one dimensional harmonic chain considered as a closed quantum mechanical system. By comparing the properties of a family of coarse-grained descriptions of the chain, we conclude that local coarse grainings in this family are more useful for prediction than nonlocal ones. A quantum mechanical system exhibits classical behavior when the probability is high for histories having the correlations in time implied by classical deterministic laws. But approximate classical determinism holds only for certain coarse grainings and then only if the initial state of the system is suitably restricted. Coarse grainings by the values of the hydrodynamic variables (integrals over suitable volumes of densities of approximately conserved quantities) define the histories usually used in classical physics. But what distinguishes this coarse graining from others? This paper approaches this question by analyzing a family of coarse grainings for the linear harmonic chain. At one extreme in the family the chain is divided into local groups of N atoms. At the other extreme the N atoms are distributed nonlocally over the whole chain. Each coarse graining follows the average (center of mass) positions of the groups and ignores the “internal” coordinates within each group, these constituting a different environment for each coarse graining. For an initial condition where long wavelength modes are excited and short wavelength modes are distributed thermally we find that the coarse-grained positions obey deterministic equations of motion accompanied by noise. The noise is greater the more nonlocal the coarse graining. Further, the deterministic equations require more time steps to evolve over a given time interval for the nonlocal coarse grainings than for the local ones. A continuum limit is possible only for the near local coarse grainings. For parameters of the model characteristic of realistic situations these features strongly favor the local coarse grainings over the nonlocal ones for prediction. Each of these differences can be traced to the approximate conservation of the local center of mass momentum. We then consider the chain quantum mechanically and show that, for realistic parameters, all the coarse grainings decohere rapidly compared to dynamical time scales. We conclude that noise, decoherence, and computational complexity favor locality over nonlocality for deterministic predictability. [S0556-2821(99)02622-3]

PACS number(s): 03.65.Bz

I. INTRODUCTION

As far as we know them, the laws of physics that apply universally to all physical systems are quantum mechanical. The universe at a fundamental level is therefore characterized by indeterminacy and distributed probabilities. The wide range of applicability of classical deterministic laws is an empirical fact to be explained from the universe’s quantum dynamics and initial quantum state. This paper investigates the origin of classical predictability for the very simple model of a linearized chain of idealized atoms in the context of the quantum mechanics of closed systems [1–3], most generally quantum cosmology. We exhibit decoherent sets of coarse-grained histories for which, given suitable restrictions on the state, the probability is high for histories exhibiting the correlations in time governed by the classical wave equation. We shall compare these quasiclassical coarse grainings with a class of others and analyze why the classical coarse

grainings are the most predictable in the class.

Why do we raise the question of the origin of classical predictability over 70 years after the initial formulation of quantum mechanics? Every quantum mechanics text contains some treatment of this question. Ehrenfest’s theorem is the starting point for one such discussion. For a nonrelativistic particle of mass m moving in one dimension in a potential $V(x)$, Ehrenfest’s theorem is the exact relation between expected values:

$$m \frac{d^2 \langle x \rangle}{dt^2} = - \left\langle \frac{\partial V(x)}{\partial x} \right\rangle. \quad (1.1)$$

This is not a deterministic equation of motion, but for certain states, typically narrow wave packets, the expected value of the force may be approximated by the force at the expected value of the position, thereby giving a classical equation of motion for that expected value:

$$m \frac{d^2 \langle x \rangle}{dt^2} = - \frac{\partial V(\langle x \rangle)}{\partial x}. \quad (1.2)$$

*Current address: Department of Physics, Carnegie Mellon University, Pittsburgh, PA 15213.

Email address: tbrun@andrew.cmu.edu

†Email address: hartle@cosmic.physics.ucsb.edu

This equation shows that the orbit of the center of a narrow wave packet obeys Newton's laws.

This kind of elementary derivation already exhibits two necessary requirements for a quantum system to exhibit classical deterministic behavior. Some coarseness in the description is needed, as well as a restriction on the initial quantum state. However, otherwise this kind of demonstration does not address the issues we hope to discuss in quantum cosmology for the following reasons:

(i) The behavior of expected values in time is not enough to define classical behavior. Equations of motion predict *correlations* in time, which in quantum mechanics are properties of the probabilities for time *histories*. The statement that the Earth moves on a classical orbit is most correctly understood in quantum theory as the assertion that, among a decoherent set of coarse-grained histories of the Earth's position in time, the probability is high for histories exhibiting the deterministic correlations in time implied by Newton's laws and low for all others. To discuss classical predictability therefore we should be dealing with the probabilities of time histories, not merely with the time dependence of expected values.

(ii) The Ehrenfest derivation relies on a close connection between the equations of motion arising from the fundamental action and the phenomenological equations of motion determining classical correlations. There is no such connection in general. In general situations we expect classical equations of motion like the Navier-Stokes equation, relating values of continuum hydrodynamic variables at different times, incorporating phenomenological equations of state, and exhibiting dissipation, noise, and irreversibility. The equations of the fundamental theory, whether one takes it to be quantum electrodynamics or M theory, exhibit none of these phenomena and are at best only distantly related in form. We need to derive the *form* of the classical equations of motion as well as the probabilities with which they are satisfied.

(iii) The Ehrenfest derivation posits the variable—the position x —in which classical deterministic behavior is exhibited. But the quantum mechanics of any closed system will exhibit a great many complementary sets of decoherent histories, some of which may exhibit deterministic correlations in time. What distinguishes coarse grainings in terms of the familiar quasiclassical variables from all other possibilities exhibited by a closed quantum mechanical system? Certainly it is not their relation to the variables of the fundamental theory, which is typically only distant, as described above. Rather, it must lie in the relative utility of different coarse grainings for prediction, with quasiclassical variables being highly predictable. A complete derivation of classical predictability must seek to distinguish classical coarse grainings from all others.

(iv) The Ehrenfest derivation deals with the expected outcomes of “measurements” on an otherwise isolated subsystem. However, in quantum cosmology we are interested in classical behavior in much more general situations, over cosmological stretches of space and time and over a wide range of systems including the universe as a whole, whether or not they are receiving the attention of observers. We are interested in sets of alternative histories that can be assigned probabilities whether or not they describe measurement situations;

in the quantum mechanics of closed systems that means the sets must decohere. Decoherence is thus a prerequisite for classical behavior.

Histories of the quasiclassical domain of everyday experience are coarse-grained by values of the usual quasiclassical variables. These include various sorts of hydrodynamic variables—averages over suitably small volumes of densities of conserved or nearly conserved quantities. Densities of energy, momentum, baryon number, nuclear and chemical species are examples. The system behaves classically when the probability is high for histories that exhibit correlations in time summarized by phenomenological classical equations of motion such as the Navier-Stokes equation.

Simple arguments [3–8] suggest why histories of these hydrodynamic, quasiclassical variables should decohere and exhibit classical correlations in time. Coarse graining is generally necessary for decoherence. Roughly speaking, a coarse graining divides the variables of the system into those that are followed by the coarse graining and those that are ignored. The ignored variables constitute the environment. An interaction between these classes of variables is necessary to dissipate the phases between different coarse-grained histories and to achieve decoherence. However, that same interaction produces noise, which causes deviations from predictability. Integrals of densities of conserved or approximately conserved quantities are natural candidates for quasiclassical variables. Their approximate conservation enables them to resist deviations from predictability caused by the noise arising from their interactions with the rest of the universe. Further, following standard arguments of nonequilibrium statistical mechanics, their approximate conservation leads to correlations in time summarized by a closed set of equations of motion. All isolated systems approach equilibrium. However, averages of approximately conserved quantities over suitable volumes approach equilibrium slowly. Closed sets of equations of motion result when the volumes can be chosen large enough that statistical fluctuations and noise are unimportant, but small enough that equilibrium is established within each volume in a time short compared to the dynamical time scales on which the variables vary (see, e.g., [9]). The constitutive relations giving equations of state, coefficients of viscosity, diffusion, etc., are then defined, permitting closure of a set of hydrodynamic equations of motion. Local equilibrium being thus established, the further equilibration of the volumes among themselves is governed by these equations.

Despite the plausibility of the above general and simple qualitative picture, its validity has been only partially investigated quantitatively. To make the argument quantitative, in light of our earlier discussion, requires at a minimum an investigation of sets of histories coarse-grained by ranges of quasiclassical variables which has the following features:

(i) Establishes the decoherence of sets of histories sufficiently coarse-grained by ranges of quasiclassical variables.

(ii) Establishes with high probability deterministic correlations in time summarized by closed systems of classical equations of motion for reasonably realistic initial conditions.

(iii) Compares the decoherence and predictability of different coarse-grained sets of histories, both within the family of coarse grainings by quasiclassical variables and with other coarse grainings of distinct character.

Despite intensive investigation of all of these points separately there is as yet no analysis which combines all three. There are many investigations of the mechanisms of decoherence of histories [10,4,5,11] and of the closely related decoherence of density matrices [12], especially in linear systems. However, these studies have typically posited a fixed division of the fundamental variables into those describing a ‘‘system’’ and those describing its ‘‘environment.’’ Coarse grainings follow variables of the system while ignoring those constituting the environment. Such a fixed system-environment split is intuitively accessible and correctly models many mechanisms of decoherence, but it is not general.

Rather, coarse graining is the general notion which, when possible, determines a family of system-environment splits. Different coarse grainings lead to different possible notions of system and environment, that division is not usually unique, and for some kinds of coarse graining no system-environment split is possible at all. (See Appendix A.) Even when a system-environment split is possible at one time, *different* system-environment splits could be needed at other moments of time. A fixed system-environment split is therefore neither general nor necessary for formulation quantum mechanics. However, as such workers as Feynman and Vernon [13], Joos and Zeh [14], Zurek [15], Caldeira and Leggett [16], and Omnès [17] fully appreciated, a system-environment split is an important tool for analyzing specific coarse grainings and for understanding the physical mechanisms of decoherence. We shall utilize this tool extensively in what follows.

The emergence of deterministic correlations in time governed by classical equations of motion has been investigated for fixed system-environment splits [4]. In a recent elegant paper, Halliwell [7] has derived classical equations of motion for hydrodynamic variables although with a special assumption about the nature of the environment. Neither of these works compared quasiclassical coarse grainings with nonclassical ones. In their pioneering paper on classical behavior in systems of interacting spins, Brun and Halliwell [6] compared a family of coarse grainings but did not derive classical equations of motion.

This paper moves the analysis of decoherence and classicality a step towards realistic coarse grainings by hydrodynamic variables in the context of a simple model—a one-dimensional chain of point masses with linear, nearest-neighbor interactions. (See Fig. 1). This is the simplest model which exhibits time correlations governed by a continuum equation of motion—the wave equation—in appropriate coarse grainings for certain initial states. Yet the Lagrangian of the model is quadratic in all coordinates, so it can be tractably analyzed with standard path integral techniques [13,16,4]. Although our analysis is only for this very simple system, and does not deal with coarse grainings by hydrodynamic variables *per se*, it does display all three features listed above.

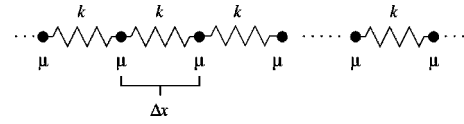


FIG. 1. The microscopic picture of the one-dimensional harmonic chain. \mathcal{N} equal masses μ are spaced an equilibrium distance Δx apart. The displacement of the j th mass is denoted x_j . The masses have a linear restoring force between them with a spring constant $k = \mu\omega^2$. The chain is assumed to have periodic boundary conditions.

The details of the model are laid out in Sec. II, where we introduce a family of coarse grainings. In the simplest, the chain of \mathcal{N} identical particles is divided into \mathcal{M} groups, each consisting of N neighboring atoms. Histories are partitioned by ranges of values of the center of mass displacement in each group. We find that the effective equations of motion for these variables are well approximated by the classical wave equation. We obtain quantitative estimates for the statistical noise causing deviations from the predictions of the wave equation.

We compare this quasiclassical coarse graining with other members of a family of sets of alternative coarse-grained histories constructed as shown in Fig. 2. The chain is divided up into \mathcal{M} groups of N atoms, each group consisting of equally spaced clumps of d atoms. We coarse grain by equal ranges Δ of the values of the average (center of mass) positions of the atoms in a group at equally spaced intervals of time Δt . A family of sets of alternative coarse-grained histories is thereby defined, parametrized by $(N, d, \Delta, \Delta t)$. When $d=N$ the N atoms in a group are all neighbors, the coarse graining entirely local, and the average position related to the approximately conserved center of mass momentum of the group. There is nothing special about the remaining members of the family except that they are amenable to analysis and range from local to highly nonlocal as d decreases from N to 1.

We find that for each decohering member of this family the probabilities of the histories can be thought of as

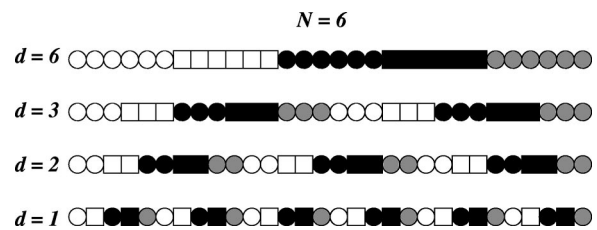


FIG. 2. The family of coarse grainings under consideration. The total number of masses, \mathcal{N} , is divided into \mathcal{M} groups of N masses each. These groups are then further subdivided into N/d clumps of d masses each. The clumps of a given group are spaced so that clumps of all the other groups occur before a clump is repeated, that is, by a distance $\mathcal{M}d$. The coarse-grained variable X_J is the average displacement of the masses in the J th group. In the figure, $\mathcal{N} = 30$, $\mathcal{M} = 5$, and $N = 6$. Masses in the same group are labeled with the same symbol, with a different symbol (including the shading) for each group. The arrangements are shown for $d = 1, 2, 3, 6$, with $d = 1$ being completely delocalized and $d = 6$ being completely localized.

obeying classical equations of motion augmented by noise [cf. Eq. (3.9)]. We compare the members of this family with respect to three properties bearing on classical behavior: decoherence, noise, and the computational complexity of their equations of motion. We find marked differences which are described in detail in the Conclusion, but which we summarize briefly here. As measured by the smallness of the ratio of the decoherence to dynamical time scales, decoherence is not a major constraint on predictability for “realistic” coarse grainings, but nonetheless favors the local coarse grainings. Noise interferes with the predictability of the nonlocal coarse grainings much more than for the local ones. The equations of motion of the local coarse grainings require many fewer steps to evolve over a given time to a given accuracy than do those for the nonlocal coarse grainings. In short, we find that the familiar local coarse grainings are more predictable than the nonlocal ones.

II. LINEAR CHAIN

A. Chain and its coarse grainings

In this section we lay out the details of the model. We consider a linear chain of \mathcal{N} “atoms,” each of mass μ , separated at rest by equal distances Δx , and with displacements $x_i, i=0, \dots, \mathcal{N}-1$. (See Fig. 1.) Each atom interacts linearly with its nearest neighbors. The action describing this system is

$$S[x_j(\tau)] = \frac{1}{2} \mu \sum_{j=0}^{\mathcal{N}-1} \int_0^{\tau} dt \{ [\dot{x}_j(t)]^2 - \omega^2 [x_{j+1}(t) - x_j(t)]^2 \} \quad (2.1)$$

where, using periodic boundary conditions, we take $x_{\mathcal{N}} \equiv x_0$.

The linear harmonic chain is the simplest model of a solid and is treated in many references.¹ The $x_j(t)$ may be conveniently analyzed in terms of spatial modes

$$x_j(t) = \sum_{l=0}^{\mathcal{N}/2} [a_l(t) f_l(j) + \text{c.c.}] \quad (2.2)$$

where

$$f_l(j) = \mathcal{N}^{-1/2} \exp(2\pi i j l / \mathcal{N}). \quad (2.3)$$

These are the normal modes of the chain and the $a_l(t)$ oscillate with frequencies

$$\omega_l = 2\omega \sin(\pi l / \mathcal{N}). \quad (2.4)$$

The action expressed in terms of normal modes takes the simple form

$$S[a_l(\tau)] = \frac{1}{2} \mu \sum_{l=0}^{\mathcal{N}/2} \int_0^{\tau} dt [|\dot{a}_l(t)|^2 - \omega_l^2 |a_l(t)|^2]. \quad (2.5)$$

¹For a classic reference see [18].

Both classically and quantum mechanically we will compare members of a family of coarse grainings defined in part by two integer parameters N and d . The \mathcal{N} particles in the chain are divided into $\mathcal{M} = \mathcal{N}/N$ groups of N atoms each. Each group consists of N/d clumps of d particles spaced by $\mathcal{M}d$. (See Fig. 2.) When $d=N$ there is only one clump. This coarse graining is local—the atoms are as closely spaced as possible in the chain. When $d=1$ there is only one particle per clump. This coarse graining is nonlocal, as the atoms are as spread out as possible in the chain. The variables followed by the coarse graining are the average displacements of the groups:

$$X_J^{(d)}(t) = \frac{1}{N} \sum_{k=0}^{N/d-1} \sum_{m=\lfloor -d/2 \rfloor + 1}^{\lfloor d/2 \rfloor} x_{Jd+m+k, \mathcal{M}d}(t). \quad (2.6)$$

The first sum is over the clumps in the group, and the second sum is over the atoms in a clump. The range of the sum over m depends on whether d is even or odd. For odd d it ranges from $-(d-1)/2$ to $(d-1)/2$. For even d the range is $-d/2+1$ to $d/2$. The brackets $\lfloor x \rfloor$ in Eq. (2.6) denote rounding down to the next lower integer. The range of J is $J=0, \dots, \mathcal{M}-1$, making a total of \mathcal{M} coarse-grained coordinates.

We consider sets of histories constructed from exhaustive sets of exclusive equal ranges Δ of $X_J^{(d)}$ separated by time intervals Δt . There is therefore a family of coarse grainings, each member of which is labeled by values of the four parameters $(N, d, \Delta, \Delta t)$.

It is convenient to expand the coarse-grained coordinates in terms of spatial modes as well:

$$X_J^{(d)}(t) = \sum_{L=0}^{\mathcal{M}/2} [A_L^{(d)}(t) F_L^{(d)}(J) + \text{c.c.}] \quad (2.7)$$

where

$$F_L^{(d)}(J) = \mathcal{M}^{-1/2} \exp(2\pi i J L / \mathcal{M}). \quad (2.8)$$

The parameter L labels the coarse-grained mode $A_L^{(d)}$ just as l labels the fine-grained mode a_l . The corresponding frequency $\Omega_L^{(d)}$ depends on the choice of coarse graining d . The $A_L^{(d)}(t)$ will be a superposition of the normal modes of the chain. Specifically,

$$A_L^{(d)}(t) = \sum_{k=0}^{d-1} c_{Lk}^{(d)} a_{m(k)N/d}(t) \quad (2.9)$$

where

$$m(k) = \begin{cases} L + k\mathcal{M}/2, & k \text{ even,} \\ -L + (k+1)\mathcal{M}/2, & k \text{ odd.} \end{cases} \quad (2.10)$$

The coefficients c_{Lk} are given by

$$c_{Lk}^{(d)} = \frac{1}{d\sqrt{N}} \frac{\sin[\pi m(k)/\mathcal{M}]}{\sin[\pi m(k)/(\mathcal{M}d)]} e^{im(k)\varphi(d)} \quad (2.11)$$

with the phase $\varphi(d)$ vanishing if d is odd and equal to $-\pi/(\mathcal{M}d)$ if d is even.

In the delocalized limit $d=1$, the $A_L^{(1)}$ are just single normal modes:

$$A_L^{(1)}(t) \propto a_{LN}(t). \quad (2.12)$$

By contrast, in the localized limit $d=N$, the $A_L^{(N)}(t)$ are superpositions of all modes higher than L , viz.

$$A_L^{(N)}(t) = \sum_{k=0}^{N-1} c_{Lk}^{(N)} a_{m(k)}(t). \quad (2.13)$$

These facts will be useful in what follows.

B. Environments

For several purposes in the subsequent analysis it will be convenient to divide up the configuration space of fine-grained modes $\{a_l\}$ into a subspace spanned by variables that are followed by the coarse grainings introduced above and a subspace spanned by variables that are ignored. The \mathcal{M} variables $\{A_L^{(d)}\}$ may be said to define the configuration space of the ‘‘system.’’ There is considerable latitude in the choice of variables $\{q_a^{(d)}\}$, $a=1,2,\dots,\mathcal{N}-\mathcal{M}$, which define the ‘‘environment.’’ The only requirement is that the $\{A_L^{(d)}\}$ and the $\{q_a^{(d)}\}$ span the whole configuration space of the fine-grained modes $\{a_l\}$. A convenient choice for our calculations will be to take the $q_a^{(d)}$ to be all but the lowest fine-grained modes that contribute to the $A_L^{(d)}$ through Eq. (2.9). That is, we take the $q_a^{(d)}$ to be the real and imaginary parts of

$$a_{m(k)N/d}, \quad k=1,2,\dots,d-1; \quad L=0,\dots,\mathcal{M}/2. \quad (2.14)$$

Each label a on q_a corresponds to a pair (L,k) ; the exact form of the correspondence will not be important for us. Thus defined, the environment variables are normal modes which classically obey

$$\ddot{q}_a^{(d)} + (\omega_a^{(d)})^2 q_a^{(d)} = 0. \quad (2.15)$$

The definition (2.14) defines a different environment for each d , and even for a given d it is but one of many possible choices, though the effect on the system must be independent of this choice.

Since only d fine-grained modes contribute to each coarse-grained mode $A_L^{(d)}$, this ‘‘system plus environment’’ only includes the full set of modes in the localized case $d=N$. For all other d , there will be some fine-grained modes that contribute to none of the coarse-grained modes, and which thus can be neglected. When $d=1$, each coarse-grained mode $A_L^{(1)}$ depends on only a single fine-grained mode, and hence has no environment at all.

C. Initial state

As we discussed in the Introduction, the classical behavior of any quantum system is exhibited through the probabilities of *certain* decoherent sets of alternative coarse-grained histories arising from *particular* initial conditions. In this paper we compare the predictability of the different members

of the family of coarse grainings introduced above for a single class of initial conditions. That is like the situation in cosmology, where the initial condition is given by fundamental theory and we search among the possible sets of coarse-grained alternative histories for sets that exhibit more predictability than other sets.

In this simple model of the harmonic chain there are no interactions between different normal modes. This is an idealization; realistically there will be interactions. These interactions mean that the normal modes will tend to equilibrate. The highest frequency modes can be expected to come into equilibrium first, the lowest frequency modes last. Thus, at an intermediate time in the approach to equilibrium, the chain can be described by a state in which the low frequency normal modes within a certain range are not yet in equilibrium, but the higher frequency modes are in equilibrium at a temperature T .

Indeed, a garden variety string would be described in this way. In a plucked violin string, for instance, the wavelengths that are reasonable fractions of the length of the string are not in equilibrium, but very short wavelengths—short compared to the transverse dimensions of the string, certainly—are likely to be in equilibrium.

Classically an initial condition is given by a distribution on the phase space of mode amplitudes a_l and their conjugate momenta π_l . We denote these collectively by $\{z_l\} = \{(a_l, \pi_l)\}$, $l=0,1,\dots,\mathcal{N}/2$. We assume that the significant expected values of z_l , denoted \bar{z}_l , occur only at low frequencies, so that for l greater than a cutoff l_C we have $z_l \approx 0$. We assume thermal fluctuations around these expected values. A distribution which gives this is

$$\rho(\{z_l\}) = \prod_{l=0}^{\mathcal{N}/2} (Z_l^{-1} e^{-H_l(z_l, \bar{z}_l)/T}). \quad (2.16)$$

Here $H_l(z_l)$ is the Hamiltonian ($|\pi_l|^2/\mu + \mu\omega_l^2|a_l|^2$)/2 for each mode, and Z_l is a normalizing factor.

The corresponding assumption in quantum mechanics would be a density matrix of the form

$$\rho = \prod_{l=0}^{\mathcal{N}/2} \exp[i(\bar{a}_l^* \hat{\pi}_l - \bar{\pi}_l^* \hat{a}_l + \text{H.c.})/2] (Z_l^{-1} e^{-\hat{H}_l/T}) \times \exp[-i(\bar{a}_l^* \hat{\pi}_l - \bar{\pi}_l^* \hat{a}_l + \text{H.c.})/2] \quad (2.17)$$

where \hat{a}_l and $\hat{\pi}_l$ are the quantum operators corresponding to the classical variables $z_l = (a_l, \pi_l)$, and the exponentials sandwiching the thermal state are phase-space displacement operators in z_l . These are the initial conditions we assume in our analysis.

A system is said to be in thermal equilibrium when its state is such that the probabilities of quasiclassical alternatives are accurately reproduced by a thermal density matrix. Typical examples are coarse grainings by volume averages of densities of conserved quantities such as energy, momentum, etc. However, the probabilities of an arbitrary set of alternatives will not be generally reproduced by the thermal density matrix. It is plausible that many (or perhaps

most) initial states of the linear chain relax after a suitable time to a state of local thermal equilibrium for which the probabilities of the *local* coarse grainings described above are reproduced by a density matrix of the form (2.17). However, we have assumed something much stronger, which is that the probabilities of the whole family of coarse grainings are accurately reproduced by these density matrices. That is a much more restrictive condition on the initial condition.

III. EQUATIONS OF MOTION FOR CLASSICAL COARSE GRAININGS

In this section we consider the *classical* linear chain. Each atom moves according to a classical equation of motion. However, with a probabilistic initial condition, a set of coarse-grained variables (such as the $X_j^{(d)}$ discussed in the previous section) need not obey *any* closed system of deterministic equations. We analyze the constraints on the initial distribution $\rho(z^0)$ necessary for the $\{X_j^{(d)}\}$ for each d to obey an open set of deterministic equations and we exhibit the form these equations take. The general kind of analysis we describe has been considered by many authors, for example Zwanzig [19] and Brun [5]. What is new here is the application of these methods to comparing different coarse grainings of the linear chain.

A. Probability of determinism

A set of functionals of the phase-space paths $F_A[z(t)]$, $A = 1, \dots, P$ and a set of ranges $\{\Delta_\alpha\}$ in \mathbf{R}^P define the most general kind of classical coarse graining. The probability p_α that the functionals F_A have values in the range Δ_α is

$$p_\alpha = \int \delta z e_\alpha\{F_A[z(t)]\} \delta[z(t) - z_t(z^0)] \rho(z^0). \quad (3.1)$$

Here, e_α is the characteristic function (1 inside, 0 outside) for the range Δ_α and $z_t(z^0)$ is the classical evolution of the initial data z^0 . The functional δ function enforces that evolution, assigning zero probability to all paths which do not conform to it. The functional integral is over all phase-space paths $z(t)$ including an integral over the initial conditions z^0 .

Utilizing this framework one can calculate the probability that the coarse-grained variables such as the $\{X_j^{(d)}\}$ exhibit deterministic correlations in time. The functionals F_A for example might define different orbits in phase space. Even more simply, one can evaluate the probability that a set of deterministic equations of motion²

$$\mathcal{E}_j(t, X(\tau)) = 0 \quad (3.2)$$

holds for a set of variables $\{X_j^{(d)}\}$ [denoted without indices in Eq. (3.2)] at time t , by calculating the probability that the functionals $\mathcal{E}_j(t, X(\tau))$ have the value zero. If that probability is high, then the coarse-grained variables obey the deterministic set of equations (3.2).

²We follow the convention that $f(t, x(\tau))$ means that f is a function of t and a functional of $x(\tau)$, for example $\int_0^t x(\tau) d\tau$.

B. Equations of motion

We now consider equations of motion for the coarse-grained average positions $X_j^{(d)}(t)$ introduced in Sec. II. Equivalently, and more conveniently, we can consider the equations of motion for the corresponding spatial modes $A_L^{(d)}(t)$ defined by Eq. (2.7) and given terms of the fine-grained modes by Eq. (2.9). It is convenient to take the system-environment split defined by Eq. (2.14) in which case the ignored coordinates are the $\{q_a^{(d)}\}$ of Eq. (2.15).

The normal modes of the chain a_l oscillate with the frequencies ω_l given in Eq. (2.4). Evidently, as a consequence of Eq. (2.9),

$$\ddot{A}_L(t) = - \sum_{k=0}^{d-1} c_{Lk} \omega_{m(k)N/d}^2 a_{m(k)N/d}(t). \quad (3.3)$$

We have suppressed the superscript (d) in this equation, as we shall do for clarity in the remainder of this section. The ignored coordinates were chosen to coincide with all but the lowest frequency normal mode in Eq. (3.3). Therefore that equation may be rewritten as

$$\ddot{A}_L(t) + \Omega_L^2 A_L(t) = f_L(t), \quad (3.4)$$

where

$$\Omega_L = \omega_{LN/d}, \quad (3.5)$$

and

$$f_L(t) = \sum_{a=1}^{d-1} (\Omega_L^2 - \omega_a^2) c_{La} q_a(t). \quad (3.6)$$

Here, ω_a , c_{La} , etc., are the values of ω_l , c_{Lk} appropriate to the value a .

The simple equation of motion (2.15) can be solved to express the $q_a(t)$ in terms of their initial values

$$q_a(t) = q_a(0) \cos(\omega_a t) + \frac{p_a(0)}{\omega_a} \sin(\omega_a t). \quad (3.7)$$

The $q_a(t)$ are probabilistically distributed with a distribution that depends on the distribution of the initial conditions through Eq. (3.7). Let $F_L(t)$ be the expected value of $f_L(t)$,

$$F_L(t) = \mathbf{M}[f_L(t)] \quad (3.8)$$

where $\mathbf{M}[f_L]$ denotes the mean over the distribution of initial conditions. (We use $\mathbf{M}[\cdot]$ for classical expected values and $\langle \cdot \rangle$ for quantum mechanical ones.) Then Eq. (3.4) becomes

$$\mathcal{E}_L(t, A_L(\tau)) \equiv \ddot{A}_L(t) + \Omega_L^2 A_L(t) - F_L(t) = \Delta f_L(t), \quad (3.9)$$

where

$$\Delta f_L(t) = f_L(t) - \mathbf{M}[f_L(t)]. \quad (3.10)$$

We can think of $\mathcal{E}_L(t, A_L(\tau))=0$ as a deterministic equation of motion and Δf_L as classical stochastic noise causing deviations from that determinism. Since the expected value of $\mathcal{E}_L(t, A_L(\tau))$ is zero, the coarse graining will approximately obey the deterministic equation $\mathcal{E}_L(t, A_L(\tau))=0$ provided the noise is small. A simple measure of its size is

$$M[\Delta f_L^*(t)\Delta f_L(t')]. \quad (3.11)$$

The situation is even simpler if, in addition, $F_L(t)$ is negligible, as it is in many realistic situations. Then the chain obeys the equation

$$\ddot{A}_L(t) + \Omega_L^2 A_L(t) = \Delta f_L(t) \approx 0 \quad (3.12)$$

with high probability—an equation whose form is independent of the initial distribution.

For our chain model $F_L(t)$ does not vanish. Because the initial condition is diagonal in the fine-grained modes rather than the A_L 's and q_a 's, there is a non-vanishing contribution to the driving force F_L proportional to $(A_L(0) - M[A_L(0)])$. However, even in terms of A_L and q_a , the initial condition is close to diagonal for large N and \mathcal{M} ; thus, this term is small compared both to the noise and the terms of the homogeneous equation of motion (3.12). The time average of $F_L(t)$ also vanishes. Hence, we can safely neglect it.

Unlike effective classical equations for many systems, Eq. (3.12) exhibits neither nonlocality in time or dissipation. These simplifying features can be traced to the conservation of the energies of the individual normal modes. The environment—the q_a 's—are all normal modes. Energy, therefore, cannot be exchanged between the A_L and the q_a on average, that is between the system and its environment. Defining the energy for a coarse-grained mode is somewhat ambiguous, but simple definitions give an energy which fluctuates about a fixed average. This is special to this linear system, which has a high level of integrability.

The initial distribution $\rho(z_l^0)$ determines whether the classical noise is small. The noise will be negligible when there is a negligible probability for any significant initial excitation for the q_a . Thus, for initial distributions that favor low frequency modes below some cutoff value, we expect low noise and a deterministic behavior of the $A_L(t)$. We shall return to this question in more detail in Sec. V.

C. Deriving the equations of motion from the Lagrangian

While the above derivation is perfectly correct, it is in some sense a shortcut to a more standard procedure. In this procedure we would substitute the change of variables (2.7) and (2.14) into the expression for the action (2.1), and derive the Euler-Lagrange equations for the new variables. This is important later in making contact with the quantum case, since that derivation proceeds from the classical Lagrangian, and there are no classical equations of motion to solve.

The action (2.5) may be expressed more compactly in matrix notation writing $\vec{a}(t)$ for the vector with components $a_l(t)$. Then

$$S[\vec{a}(\tau)] = \frac{1}{2} \int_0^{\tau_f} dt [(\dot{\vec{a}} \boldsymbol{\mu} \dot{\vec{a}}) - (\vec{a} \boldsymbol{\mu}^{1/2} \boldsymbol{\omega}^2 \boldsymbol{\mu}^{1/2} \vec{a})]. \quad (3.13)$$

We use a Hermitian inner product indicated only implicitly, so the $\vec{a} \vec{b} = \sum_l a_l^* b_l$. Sandwiched in inner products like those of Eq. (3.13), $\boldsymbol{\omega}$ and $\boldsymbol{\mu}$ denote the diagonal matrices of normal mode frequencies and masses (all equal) respectively. For this case, $\boldsymbol{\mu}^{1/2} \boldsymbol{\omega}^2 \boldsymbol{\mu}^{1/2} = \boldsymbol{\mu} \boldsymbol{\omega}^2$.

The coarse-grainings are by the variables $X_j^{(d)}$ or, equivalently, by their modes $A_L^{(d)}$. The coordinates $q_a^{(d)}$ are the fine-grained modes that are not followed by the coarse-graining. Continuing to suppress superscript (d), we write

$$a_l = \sum_L S_{lL} A_L + \sum_a T_{la} q_a \quad (3.14)$$

or, in matrix notation,

$$\vec{a} = \mathbf{S} \vec{A} + \mathbf{T} \vec{q}. \quad (3.15)$$

In general, there is considerable arbitrariness in the matrices \mathbf{S} and \mathbf{T} depending on how the variables q_a are chosen. The only requirements are that Eq. (3.15) must reproduce the definition of the A_L 's (2.6) and (2.7), and the set of $\{A_L, q_a\}$ must span the space of the $\{a_l\}$. The choice (2.14) specifies a definite \mathbf{T} and \mathbf{S} .

Inserting the transformation (3.15) into the action (3.13) one has

$$\begin{aligned} S[\vec{A}(t), \vec{q}(t)] = & \frac{1}{2} \int_0^{\tau_f} dt [(\dot{\vec{A}} \mathbf{M}_{SS} \dot{\vec{A}}) + (\dot{\vec{q}} \mathbf{M}_{TT} \dot{\vec{q}}) + (\dot{\vec{A}} \mathbf{M}_{ST} \dot{\vec{q}}) \\ & + (\dot{\vec{q}} \mathbf{M}_{TS} \dot{\vec{A}}) - (\vec{A} \mathbf{V}_{SS} \vec{A}) - (\vec{q} \mathbf{V}_{TT} \vec{q}) \\ & - (\vec{A} \mathbf{V}_{ST} \vec{q}) - (\vec{q} \mathbf{V}_{TS} \vec{A})] \end{aligned} \quad (3.16)$$

where (with AB standing for S or T)

$$\mathbf{M}_{AB} \equiv \mathbf{A}^\dagger \boldsymbol{\mu} \mathbf{B} \quad (3.17a)$$

and

$$\mathbf{V}_{AB} \equiv \mathbf{A}^\dagger \boldsymbol{\mu}^{1/2} \boldsymbol{\omega}^2 \boldsymbol{\mu}^{1/2} \mathbf{B}. \quad (3.17b)$$

With the action in this form, it is a simple matter to derive the equations of motion for \vec{A} and \vec{q} :

$$\mathbf{M}_{SS} \ddot{\vec{A}} + \mathbf{M}_{ST} \ddot{\vec{q}} = -\mathbf{V}_{SS} \vec{A} - \mathbf{V}_{ST} \vec{q}, \quad (3.18a)$$

$$\mathbf{M}_{TT} \ddot{\vec{q}} + \mathbf{M}_{TS} \ddot{\vec{A}} = -\mathbf{V}_{TT} \vec{q} - \mathbf{V}_{TS} \vec{A}. \quad (3.18b)$$

Equation (3.18) looks complicated, but in fact we can easily recover our earlier result. Because the q variables are normal modes, they obey the usual harmonic oscillator motion (2.15). By plugging the second equation into the first, the equation becomes

$$\begin{aligned}
& (\mathbf{M}_{SS} - \mathbf{M}_{ST}\mathbf{M}_{TT}^{-1}\mathbf{M}_{TS})\ddot{\vec{A}} + (\mathbf{V}_{SS} - \mathbf{M}_{ST}\mathbf{M}_{TT}^{-1}\mathbf{V}_{TS})\dot{\vec{A}} \\
& = -(\mathbf{V}_{ST} - \mathbf{M}_{ST}\mathbf{M}_{TT}^{-1}\mathbf{V}_{TT})\dot{\vec{q}}. \tag{3.19}
\end{aligned}$$

If we then plug in the simple harmonic solution (3.7) for the ignored modes \vec{q} , the equation reduces to the simple equation (3.12) above multiplied by the diagonal matrix $(\mathbf{M}_{SS} - \mathbf{M}_{ST}\mathbf{M}_{TT}^{-1}\mathbf{M}_{TS})$. (See Appendix B for the proof of this.)

This is a slightly more complicated derivation of the equation of motion, but it still relies on the shortcut of knowing the solution for the motion of \vec{q} . That will not be available in quantum mechanics. Without making use of this, we could solve the linear equation (3.18b) above for $\vec{q}(t)$ and insert it into Eq. (3.19). The solution for $\vec{q}(t)$ is

$$\begin{aligned}
\mathbf{M}_{TT}^{1/2}\vec{q}(t) &= \cos[\boldsymbol{\Omega}t]\mathbf{M}_{TT}^{1/2}\vec{q}(0) + \boldsymbol{\Omega}^{-1}\sin[\boldsymbol{\Omega}t]\mathbf{M}_{TT}^{1/2}\dot{\vec{q}}(0) \\
&\quad - \boldsymbol{\Omega}^{-1}\int_0^t dt' \sin[\boldsymbol{\Omega}(t-t')]\mathbf{M}_{TT}^{-1/2} \\
&\quad \times [\mathbf{M}_{TS}\ddot{\vec{A}}(t') + \mathbf{V}_{TS}\dot{\vec{A}}(t')], \tag{3.20}
\end{aligned}$$

where

$$\boldsymbol{\Omega}^2 = \mathbf{M}_{TT}^{-1/2}\mathbf{V}_{TT}\mathbf{M}_{TT}^{-1/2}, \tag{3.21}$$

and it gives us the very complicated-looking equation of motion

$$\begin{aligned}
& (\mathbf{M}_{SS} - \mathbf{M}_{ST}\mathbf{M}_{TT}^{-1}\mathbf{M}_{TS})\ddot{\vec{A}} + (\mathbf{V}_{SS} - \mathbf{M}_{ST}\mathbf{M}_{TT}^{-1}\mathbf{V}_{TS})\dot{\vec{A}} \\
& \quad + (\mathbf{V}_{ST} - \mathbf{M}_{ST}\mathbf{M}_{TT}^{-1}\mathbf{V}_{TT})\mathbf{M}_{TT}^{-1/2}\boldsymbol{\Omega}^{-1} \\
& \quad \times \int_0^t dt' \sin[\boldsymbol{\Omega}(t-t')]\mathbf{M}_{TT}^{-1/2}[\mathbf{M}_{TS}\ddot{\vec{A}}(t') + \mathbf{V}_{TS}\dot{\vec{A}}(t')], \\
& = -(\mathbf{V}_{ST} - \mathbf{M}_{ST}\mathbf{M}_{TT}^{-1}\mathbf{V}_{TT})\mathbf{M}_{TT}^{-1/2}\{\cos[\boldsymbol{\Omega}t]\mathbf{M}_{TT}^{1/2}\dot{\vec{q}}(0) \\
& \quad + \boldsymbol{\Omega}^{-1}\sin[\boldsymbol{\Omega}t]\mathbf{M}_{TT}^{1/2}\dot{\vec{q}}(0)\}. \tag{3.22}
\end{aligned}$$

Two observations can be made. First, the solution (3.20), while still harmonic motion, appears to be at quite different frequencies from (3.7), and also includes a driving term absent in that case. Second, Eq. (3.22) appears very different from the rather simple harmonic oscillator equation (3.12). These differences, however, must be apparent rather than real; both Eqs. (3.7) and (3.20) follow from the same Lagrangian, as do Eqs. (3.12) and (3.22). In fact, the more complicated form (3.22) of the equation of motion is related to the simple form (3.12) by an invertible transformation, and thus has exactly the same solutions. (See Appendix C.)

D. Transforming the classical noise

The fact that classical equations of motion can be represented in widely different forms is nothing new, of course. But the apparent complexity masking the comparatively

simple underlying dynamics only complicates the analysis of the quantum case. For the classical case, it is best to stick with the simple form (3.12).

The two forms do differ in one important respect. The retarded term in Eq. (3.22) is most readily identified as part of the homogeneous equation of motion, while in Eq. (3.12) it is implicitly included in the noise terms. We shall see that this ambiguity in the definition of the noise becomes important in comparing the classical and quantum cases: one definition is most natural in the classical case, while the other is most natural in the quantum case [where $\vec{A}(t)$ need not obey the classical equation of motion].

Let us restrict ourselves to a single coarse-grained mode $A_L^{(d)}(t)$ and its associated modes $\vec{q}(t)$. If we define the two forms of the noise to be the right hand sides of Eqs. (3.12) and (3.22), respectively, they can then be expressed as

$$\begin{aligned}
\Delta f_L(t) &= \vec{c}(\Omega_L^2\mathbf{I} - \boldsymbol{\Omega}_Q^2)\{\cos[\boldsymbol{\Omega}_Q t]\Delta\vec{q}(0) \\
&\quad + \boldsymbol{\Omega}_Q^{-1}\sin[\boldsymbol{\Omega}_Q t]\Delta\dot{\vec{q}}(0)\} \tag{3.23a}
\end{aligned}$$

and

$$\begin{aligned}
\Delta f_L'(t) &= N\vec{c}(\Omega_L^2\mathbf{I} - \boldsymbol{\Omega}_Q^2)\mathbf{M}_{TT}^{-1/2}\{\cos[\boldsymbol{\Omega}t]\mathbf{M}_{TT}^{1/2}\Delta\vec{q}(0) \\
&\quad + \boldsymbol{\Omega}^{-1}\sin[\boldsymbol{\Omega}t]\mathbf{M}_{TT}^{1/2}\dot{\vec{q}}(0)\}, \tag{3.23b}
\end{aligned}$$

where \vec{c} is a vector in the space of the q 's with elements equal to the coefficients c_b , $\boldsymbol{\Omega}_Q$ is a diagonal matrix on the space of the q_b 's with diagonal elements ω_b , and $\boldsymbol{\Omega}$ is the effective frequency matrix defined by Eq. (3.21). The structure of these two expressions is closely parallel, and in Appendix C we show that we can switch from one form of the noise to the other by means of an invertible linear transformation. As far as determining the classical dynamics and predictability, they are equivalent.

However, if we look at the absolute strength of the noise as a function of L or d , the form of the noise *can* make a difference. We assess this by looking at the correlation function (3.11) for the two forms of the noise.

In the initial state (2.16) we find the expectation values

$$\begin{aligned}
\mathbf{M}[\Delta q_b(0)\Delta q_{b'}^*(0)] &= k_B T(\mathbf{V}_{TT}^{-1})_{bb'}, \\
\mathbf{M}[\Delta \dot{q}_b(0)\Delta \dot{q}_{b'}^*(0)] &= k_B T(\mathbf{M}_{TT}^{-1})_{bb'}. \tag{3.24}
\end{aligned}$$

We can use these to calculate the correlation functions (3.11):

$$\begin{aligned}
\mathbf{M}[\Delta f_L^*(t)\Delta f_L(t')] &= k_B T\vec{c}(\Omega_L^2\mathbf{I} - \boldsymbol{\Omega}_Q^2) \\
&\quad \times (\cos[\boldsymbol{\Omega}_Q t]\mathbf{V}_{TT}^{-1}\cos[\boldsymbol{\Omega}_Q t'] \\
&\quad + \boldsymbol{\Omega}_Q^{-1}\sin[\boldsymbol{\Omega}_Q t]\mathbf{M}_{TT}^{-1}\sin[\boldsymbol{\Omega}_Q t']\boldsymbol{\Omega}_Q^{-1}) \\
&\quad \times (\Omega_L^2\mathbf{I} - \boldsymbol{\Omega}_Q^2)\vec{c} \tag{3.25}
\end{aligned}$$

and

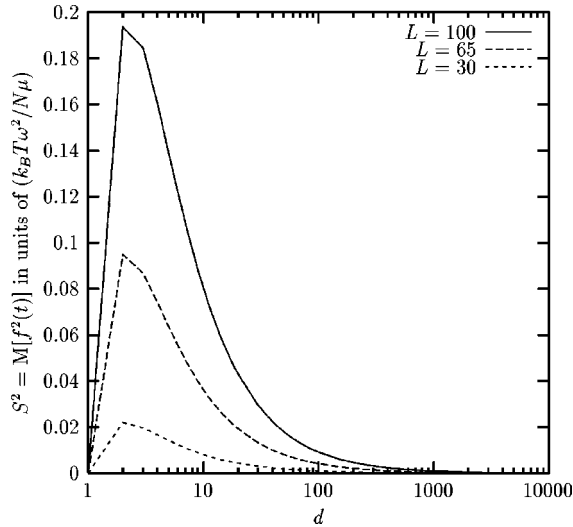


FIG. 3. The time-averaged mean force squared of the noise, S^2 [Eq. (3.27)], for the harmonic chain as a function of the coarse graining d . This noise is chosen for three typical coarse-grained modes $L=30, 65, 100$, with $\mathcal{M}=630$ and N assumed to be very large; the N dependence is absorbed into the units, $k_B T \omega^2 / N \mu$. Note that the noise vanishes for $d=1$, but otherwise assumes its highest values at low d , dropping off like $1/d$ at high d , as predicted by the analytical result (5.6).

$$\begin{aligned} \mathbf{M}[\Delta f_L^*(t) \Delta f_L'(t')] &= N k_B T \vec{c} (\Omega_L^2 \mathbf{I} - \Omega_Q^2) \\ &\times \mathbf{M}_{TT}^{-1/2} (\cos[\Omega t] \Omega^{-2} \cos[\Omega t']) \\ &+ \Omega^{-1} \sin[\Omega t] \sin[\Omega t'] \Omega^{-1}) \\ &\times \mathbf{M}_{TT}^{-1/2} (\Omega_L^2 \mathbf{I} - \Omega_Q^2) \vec{c}. \end{aligned} \quad (3.26)$$

Using these expressions, we can estimate the mean strength of the noise by taking the average over time:

$$S^2 = \lim_{t_f \rightarrow \infty} \frac{1}{t_f} \int_0^{t_f} \mathbf{M}\{|f_L(t) - F_L(t)|^2\} dt. \quad (3.27)$$

In Fig. 3 we plot S^2 as a function of the coarse graining d . We see that the noise strength falls off steeply as a function of d . Thus, the noise becomes lower in the highly localized case, and the motion of the localized coarse graining is most predictable. Later we shall see that the Lagrangian form of the noise is closely related to the strength of decoherence in the quantum case, and closely resembles this ‘‘simple’’ noise.

IV. WAVE EQUATION

The classical wave equation for the string does not follow directly from the deterministic equations for the chain (3.12). A restriction on the initial distribution is required beyond that necessary for determinism. This is the requirement that only very long wavelength modes of the chain are excited. We assumed such a restriction on the initial distribution in Sec. II C, but in this section we will examine the requirements on the short wavelength cutoff l_C . This small gradient

approximation is necessary for the validity of the wave equation as for other familiar continuum equations such as the Navier-Stokes equation.³

A. Small gradient approximation

The expansion (2.7) of the coarse-grained coordinates $X_J^{(d)}(t)$ in terms of coarse-grained modes $A_L^{(d)}(t)$ connects the equation of motion (3.12) for the $A_L^{(d)}(t)$ to an equation of motion for the $X_J^{(d)}(t)$. The character of these equations for the $X_J^{(d)}(t)$ is determined by the dispersion relation for $\Omega_L^{(d)}$ which is [cf. Eqs. (3.5), (2.4)]:

$$\Omega_L^{(d)} = 2\omega \sin\left(\frac{\pi L}{\mathcal{M}d}\right). \quad (4.1)$$

Since Eq. (4.1) is not linear in L , the equations for $X_J^{(d)}(t)$ following from Eq. (3.12) will generally relate $\ddot{X}_J^{(d)}(t)$ to all the other coordinates $X_K^{(d)}(t)$ of the chain. The form of the equations for $X_J^{(d)}(t)$ simplifies if the initial distribution is such that only modes with

$$l \ll \mathcal{N} \quad (4.2)$$

have any significant probabilities, that is $l_C \ll \mathcal{N}$. Then from Eq. (2.4), $\omega_l \approx 2\pi\omega l/\mathcal{N}$ and in particular

$$\Omega_L^{(d)} \approx \frac{2\pi\omega L}{\mathcal{M}d}. \quad (4.3)$$

In this small gradient approximation, the equation of motion for the $X_J^{(d)}(t)$ implied by Eqs. (3.12) and (2.7) is

$$\ddot{X}_J^{(d)}(t) = \frac{\omega^2}{d^2} [X_{J+1}^{(d)}(t) - 2X_J^{(d)}(t) + X_{J-1}^{(d)}(t)]. \quad (4.4)$$

Only nearest neighbor interactions are involved in the small gradient approximations.

Usually a much stronger condition is meant by the small gradient approximation, namely that the only modes with significant probabilities are those with

$$l \ll \mathcal{M} \ll \mathcal{N}, \quad (4.5)$$

that is $l_C \ll \mathcal{M}$. For $d=N$ this condition ensures that many groups will fit into a wavelength so that the X_J vary only slightly from one J to the next. We will see below that this is essential to deriving the continuum wave equations.

Condition (4.5) can be very much stronger than Eq. (4.2). In a 10 cm length of string with typical interatomic spacings, $\mathcal{N} \sim 10^9$. Dividing the string into .1 mm lengths constituting the groups in the $d=N$ case gives $N \sim 10^6$.

For the nonlocal coarse graining $d=1$, the condition (4.5) would imply that no values of $A_L^{(1)}(t)$ would be excited above $L=0$, since the l values contributing to any $d=1$ mode are all larger than N [cf. Eq. (2.9)] except

³See, e.g., [20,9].

$l=0$. That makes the equation of motion (4.4) in the delocalized case not incorrect, but rather trivial since both sides are negligible.

B. Continuum approximation

For the localized coarse graining $d=N$, the difference equation (4.4) is well approximated by the wave equation when N is large. The derivation is standard, but we briefly repeat its essential features here.

Recall that we denoted the mass of an atom by μ and the spacing between atoms in the unexcited chain by Δx . The mass density σ is therefore

$$\sigma = \mu / \Delta x. \quad (4.6)$$

Multiplying both sides of Eq. (4.4) by σ it can be written as

$$\sigma \ddot{X}_J^{(N)}(t) = \mu \omega^2 \Delta x \left[\frac{X_{J+1}^{(N)}(t) - 2X_J^{(N)}(t) + X_{J-1}^{(N)}(t)}{(N\Delta x)^2} \right]. \quad (4.7)$$

The length $N\Delta x$ is the distance between the centers of the groups in the unexcited string. Assuming the strong form of the slow approximation gradient (4.5), we can approximate Eq. (4.7) by the continuum equation

$$\sigma \frac{\partial^2 X(x,t)}{\partial t^2} = Y \frac{\partial^2 X(x,t)}{\partial x^2}, \quad (4.8)$$

where Young's modulus Y is $\mu \omega^2 \Delta x$. Equation (4.8) is the wave equation for the propagation of compressional modes along the string.

V. CLASSICAL PREDICTABILITY

The fine-grained variables of a classical system obey a closed system of deterministic equations of motion. However, there is no guarantee that coarse-grained variables will. There may be no deterministic equations at all, or the set of those that do hold may not close, in the sense that there may not be a complete set of equations to solve for all the variables. In Sec. III B we demonstrated that the probabilities of the evolution of the coarse-grained modes $A_L^{(d)}(t)$ of the linear harmonic chain are reproduced by a classical equation of motion (3.9) modified by noise,

$$\ddot{A}_L^{(d)}(t) - \Omega_L^2 A_L^{(d)}(t) - F_L^{(d)}(t) = \Delta f_L^{(d)}(t), \quad (5.1)$$

for the family of coarse grainings under consideration. The time evolution of the $A_L^{(d)}(t)$ will be classically predictable by the left hand side of Eq. (5.1) if the noise term on the right hand side is negligible. In this section we analyze this requirement for classical predictability as a function of d .

A simple estimate of the noise can be obtained by assuming a completely thermal initial state characterized by a temperature T . That is, we assume Eq. (2.16) with $l_C=0$. In this initial state, $M[f_L^{(d)}(t)] \approx 0$. A measure of the magnitude of the noise fluctuations is $M\{[f_L^{(d)}(t)]^2\}$. In a thermal state

$$M[a_l^*(t)a_{l'}(t)] = \delta_{ll'} k_B T / (2\mu \omega_l^2). \quad (5.2)$$

We therefore have, from Eq. (3.6),

$$M\{|f_L^{(d)}(t)|^2\} = \frac{k_B T}{\mu} \sum_{k=1}^{d-1} |c_{Lk}|^2 \omega_{l(k)}^2 \times \left(1 - \frac{\omega_{l(0)}^2}{\omega_{l(k)}^2} \right)^2 \frac{\mu}{2} (\omega_{l(k)}^2 \mathbf{V}_{TT}^{-1} + \mathbf{M}_{TT}^{-1})_{kk} \quad (5.3)$$

where the final factor (arising from the initial condition) is very close to 1 for $\mathcal{M} \gg L$, that is, $(\mu/2)(\omega_{l(k)}^2 \mathbf{V}_{TT}^{-1} + \mathbf{M}_{TT}^{-1})_{kk} = 1 + O(L^2/\mathcal{M}^2)$, where $l(k) \equiv m(k)N/d$ is

$$l(k) = (L + k\mathcal{M}/2)N/d, \quad \text{for } k \text{ even}, \quad (5.4a)$$

$$l(k) = [-L + (k+1)\mathcal{M}/2]N/d, \quad \text{for } k \text{ odd}. \quad (5.4b)$$

Every term on the right hand side of Eq. (5.3) depends on d although we have not indicated the dependence explicitly.

Figure 3 shows a plot of the expected value of the square of the fluctuations (5.3) as a function of d for some representative values of L . The plot is for $\mathcal{M}=630$; the value of N cancels out of the plotted function, but is assumed to be very large in order to have a sufficient number of factors d . As is evident from Eq. (5.3), the noise vanishes for $d=1$. That is because, as we noted in (2.12), $A_L^{(1)}$ is a single fine-grained mode not coupled to any other fine-grained modes. This special situation results from our idealized linear model of the chain. Even a tiny amount of nonlinearity would couple this mode to others and produce noise.

Figure 3 shows that the noise generally increases with L and decreases with d . Analytic estimates can be derived from Eq. (5.3) when $L \ll \mathcal{M} < N$. Assuming that the final factor in Eq. (5.3) is well approximated by unity, we have, for $d=2$,

$$M\{|f_L^{(d)}(t)|^2\} \approx \frac{k_B T \omega^2}{N\mu} (\pi L / \mathcal{M})^2, \quad (5.5)$$

while, for large d comparable to N ,

$$M\{|f_L^{(d)}(t)|^2\} \approx \frac{k_B T \omega^2}{N\mu} \frac{(\pi L / \mathcal{M})^2}{d}. \quad (5.6)$$

The noise thus varies inversely with d . For the ‘‘realistic’’ coarse graining discussed at the end of Sec. IV A, where $N \sim 10^6$, the noise is 10^6 times smaller for $d=N$ than it is for $d=2$. That is a vast advantage in predictability of the local coarse grainings over the nonlocal ones. The origin of this advantage can be traced to the approximate conservation of the center of mass momentum of the local groups of atoms.

The noise term on the right hand side of the equation of motion (5.1) must be compared with the characteristic size of the deterministic terms on the left hand side to get a true estimate of the effect of noise on predictability. In Eq. (2.16) we assumed an initial state in which only fine-grained modes with $l < l_C$ had significant excitations above thermal noise.

But, as we remarked earlier, the coarse-grained modes $A_L^{(d)}$ are superpositions of fine-grained modes with $l > LN/d$, as Eq. (2.9) shows. Thus, for $d < LN/l_C$, there will be no significant excitation of $A_L^{(d)}$ above the level of thermal noise. The subsequent dynamics is predictable only in a trivial sense. The string exhibits no motion except in response to thermal fluctuations. For true classical predictability, d must be large, so the noise is low, but also so the deterministic terms in the equation of motion dominate the noise terms. We shall return to a more quantitative comparison of the noise and dynamical force terms in the Conclusion.

Even leaving aside the competition between noise and predictability, the classical equations of motion for nonlocal coarse grainings are distinguished from the local ones by their computational complexity. Consider the classical equations (3.12) for the coarse-grained modes or, equivalently, in the small gradient approximation, Eqs. (4.4), for the center of mass positions of the groups. The characteristic dynamical time scales are of order $\mathcal{M}d/\omega L$. The local coarse grainings therefore vary the most slowly as would be expected from their association with approximately conserved quantities. Thus computing the evolution of the coarse-grained quantity $A_L^{(d)}$ or $X_J^{(d)}$ over a given time interval to a given accuracy will take a factor of N more time steps for the nonlocal equations than the local ones. For the ‘‘realistic’’ case when $N \sim 10^6$ that is a significant advantage in computational complexity for the local coarse grainings.

Thus, whether one considers the absolute value of the noise, the relative size of the noise and deterministic forces, or the effort needed to solve the classical equations of motion, the local coarse grainings are more predictable than the nonlocal ones in the family we have considered. In the next section we turn to the same questions in quantum theory.

VI. DECOHERENCE

A. Quantum mechanics of the linear chain

In this section we turn to the classical behavior of the *quantum* linear harmonic chain. A quantum system behaves classically when the probability is high that coarse-grained histories exhibit the correlations implied by classical equations of motion. We will be concerned with the histories of the linear harmonic chain coarse-grained by values of the position averages $\{X_J^{(d)}(t)\}$ defined in Sec. II. More specifically we shall consider, for each d , sets of histories defined by an exhaustive set of exclusive regions $\{\Delta_{\alpha_k}^k\}$, $\alpha_k = 1, 2, 3, \dots$, of the \mathcal{M} -dimensional configuration space spanned by the $\{X_J^{(d)}(t)\}$ at a series of times t_k , $k = 1, 2, \dots, n$, with $t_1 < t_2 < \dots < t_n$. We take the same set of regions for each value of d and usually take them to be ‘‘cubes’’ of equal sides Δ . An individual history is then labeled by the particular sequence of intervals $(\alpha_1, \dots, \alpha_n) \equiv \alpha$. We then compare the probabilities that these histories are correlated by the classical equations of motion discussed in Sec. III for different values of d .

Quantum interference between the individual members of a coarse-grained set of histories must be negligible for probabilities to be consistently assigned to its individual mem-

bers. When this condition is satisfied the set of histories is said to decohere. Decoherence is a prerequisite for probabilities.

The interference between histories α and α' is measured by the decoherence functional

$$D^{(d)}(\alpha', \alpha) = \text{Tr}[P_{\alpha'_n}^d(t_n) \cdots P_{\alpha'_1}^d(t_1) \rho P_{\alpha_1}^d(t_1) \cdots P_{\alpha_n}^d(t_n)]. \quad (6.1)$$

Here, $\{P_{\alpha_k}^d(t_k)\}$ are an exhaustive set of mutually orthogonal Heisenberg picture projection operators projecting on the regions $\{\Delta_{\alpha_k}^k\}$ of $\{X_J^{(d)}\}$ at time t_k . The operator ρ is the Heisenberg picture density matrix of the system. The set of histories decoheres when the ‘‘off-diagonal’’ elements of $D^{(d)}$ are negligible:

$$D^{(d)}(\alpha', \alpha) \approx 0, \quad \alpha' \neq \alpha. \quad (6.2)$$

There is an equivalent path integral expression for the decoherence functional of sets of histories coarse grained by ranges of configuration space such as those under discussion here. Suppose the coarse graining is entirely confined to times less than a final time t_f , i.e., $t_n < t_f$. Then, for the linear chain coarse grained by ranges of $X_J^{(d)}(t)$,

$$D^{(d)}(\alpha', \alpha) = \int_{\alpha'} \delta \vec{a}' \int_{\alpha} \delta \vec{a} \delta(\vec{a}'_f - \vec{a}_f) \times \exp(i\{S[\vec{a}'(\tau)] - S[\vec{a}(\tau)]\}/\hbar) \rho(\vec{a}'_0, \vec{a}_0). \quad (6.3)$$

One integral in Eq. (6.3) is over paths $\vec{a}(\tau)$ on the interval $[0, t_f]$ which start at \vec{a}_0 at $t=0$ and end at \vec{a}_f at $t=t_f$ including integrations over those end points. The integral is only over paths which pass through the regions $\{\Delta_{\alpha_k}^k\}$ in $\{X_J^{(d)}\}$ at the times t_k . The constraint on the $X_J^{(d)}$ translates linearly into a constraint on the \vec{a} through Eq. (2.2). An integral over $\vec{a}'(\tau)$ is similar except that it is constrained by the coarse grainings of α' . The sum in Eq. (6.3) could have been expressed in terms of any configuration space variables. We have chosen the modes a_l because the action takes the simple form (2.5). Equally well, we could have used the coordinates of the individual atoms, x_i , $i = 1, \dots, \mathcal{N}$.

Path integrals of the form (6.3) have been extensively studied for quadratic actions and thermal density matrices by many authors [13,16,4,5]. All integrals are Gaussian in this situation and can be evaluated explicitly. The simplest way to review this is to recall a simple example.

B. Simple example

The sum-over-histories techniques used in this paper to calculate the decoherence functional for sets of alternative coarse-grained histories of the linear harmonic chain are generalizations of those used for more straightforward coarse grainings of simpler linear systems [4,5]. In turn, these methods extend those pioneered by Feynman and Vernon [13] and Caldeira and Leggett [16]. While the results of this paper

are algebraically more complex, the basic ideas are similar to those in simpler cases. To emphasize this connection with previous work, and to explain the ideas in an algebraically simple context, we review a version of these simple models.

The model consists of the linear chain under discussion but with a particle of mass M and position $X(t)$ coupled by a linear interaction to atom 0. The total action is

$$S_{\text{tot}}[X(\tau), \vec{x}(\tau)] = S[\vec{x}(\tau)] + S_X[X(\tau)] + S_{\text{int}}[x_0(\tau), X(\tau)], \quad (6.4)$$

where $S[\vec{x}(\tau)]$ is given by Eq. (2.1), $S_X[X(\tau)]$ is

$$S_X[X(\tau)] = \int_0^{t_f} d\tau \frac{1}{2} M \dot{X}^2(\tau) \quad (6.5)$$

and the interaction term is

$$S_{\text{int}}[x_0(\tau), X(\tau)] = -\kappa \int_0^{t_f} d\tau X(\tau) x_0(\tau). \quad (6.6)$$

We consider coarse grainings where only histories of X are followed. Thus the entire chain serves as the environment.

The action $S[\vec{x}(\tau)]$ is Eq. (2.1), which is Eq. (2.5) when expressed in terms of normal modes. The interaction is

$$S_{\text{int}}[\vec{a}(\tau), X(\tau)] = -2\kappa \mathcal{N}^{-1/2} \sum_l \int_0^{t_f} d\tau \text{Re } a_l(\tau) X(\tau). \quad (6.7)$$

The problem summarized by Eq. (6.4) can be mapped onto a problem studied by many authors following Caldeira and Leggett [16]. We will follow the calculation of the decoherence functional described in [4] but in a notation that is designed to stress the analogy with the subjects of this paper. The translations are as follows, the first being the notation of this paper, the second of [4]:

$$\begin{aligned} \text{Re } a_l &\leftrightarrow Q_A, & \omega_l &\leftrightarrow \omega_A, \\ X(t) &\leftrightarrow x(t), & \mu &\leftrightarrow m, \\ 2\kappa \mathcal{N}^{-\frac{1}{2}} &\leftrightarrow C_A, & M &\leftrightarrow M. \end{aligned} \quad (6.8)$$

We assume an initial condition that is a product of a density matrix $\tilde{\rho}(x'_0, x_0)$ for the particle and a thermal density matrix $\rho_T(\vec{a}'_0, \vec{a}_0)$ at temperature T for the environment.

We consider a set of alternative coarse-grained histories defined by exhaustive sets of ranges for X , $\{\Delta_{\alpha'}^1\}$, $\{\Delta_{\alpha'}^2\} \dots \{\Delta_{\alpha'}^n\}$, $\alpha = 1, 2, \dots$, at a series of times $t_1 < \dots < t_n$. The decoherence functional for this coarse-grained set of histories is given generally by

$$\begin{aligned} D(\alpha', \alpha) &= \int_{\alpha'} \delta X' \int_{\alpha} \delta X \int \delta a' \int \delta a \delta(X'_f - X_f) \delta(\vec{a}'_f - \vec{a}_f) \\ &\times \exp(i\{S_{\text{tot}}[X'(\tau), \vec{a}'(\tau)] - S_{\text{tot}}[X(\tau), \vec{a}(\tau)]\}/\hbar) \\ &\times \tilde{\rho}(X'_0, X_0) \rho_T(\vec{a}'_0, \vec{a}_0). \end{aligned} \quad (6.9)$$

The integral over the X 's is restricted to paths that traverse the regions $\Delta_{\alpha'_1}^1, \dots, \Delta_{\alpha'_n}^n$ defining the coarse-grained history $\alpha \equiv (\alpha_1, \dots, \alpha_n)$ and similarly for X' 's. The integrals over the a'_l and a_l are unrestricted and, given the assumed thermal initial condition, reduce to Gaussian integrals which can be carried out explicitly. The result, expressed in terms of the variables

$$\bar{X}(t) = \frac{1}{2} [X'(t) + X(t)], \quad (6.10a)$$

$$\xi(t) = X'(t) - X(t), \quad (6.10b)$$

is

$$\begin{aligned} D(\alpha', \alpha) &= \int_{\alpha'_\xi} \delta \xi \int_{\alpha_{\bar{x}}} \delta \bar{x} e^{i\mathcal{A}[\bar{X}(\tau), \xi(\tau)]} \\ &\times \tilde{\rho}\left(\bar{X}_0 + \frac{\xi_0}{2}, \bar{X}_0 - \frac{\xi_0}{2}\right) \end{aligned} \quad (6.11)$$

where α_ξ and $\alpha_{\bar{x}}$ are the limits on $\xi(\tau)$ and $\bar{x}(\tau)$ given that $x(\tau)$ and $x'(\tau)$ lie within the limits α and α' , respectively, and

$$\begin{aligned} \mathcal{A}[\bar{X}(\tau), \xi(\tau)] &= -\xi_0 M (d\bar{X}/dt)|_{t=0} \\ &+ \int_0^{t_f} dt \xi(t) e(t, \bar{X}(\text{tan})) \\ &+ \frac{i}{4} \int_0^{t_f} dt \int_0^{t_f} dt' \xi(t') k_I(t' - t) \xi(t). \end{aligned} \quad (6.12)$$

The ingredients in Eq. (6.12) are the equation of motion

$$e(t, X(\tau)) = -M \frac{d^2 \bar{X}}{dt^2}(t) + \int_0^t dt' k_R(t - t') \bar{X}(t'), \quad (6.13)$$

together with the kernels

$$k_R(t) = -4\kappa^2 (\mu \mathcal{N})^{-1} \sum_l \omega_l^{-1} \sin(\omega_l t) \quad (6.14)$$

and

$$k_I(t) = 4\kappa^2 (\mu \mathcal{N})^{-1} \sum_l \omega_l^{-1} \coth\left(\frac{\hbar \omega_l}{2kT}\right) \cos(\omega_l t). \quad (6.15)$$

The imaginary term in Eq. (6.12) favors $\xi(t) = 0$, that is $X'(t) = X(t)$. If it is large, the off-diagonal elements of $D(\alpha', \alpha)$ will be negligible and decoherence achieved. The

characteristic time scale t_{decoh} over which enough imaginary exponent is built up to make the off-diagonal elements of D negligible is

$$t_{\text{decoh}} \sim (k_I \Delta^2)^{-1/2}, \quad (6.16)$$

where k_I and Δ denote characteristic sizes of the kernel (6.15) and the intervals $\Delta_{\alpha_i}^i$.

If the set of histories decoheres, then the restrictions on the integrals over $\xi(t)$ in Eq. (6.11) defining the diagonal elements of $D(\alpha', \alpha)$ can be ignored and the resulting Gaussian integral over $\xi(t)$ carried out. The result is the following expression for the probabilities of the coarse-grained history α :

$$\begin{aligned} p(\alpha) = & \int_{\alpha} \delta \bar{X} [\det(k_I)/4\pi]^{-1/2} \\ & \times \exp \left\{ -\frac{1}{\hbar} \int_0^{t_f} dt' \int_0^{t_f} dt e(t', \bar{X}(\tau)) \right. \\ & \left. \times k_I^{\text{inv}}(t' - t) e(t, \bar{X}(\tau)) \right\} w(\bar{X}_0, \bar{P}_0). \end{aligned} \quad (6.17)$$

Here, $k_I^{\text{inv}}(t, t')$ is the inverse of $k_I(t, t')$ and $w(\bar{X}_0, \bar{P}_0)$ is the Wigner distribution of the density matrix $\tilde{\rho}$.

Equation (6.17) shows that probabilities peak on histories obeying the deterministic equation of motion $e(t, X(\tau)) = 0$, but with a width in this distribution related to $k_I(t' - t)$. The same probabilities follow from a Langevin equation

$$e(t, X(\tau)) + l(t) = 0, \quad (6.18)$$

with a stochastic noise force distributed with a correlation function

$$M[l(t')l(t)] = \frac{1}{2} \hbar k_I(t' - t). \quad (6.19)$$

Thus, decoherence and noise are connected. The stronger the coupling between system and environment, the more rapidly interference between histories is dissipated, but also the more noise which disturbs the deterministic dynamics and reduces predictability.

The deterministic equation $e(t, X(\tau)) = 0$ is exactly the same as the classical equation of motion which would be derived from the Lagrangian for this system, in the limit of zero noise. This result is generally true for systems with quadratic Lagrangians, and may hold approximately for systems with greater nonlinearities. More details than we have given here are presented in [4]. We will follow the basic ideas of this model in our treatment of the family of coarse grainings of the linear chain.

C. Decoherence functional for the linear chain

We now apply essentially the same procedure to the linear chain, analyzing decoherence and deriving equations of motion for the coarse-grained position averages $X_J^{(d)}$.

Using the initial condition (2.17) the integrals over q_a can be carried out in Eq. (6.3), yielding an expression for the decoherence functional of the coarse-grained modes, $D^{(d)}[\vec{A}'(\tau), \vec{A}(\tau)]$, analogous to Eq. (6.9). The magnitude of $D^{(d)}$ in the limit $\Delta, \Delta t \rightarrow 0$ is

$$\begin{aligned} & |D^{(d)}[\vec{A}'(\tau), \vec{A}(\tau)]| \\ & = \exp \left[-\frac{1}{2} \int_0^{t_f} dt' \int_0^{t_f} dt [\vec{\xi}(t') \mathbf{K}_I^{(d)}(t', t) \vec{\xi}(t)] \right] \\ & \quad \times \left| \rho \left(\vec{A}_0 + \frac{\vec{\xi}_0}{2}, \vec{A}_0 - \frac{\vec{\xi}_0}{2} \right) \right| \end{aligned} \quad (6.20)$$

where

$$\vec{\xi}(t) = \vec{A}'(t) - \vec{A}(t), \quad (6.21a)$$

$$\mathcal{A}(t) = \frac{1}{2} [\vec{A}'(t) + \vec{A}(t)]. \quad (6.21b)$$

The all-important kernel $\mathbf{K}_I^{(d)}(t', t)$ is given by

$$\begin{aligned} \mathbf{K}_I^{(d)}(t', t) = & \frac{N^2 \mu^2 k_B T}{4 \hbar^2} \vec{c} (\Omega_L^2 \mathbf{I} - \Omega_Q^2) \\ & \times \mathbf{M}_{TT}^{-1/2} \Omega^{-1} (\cos[\Omega t'] \cos[\Omega t]) \\ & + \sin[\Omega t'] \sin[\Omega t] \Omega^{-1} \mathbf{M}_{TT}^{-1/2} (\Omega_L^2 \mathbf{I} - \Omega_Q^2) \vec{c}, \end{aligned} \quad (6.22)$$

which is proportional to the correlation function (3.26) of the classical noise derived from the Lagrangian. Thus the ‘‘off-diagonal’’ elements of the decoherence functional decay exponentially with increasing difference between $\vec{A}'(\tau)$ and $\vec{A}(\tau)$. The set of histories with $\Delta, \Delta t \rightarrow 0$ is clearly not decoherent, since $\vec{A}(\tau)$ and $\vec{A}'(\tau)$ can be arbitrarily close; but, by introducing suitably large regions $\Delta_{\alpha_k}^k$ at suitably spaced intervals Δt of time, decoherence can be achieved. We shall return to a detailed discussion of decoherence times as a function of d below, but first we consider the equations of motion.

The probability of a given coarse-grained history α is given by

$$p(\alpha) = \int_{\alpha} \delta \vec{A} D[\vec{A}(\tau), \vec{A}(\tau)] \quad (6.23)$$

which in analogy to Eq. (6.17) can be expressed as

$$\begin{aligned} p(\alpha) = & \int_{\alpha} \delta \vec{A} [\det(\mathbf{K}_I^{(d)})/4\pi]^{-1/2} \\ & \times \exp \left\{ -\frac{1}{\hbar} \int_0^{t_f} dt' \int_0^{t_f} dt \{ \vec{\mathcal{E}}'(t', \vec{A}(\tau)) \right. \\ & \left. \times \mathbf{K}_I^{(d)\text{inv}}(t', t) \vec{\mathcal{E}}(t, \vec{A}(\tau)) \right\}. \end{aligned} \quad (6.24)$$

$\vec{\mathcal{E}}'(t, \vec{A}(\tau))$ is a linear functional of $\vec{A}(\tau)$ analogous to Eq. (6.13), whose exact form we return to below; $\mathbf{K}^{(d)\text{inv}}(t', t)$ is the inverse of $\mathbf{K}^{(d)}(t', t)$ defined in Eq. (6.22).

Equation (6.24) shows that the probability of histories is sharply peaked about those obeying the equations of motion

$$\vec{\mathcal{E}}'(t, \vec{A}(\tau)) = 0, \quad (6.25)$$

but with Gaussian noise causing deviations from this predictability related to the size of the kernel $\mathbf{K}_I^{(d)\text{inv}}(t', t)$. The form of the equations of motion (6.25) could be worked out by following the procedure used in the simple example above. However, it is more direct to note that the result of that calculation is exactly the equation of motion that would be obtained by a completely classical analysis of the coarse-grained dynamics, just as in Eq. (6.17) for the simple model. *The equations of motion $\vec{\mathcal{E}}'(t, X(\tau)) = 0$ are therefore equivalent to the classical equations* derived in Secs. III and IV. This is an important simplification because a straightforward extension of the above analysis would lead to nonlocal terms such as occur in Eq. (6.13), as we saw in Sec. III C. In the end, these all cancel to give the simple equations of motion exhibited in Sec. III. This is checked explicitly in Appendix C.

The size of the kernel $\mathbf{K}_I^{(d)}(t, t')$ in Eq. (6.20) controls the efficacy of decoherence—the larger the kernel, the shorter the decoherence time scale. We study it as a function of d , holding all other parameters fixed, including the temperature of bath T . The kernel is necessarily positive [5]. A simple measure of its size is the time-averaged trace

$$\mathcal{K}_I(d) = \lim_{t_f \rightarrow \infty} \frac{1}{t_f} \int_0^{t_f} dt \text{Tr}[\mathbf{K}^{(d)}(t, t)]. \quad (6.26)$$

Figure 4 shows \mathcal{K}_I plotted as a function of d . Since the form of the kernel is closely related to the classical noise correlation function $M[\Delta f'^*(t)\Delta f'(t')]$ from Eq. (3.26), it is not surprising that the shape of the result is virtually identical to Fig. 3. While Fig. 3 was computed from the form (3.25) for the noise, which is different, the difference amounts to a constant factor of N^2 and a d -dependent factor very close to 1. From the two graphs, where the N dependence has been absorbed into the choice of units, it is evident that the dependence on d of the two forms of noise is almost exactly the same.

Since the kernel $\mathbf{K}_I^{(d)}$ is a factor of N^2 larger than the classical noise correlation function, increasing the level of coarse graining N exponentially improves decoherence, but actually reduces the classical noise [cf. Eq. (5.6)]. Because of this, for realistically large values of N , the decoherence rate is rapid compared to dynamical time scales even in the completely localized case, where the absolute strength of the noise is weakest. One can understand this as increasing the absolute level of decoherence, but simultaneously increasing the inertia of the coarse-grained variables to resist the increased noise, since the inertia of a group just goes like its total mass $N\mu$. We discuss this trade-off more thoroughly below.

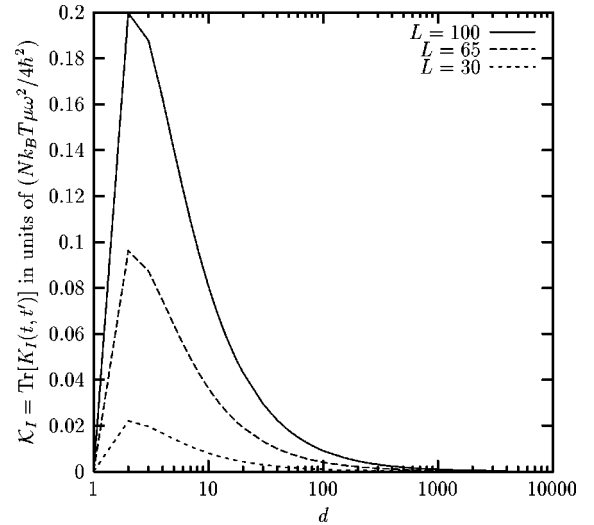


FIG. 4. The time-averaged trace $\mathcal{K}_I(d)$ of the decoherence kernel $\mathbf{K}_I^{(d)}(t, t')$, in units of $Nk_B T \mu \omega^2 / 4 \hbar^2$, vs the coarse graining d , for $\mathcal{M} = 630$ and $L = 30, 65, 100$. The form of these curves is virtually identical to the classical noise correlation function, plotted in Fig. 3. Note that an overall factor of N^2 has been divided out to make comparison to Fig. 3 more exact.

VII. CONCLUSIONS: CLASSICALITY

For a system with many degrees of freedom, useful dynamical predictions concern regularities emerging from coarse-grained descriptions. To be sure, at a fine-grained level the system will display the regularities arising from its fundamental equations of motion if it is classical or from the Schrödinger equation if quantum mechanical. However, these regularities are usually impossible to extract or apply if the number of degrees of freedom is very large. The useful predictions arise from much smaller numbers of coarse-grained variables correlated in time according to phenomenological equations of motion.

There are arbitrarily many sets of alternative coarse-grained histories that can be assigned probabilities on the basis of a closed system's initial condition and fundamental dynamics. Which of these will exhibit useful regularities in time governed by phenomenological equations of motion? How much, and what, coarse graining is needed to obtain useful predictability? This, very roughly, is the problem of characterizing classicality that we mentioned in the Introduction. In this conclusion we describe how our results for the linear harmonic chain bear on this question.

Which coarse-grained descriptions are predictable is an important problem even in classical physics. However, it is especially important in quantum mechanics where probabilities can be assigned only to *decoherent* sets of histories, and two such sets are generally mutually incompatible. Further, in a loose sense, the number of sets of coarse-grained histories is much larger in quantum mechanics than it is in classical physics. It is therefore important to explain *within* quantum mechanics (and a theory of the cosmological initial condition) why we find it useful to employ only a narrow class of the possible coarse grainings by which the universe could in principle be described. Many see this as the central

problem in understanding quantum mechanics.

Characterizing classicality involves comparing the utility for prediction of various sets of coarse grained alternative histories. In this paper we have considered only a family of coarse grainings of the simplest linear system exhibiting a continuum description of the kind usually found in classical physics—the linear harmonic chain.

Four parameters characterize the family of coarse grainings we have considered. The atoms of the chain are divided into groups of N , consisting of equally spaced clumps of d neighboring atoms. (See Fig. 2.) The center of mass coordinates of each group are coarse grained by exhaustive sets of equal ranges Δ spaced by equal time intervals Δt . The four parameters are therefore N , d , Δ , and Δt .

The probabilities of the individual members of a decoherent set of histories follow from the initial state, so that any comparison of the predictability of different coarse grainings will depend crucially on the nature of this initial condition. We assumed an initial condition in which the short wavelength modes of the string were in thermal equilibrium at a temperature T , while the long wavelength modes were excited well above the level of thermal fluctuations. This is an initial state of local but not global thermal equilibrium.

Both classically and quantum mechanically the probabilities of these decoherent sets of alternative coarse-grained histories can be characterized as arising from equations of motion augmented by noise. The dynamical time scale of the equations of motion (3.12) is given roughly by

$$t_{dyn} \sim \frac{d}{\omega} \left(\frac{\mathcal{M}}{L} \right). \quad (7.1)$$

The local coarse grainings $d \sim N$ have the longest dynamical time scales because the center of mass momenta of the local groups are approximately conserved.

The utility of these equations of motion for prediction depends on the size of the deviations from the regularity in time they describe that is caused by the noise. The noise forces were estimated roughly in Eq. (5.6). (The force is $N\mu$ times the force per unit mass $\Delta f_L^{(d)}$.) For large N , d comparable to N , and L small compared to \mathcal{M} ,

$$F_{noise} \sim (k_B T \omega^2 \mu)^{1/2} (N/d)^{1/2} (L/\mathcal{M}). \quad (7.2)$$

With these basic estimates in hand, we can compare the different members of this family of coarse grainings with respect to three properties bearing on classicality: the rate of decoherence, the deviations from predictability caused by the noise, and the computational complexity required to use the equations of motion to make predictions. The results are as follows:

Decoherence. Decoherence and noise are connected. The kernel which governs the size of the imaginary part of the influence phase and effects decoherence is the correlation function of the noise force [cf. Eqs. (6.15) and (6.19)]. From Eq. (6.20) we can obtain the following rough estimate for the decoherence time t_{decoh} which Δt must exceed if the coarse-grained set of decoherent histories is to decohere:

$$t_{decoh} \sim \hbar / (F_{noise} \Delta). \quad (7.3)$$

This time increases with the locality of the coarse graining d because F_{noise} decreases with d , as Eq. (7.2) shows. Since the more local coarse grainings are dominated by low frequency modes, the dynamical timescale also increases with d , so that the *ratio* of the two times favors the more local coarse-grainings; combining Eqs. (7.1) and (7.2) we have

$$\frac{t_{decoh}}{t_{dyn}} \sim \left(\frac{\lambda_{DB}}{\Delta} \right) (Nd)^{-1/2}, \quad (7.4)$$

where λ_{DB} is the thermal de Broglie wavelength introduced by Zurek [21]:

$$\lambda_{DB} = \hbar / (k_B T \mu)^{1/2}. \quad (7.5)$$

The decoherence time scale must be less than the dynamical time scale to use the equations of motion at all. This can be achieved by taking N or Δ or both sufficiently large, and for both local and non-local coarse grainings is not a very constraining condition given “realistic” parameter values, as was stressed by Zurek [21] in simpler cases. For $d \sim 1$, $N \sim 10^6$, $\mu \sim 10$ amu, and $T \sim 300^\circ$,

$$t_{decoh}/t_{dyn} \sim (10^{-13} \text{ cm})/\Delta. \quad (7.6)$$

For such coarse grainings, decoherence is not a major restriction on predictability.

Noise. As Eq. (7.2) shows, the noise force decreases as d increases for fixed N ; that is, it decreases as the coarse graining becomes more local. However, it is not the absolute scale of the noise that is important for predictability, but rather its size relative to the dynamical force terms F_{dyn} that occur in the equation of motion. If \mathcal{L} is the characteristic size of the excitations of the chain that occur in the coarse graining, then roughly

$$F_{dyn} \sim N\mu \mathcal{L} / t_{dyn}^2. \quad (7.7)$$

The size of \mathcal{L} is determined by the initial condition and varies with both N and d . In Eqs. (2.16) and (2.17) we assumed an initial condition in which the fine-grained modes above a mode number l_C were thermally excited, while modes below l_C were much more highly excited. The connection between fine- and coarse-grained modes given by Eqs. (2.7) and (2.9) shows that the fine-grained modes below l_C contribute to coarse-grained modes only when $d > N(L/l_C)$. Thus, if d lies much below N , we have

$$\frac{F_{noise}}{F_{dyn}} \sim 1, \quad d \ll N, \quad (7.8)$$

and the regularities of the equation of motion will be swamped by the noise.

By contrast, when $d \sim N$

$$\frac{F_{noise}}{F_{dyn}} \sim \frac{\mathcal{L}_T}{\mathcal{L}} \sqrt{N}, \quad d \sim N \quad (7.9)$$

where \mathcal{L}_T is the characteristic scale of thermal excitations of the mode:

$$\mathcal{L}_T \sim [(k_B T)/(N\mu\Omega_L^2)]^{1/2}. \quad (7.10)$$

If the size of excitations of long wavelength modes is much greater than that of thermal fluctuations, the effect of the noise on the equation of motion will be negligible. Thus the local coarse grainings exhibit more regularity in time if the initial condition has this property. For the realistic string described above with $N \sim 10^6$, typical thermal excitations of the $L=10$ mode would be $\mathcal{L}_T \sim 10^{-7}$ m.

Computational complexity. Even when coarse grainings decohere so that probabilities can be assigned to histories, even when noise is negligible so that histories exhibit the regularities in time summarized by classical equations of motion, coarse grainings can be distinguished by the effort needed to calculate these regularities. The number of operations N_S necessary to evolve the equations of motion over a time interval T is roughly proportional to

$$N_S \propto (\mathcal{M}/t_{dyn})T \sim (L\omega T/d). \quad (7.11)$$

Thus prediction becomes easier as both N and d increase. For ‘‘realistic’’ coarse grainings where $N \sim 10^6$ there can be a significant difference between the local coarse grainings with $d \sim 10^6$ and the nonlocal ones with $d \sim$ few.

In summary, *decoherence, resistance to noise and computational simplicity all favor local coarse grainings over non-local ones*—all these comparisons being contingent on large N and an initial condition in which long wavelength modes are more excited than short wavelength ones.

These quantitative results for the linear harmonic chain support the heuristic arguments for the predictability of more general kinds of quasiclassical variables that were sketched in the Introduction. In our family of coarse grainings, the ones more useful for prediction are the more local ones associated with an approximately conserved quantity. Our analysis of the harmonic chain is a step towards a more realistic analysis of classicality in at least three ways: (1) It considered a system which permits a continuum approximation of the kind usually found in classical physics. (2) It employed a system-environment split which follows from the coarse grainings needed to realize that approximation rather than being posited *ad hoc* in terms of fundamental coordinates. (3) Different coarse grainings were compared quantitatively with respect to decoherence, noise and computational complexity.

However, these positive features should not obscure how short this analysis falls from the kind of treatment of classicality envisaged by [3,4,6,22,23]. We considered only linear interactions, not a realistic Hamiltonian. We did not compare all possible sets of alternative coarse-grained histories, but only a four-parameter family of them. We did not propose a unified quantitative measure for classicality, but rather dealt separately with some of its attributes: decoherence, resistance to noise, and computational simplicity. We did not start from the initial condition of the universe or exhibit the important role played by gravity in creating the conditions for local equilibrium while ensuring the absence of global equilibrium. Rather we assumed these properties in our initial condition. Future analyses will do better.

ACKNOWLEDGMENTS

The authors are grateful for conversations with M. Gell-Mann over a long period of time concerning the issues addressed in this paper, as well as discussions with J.J. Halliwell. The work of both authors was supported in part by NSF grant PHY94-07194 at the Institute for Theoretical Physics. That of J.B.H. was also supported by NSF grant PHY95-07065, while T.A.B. was also supported by NSF grant PHY96-02084.

APPENDIX A: SYSTEM-ENVIRONMENT SPLITS

In this appendix we describe the circumstances under which—for a given coarse-grained set of alternatives—the Hilbert space \mathcal{H} of a closed system can be written as a tensor product $\mathcal{H}^s \otimes \mathcal{H}^e$ where \mathcal{H}^s contains the quantities followed by the coarse graining and \mathcal{H}^e contains the quantities that are ignored. Such a tensor product factorization is called a system-environment split.

We begin by considering a Hilbert space \mathcal{H} and a set of alternatives at a single moment of time represented by an exhaustive set of orthogonal projection operators $\{P_\alpha\}$, $\alpha = 1, 2, \dots$, satisfying

$$P_\alpha P_\beta = \delta_{\alpha\beta} P_\beta, \quad \sum_\alpha P_\alpha = I. \quad (A1)$$

We seek to write

$$\mathcal{H} = \mathcal{H}^s \otimes \mathcal{H}^e \quad (A2)$$

such that

$$P_\alpha = P_\alpha^s \otimes I^e, \quad \alpha = 1, 2, \dots \quad (A3)$$

The decomposition (A2) is then a system-environment split. If \mathcal{H}^s were to contain *just* the quantities followed by the coarse graining, we would naturally impose $\dim(P_\alpha^s) = 1$, where $\dim(P)$ is the dimension of the subspace projected on by P . However, other notions of an environment can be useful in which $(\dim P_\alpha^s) > 1$, and we shall consider the general case.

Only two simple mathematical facts are needed to analyze the above question. First, the decomposition (A3) requires the relation between dimensions,

$$\dim(P_\alpha) = \dim(P_\alpha^s) \dim(\mathcal{H}^e), \quad (A4)$$

and, as a special case,

$$\dim(\mathcal{H}) = \dim(\mathcal{H}^s) \dim(\mathcal{H}^e). \quad (A5)$$

Second, two separable Hilbert spaces of a given dimension are isomorphic—a consequence of the fact that they both have countable bases.

Realistic cases have $\dim(\mathcal{H}) = \infty$, but we pause to note some evident results from Eq. (A4) when $\dim(\mathcal{H})$ is finite. Then all the $\dim(P_\alpha)$ are finite. A system-environment split is not always possible, only when the $\dim(P_\alpha)$ are all divisible by a common factor. In particular, if $\dim(P_\alpha^s)$ is

quired to be unity, then a system-environment split is possible only when all the P_α 's have the same dimension.

When $\dim(\mathcal{H})$ is infinite, there are a number of subcases which are convenient to treat separately. The most important of these is when $\dim(P_\alpha) = \infty$ for all α . The requirements (A1) imply that the P_α all commute and can be simultaneously diagonalized. Let $\{|i\rangle\}$, $i=1,2,\dots$, be a basis in which they are all diagonal. Then to each P_α there is a subset of these basis vectors spanning the corresponding subspace. We write

$$P_\alpha = \sum_{i \in \alpha} |i\rangle\langle i|. \quad (\text{A6})$$

However, it is then a simple matter of relabeling to define an isomorphism between the infinite dimensional Hilbert spaces \mathcal{H} and $\mathcal{H}^s \otimes \mathcal{H}^e$. We write

$$|i\rangle = |\alpha, A\rangle \quad (\text{A7})$$

where i ranges over the infinity of states in P_α and $A = 1, 2, \dots$ is another labeling of them. This relabeling defines the tensor product $\mathcal{H}^s \otimes \mathcal{H}^e$. Operators acting only on \mathcal{H}^s have the form

$$\langle \alpha' A' | \mathcal{O} | \alpha A \rangle = \langle \alpha' | \mathcal{O}^s | \alpha \rangle \delta_{AA'}, \quad (\text{A8a})$$

while those on \mathcal{H}^e have matrix elements

$$\langle \alpha' A' | \mathcal{O} | \alpha A \rangle = \delta_{\alpha' \alpha} \langle A' | \mathcal{O}^e | A \rangle. \quad (\text{A8b})$$

In particular,

$$P_\alpha = P_\alpha^s \otimes I^e = (|\alpha\rangle\langle\alpha|) \otimes I^e \quad (\text{A9})$$

and $\dim(P_\alpha^s) = 1$. We have constructed a system-environment split defined by the coarse-graining $\{P_\alpha\}$.

If the condition $\dim(P_\alpha^s) = 1$ is relaxed, it is possible to define many other system-environment splits for this coarse graining. One simply relabels including more states in \mathcal{H}^s , viz.

$$|i\rangle = |\alpha, A\rangle \quad (\text{A10})$$

such that the subspace P_α^s contains several different values of α .

Many calculations use a system-environment split of this kind. For example, in studies of Brownian motion the labels α correspond to the coordinates of the massive particle and A to the coordinates of the particles of the bath. The coordinates of the bath are ignored, but typically the coordinates of the Brownian particle are followed only to some accuracy. Thus, for a given choice of ranges, coordinates other than those in the bath are ignored corresponding to $\dim(P_\alpha^s) > 1$. There is no unique system-environment split.

The key to the above construction is that the relation (A4) is easily satisfied because $\dim(P_\alpha)$ and $\dim(\mathcal{H})$ are both infinite. Finite dimensional members of the set of alternatives are obstacles to a system-environment split. If $\dim(P_\alpha)$ is finite for some α , then Eq. (A4) can only be satisfied if $\dim(P_\alpha^s)$ and $\dim(\mathcal{H}^e)$ are both finite—already a restrictive condition. Furthermore, the dimensions of all the finite dimensional P_α must be divisible by common factor—

$\dim(\mathcal{H}^e)$ —and this is not always possible. The only case in which the condition $\dim(P_\alpha^s) = 1$ could be enforced is if all the finite dimensional P_α have the *same* dimension. Clearly, a system-environment split is generally possible only when the dimensions of all of the P_α are infinite.

APPENDIX B: MATRICES FOR THE CHAIN OF OSCILLATORS

In this appendix we complete a calculation begun in Sec. III C. This is the explicit demonstration that when the variables in the action are changed according to Eqs. (2.9) and (2.14), the result yields the same equations of motion as are obtained by making these changes in the fine-grained equations of motion directly. Specifically we check that when Eq. (3.7) is used to eliminate the q 's from Eq. (3.19) it yields Eq. (3.12).

Since the coarse-grained modes $A_L^{(d)}(t)$ are all decoupled from each other, and interact with separate collections of high-frequency modes, we can consider them one at a time, which somewhat simplifies our notation. In this case, the matrix \mathbf{S} reduces to a diagonal matrix with elements making up a single vector with d components S_a , and \mathbf{T} is a d by $d-1$ matrix with components T_{ab} , where a ranges from 0 to $d-1$ and b ranges from 1 to $d-1$. Thus \mathbf{M}_{SS} and \mathbf{V}_{SS} become scalars, and \mathbf{M}_{ST} , \mathbf{M}_{TS} , \mathbf{V}_{ST} and \mathbf{V}_{TS} are vectors in the space of the q 's. These matrices have the simple form

$$S_0 = \frac{1}{c_0}, \quad S_a = 0, \quad \text{for } a > 0, \quad (\text{B1})$$

and

$$T_{0b} = -\frac{c_b}{c_0}, \quad T_{ab} = \delta_{ab}, \quad \text{for } a > 0, \quad (\text{B2})$$

where the numbers c_a are the coefficients $c_{Lk}^{(d)}$ defined by Eqs. (2.11) and (3.6), forming the components of the vector \vec{c} . The matrix ω is diagonal with components ω_a and the mass is a constant μ .

With these definitions, the matrices defined in Eqs. (3.17a), (3.17b) are

$$\begin{aligned} M_{SS} &= \frac{\mu}{|c_0|^2}, \\ (\mathbf{M}_{TT})_{bb'} &= \mu \delta_{bb'} + \mu \frac{c_b c_{b'}^*}{|c_0|^2}, \\ (\vec{M}_{ST})_b &= -\mu \frac{c_b}{|c_0|^2} = (\vec{M}_{TS})_b, \\ V_{SS} &= \mu \omega_0^2, \\ (\mathbf{V}_{TT})_{bb'} &= \mu \omega_b^2 \delta_{bb'} + \mu \omega_0^2 \frac{c_b c_{b'}^*}{|c_0|^2}, \\ (\vec{V}_{ST})_b &= -\mu \omega_0^2 \frac{c_b}{|c_0|^2} = (\vec{V}_{TS})_b. \end{aligned} \quad (\text{B3})$$

In these expressions when the matrices \mathbf{M}_{SS} , etc., have been reduced to scalars or vectors we have changed the notation in

what we hope is an obvious way. With Eqs. (B3) we can now show that Eq. (3.19) is identical to Eq. (3.12) aside from a multiplicative factor. With a little algebra we find that

$$\begin{aligned} (M_{SS} - \vec{M}_{ST} \mathbf{M}_{TT}^{-1} \vec{M}_{TS}) &= \left(\frac{\mu}{|c_0|^2 + \sum_b |c_b|^2} \right), \\ (V_{SS} - \vec{M}_{ST} \mathbf{M}_{TT}^{-1} \vec{V}_{TS}) &= \left(\frac{\mu}{|c_0|^2 + \sum_b |c_b|^2} \right) \omega_0^2, \\ -(\vec{V}_{ST} - \vec{M}_{ST} \mathbf{M}_{TT}^{-1} \mathbf{V}_{TT})_b &= \left(\frac{\mu}{|c_0|^2 + \sum_{b'} |c_{b'}|^2} \right) \\ &\quad \times c_b (\omega_0^2 - \omega_b^2). \end{aligned} \quad (\text{B4})$$

Since $\omega_0 \equiv \Omega_L$, plugging these back into Eq. (3.19) simply yields the equation

$$\begin{aligned} &\left(\frac{\mu}{|c_0|^2 + \sum_b |c_b|^2} \right) [\ddot{A}_L^{(d)}(t) + \Omega_L^2 A_L^{(d)}(t)] \\ &= \left(\frac{\mu}{|c_0|^2 + \sum_b |c_b|^2} \right) \Delta f(t), \end{aligned} \quad (\text{B5})$$

that is, simply Eq. (3.12) multiplied by a constant factor. This factor is independent of the choice of coarse-grained mode L or the coarse graining d :

$$\left(\frac{\mu}{|c_0|^2 + \sum_b |c_b|^2} \right) = \left(\frac{\mu}{|c_0|^2 + \vec{c}\vec{c}} \right) = N\mu. \quad (\text{B6})$$

APPENDIX C: TRANSFORMING THE EQUATION OF MOTION

In Sec. III we derived the classical equation of motion for the coarse-grained variables $A_L(t)$ utilizing two different ways of eliminating the environmental coordinates q_a . First, using the fact that the q 's were themselves fine-grained coordinates, we solved the classical equations of motion for the q 's and substituted the solution into the fine-grained equations of motion. Second, we derived the equations of motion from the Lagrangian written in terms of the A 's and q 's and then solved for the q 's to eliminate them. In this appendix we complete the demonstration that the ostensibly different equations for the A 's that result are, in fact, equivalent.

Suppose we have an equation of motion of the form (3.9) for a single coarse-grained mode A_L , which in this appendix we call $\mathcal{E}_L=0$. We wish to write it in a new form (3.22) which we call $\mathcal{E}'_L=0$ by a transformation of the form

$$\begin{aligned} \mathcal{E}'_L(t, A_L(\tau)) &= C \left(\mathcal{E}_L(t, A_L(\tau)) \right. \\ &\quad \left. + \int_0^t dt' G_L(t, t') \mathcal{E}_L(t', A_L(\tau)) \right) \\ &= \Delta f'_L(t), \end{aligned} \quad (\text{C1})$$

with, of course, a transformed noise function

$$\Delta f'_L(t) = C \left(\Delta f_L(t) + \int_0^t dt' G_L(t, t') \Delta f_L(t') \right). \quad (\text{C2})$$

Here, C is a positive constant and $G_L(t, t')$ is a particular Green's function for the equation $\mathcal{E}_L=0$, that is in operator shorthand $\mathcal{E}_L G_L = I$. In a similar shorthand we refer to the transformation (C1) as $C(I+G)$. Clearly, the solutions to the two equations (3.9) and (C1) will be the same only if $(I+G)$ is invertible. This will be true if the equation

$$f_L(t) + \int_0^t G_L(t, t') f_L(t') dt' = 0 \quad (\text{C3})$$

can only be solved by $f_L(t)=0$. From Eq. (C3) it is clear that any solution $f_L(t)$ must have $f_L(0)=0$, and is a solution to a second-order linear equation.

In the case of the chain of oscillators, the original form of the equation is Eq. (3.12) and the transformed equation is Eq. (3.22). From Appendix B we see that the positive constant is

$$C = \left(\frac{\mu}{|c_0|^2 + \vec{c}\vec{c}} \right) = N\mu, \quad (\text{C4})$$

and from Eqs. (3.22) and (B4) the kernel $G_L(t, t')$ is

$$\begin{aligned} G_L(t, t') &= \frac{\mu}{|c_0|^2} \vec{c} (\Omega_L^2 \mathbf{I} - \Omega_Q^2) \mathbf{M}_{TT}^{-1/2} \Omega^{-1} \\ &\quad \times \sin[\Omega(t-t')] \mathbf{M}_{TT}^{-1/2} \vec{c}, \end{aligned} \quad (\text{C5})$$

where Ω_L^2 is the constant ω_0^2 and Ω_Q^2 is the diagonal matrix ω restricted to the q 's, with diagonal elements ω_b^2 .

From Eq. (C5) we know that $G_L(t, t)=0$ for all t , which implies

$$\frac{df_L}{dt}(t) = - \int_0^t dt' \frac{dG_L}{dt}(t, t') f_L(t') \quad (\text{C6})$$

and hence $(df_L/dt)(0)=0$. Thus, since both f_L and (df_L/dt) vanish at $t=0$, the only solution to Eq. (C3) is $f_L(t)=0$ and $(I+G)$ is indeed invertible.

Now we need to show that $C(I+G)\Delta f'_L(t) = \Delta f'_L(t)$ for our harmonic chain. The two forms of the noise are given by Eqs. (3.23a) and (3.23b), respectively. Let Ω^2 be the transformed frequency matrix defined by Eq. (3.21), with eigenvalues ν_k^2 and orthonormal eigenvectors \vec{v}_k , and Ω_Q^2 be the diagonal frequency matrix with eigenvalues ω_a^2 . Then the requirement (C2) can be written as

$$\begin{aligned}
 & N\mu\vec{c}(\Omega_L^2\mathbf{I}-\Omega_Q^2)[\cos(\Omega_Q t)\Delta\vec{q}(0)+\Omega_Q^{-1}\sin(\Omega_Q t)\Delta\dot{q}(0)]+\frac{N\mu^2}{|c_0|^2}\vec{c}\mathbf{M}_{TT}^{-1/2}(\Omega_L^2\mathbf{I}-\Omega_Q^2)\Omega^{-1}\int_0^t\sin[\Omega(t-t')]\mathbf{M}_{TT}^{-1/2}\vec{c} \\
 & \quad \times\vec{c}(\Omega_L^2\mathbf{I}-\Omega_Q^2)[\cos(\Omega_Q t)\Delta\vec{q}(0)+\Omega_Q^{-1}\sin(\Omega_Q t)\Delta\dot{q}(0)]dt' \\
 & =N\mu\vec{c}(\Omega_L^2\mathbf{I}-\Omega^2)[\cos(\Omega t)\mathbf{M}_{TT}^{1/2}\Delta\vec{q}(0)+\Omega^{-1}\sin(\Omega t)\mathbf{M}_{TT}^{1/2}\Delta\dot{q}(0)]. \tag{C7}
 \end{aligned}$$

By writing the vectors in terms of eigenvectors of Ω^2 we can break the integral in Eq. (C7) into a sum over many integrals having the forms

$$\int_0^t\sin[\nu(t-t')]\sin(\omega t')dt'=\frac{1}{\nu^2-\omega^2}[\nu\sin(\omega t)-\omega\sin(\nu t)] \tag{C8}$$

and

$$\int_0^t\sin[\nu(t-t')]\cos(\omega t')dt'=\frac{\nu}{\nu^2-\omega^2}[\cos(\omega t)-\cos(\nu t)]. \tag{C9}$$

Substituting these values into Eq. (C7), the result we wish to show becomes

$$\begin{aligned}
 & \sum_a c_a(\Omega_L^2-\omega_a^2)\left(\cos(\omega_a t)\Delta q_a(0)+\frac{1}{\omega_a}\sin(\omega_a t)\Delta\dot{q}_a(0)\right)+\frac{\mu}{|c_0|^2}\sum_{a,k}|\vec{c}\mathbf{M}_{TT}^{-1/2}\vec{v}_k|^2c_a\frac{(\Omega_L^2-\nu_k^2)(\Omega_L^2-\omega_a^2)}{(\nu_k^2-\omega_a^2)} \\
 & \quad \times\left[\cos(\omega_a t)\Delta q_a(0)-\cos(\nu_k t)\Delta q_a(0)+\frac{1}{\omega_a}\sin(\omega_a t)\Delta\dot{q}_a(0)-\frac{1}{\nu_k}\sin(\nu_k t)\Delta\dot{q}_a(0)\right] \\
 & =\sum_k(\vec{c}\mathbf{M}_{TT}^{-1/2}\vec{v}_k)(\Omega_L^2-\nu_k^2)\left(\cos(\nu_k t)[\vec{v}_k\mathbf{M}_{TT}^{1/2}\Delta\vec{q}(0)]+\frac{1}{\nu_k}\sin(\nu_k t)[\vec{v}_k\mathbf{M}_{TT}^{1/2}\Delta\dot{q}(0)]\right). \tag{C10}
 \end{aligned}$$

We wish this to hold at arbitrary times t , which implies that each frequency must be equated separately. This requires that the following two conditions hold true:

$$\mathbf{I}+\frac{\mu}{|c_0|^2}\vec{c}\mathbf{M}_{TT}^{-1/2}(\Omega_L^2\mathbf{I}-\Omega^2)(\Omega^2-\omega_a^2\mathbf{I})^{-1}\mathbf{M}_{TT}^{-1/2}\vec{c}=0, \tag{C11a}$$

$$\begin{aligned}
 & [\vec{v}_k\mathbf{M}_{TT}^{1/2}\Delta\vec{q}(0)] \\
 & +\frac{1}{|c_0|^2}(\vec{v}_k\mathbf{M}_{TT}^{-1/2}\vec{c})\sum_a c_a\frac{(\Omega_L^2-\omega_a^2)}{(\nu_k^2-\omega_a^2)}\Delta q_a(0)=0. \tag{C11b}
 \end{aligned}$$

The first condition (C11a) must hold for all a . The last condition (C11b) must hold for arbitrary initial vector $\Delta\vec{q}(0)$ and all k .

We can readily evaluate Eq. (C11a) from the matrix definitions (B3). The inverse matrix is

$$(\Omega^2-\omega_a^2\mathbf{I})^{-1}=\mathbf{M}_{TT}^{1/2}(\mathbf{V}_{TT}-\omega_a^2\mathbf{M}_{TT})^{-1}\mathbf{M}_{TT}^{1/2}, \tag{C12}$$

and the matrix $(\mathbf{V}_{TT}-\omega_a^2\mathbf{M}_{TT})$ has the simple form $\mathbf{M}_{ij}=f_i\delta_{ij}+g_i g_j$ and hence can be analytically inverted (even though one of the f_i vanishes). Carrying out this inverse and

performing the sum, we see that the a dependence of Eq. (C11a) does indeed drop out, and the equation is satisfied.

The second condition (C11b) looks even more difficult to evaluate, since we have no explicit expressions for the eigenvalues ν_k^2 and eigenvectors \vec{v}_k . However, these are not necessary. Note that if \vec{v}_k is an eigenvector of $\Omega^2=\mathbf{M}_{TT}^{-1/2}\mathbf{V}_{TT}\mathbf{M}_{TT}^{-1/2}$ with eigenvalue ν_k^2 , then $\mathbf{M}_{TT}^{1/2}\vec{v}_k$ is an eigenvector of $\mathbf{V}_{TT}\mathbf{M}_{TT}^{-1}$ with the same eigenvalue. Using the definitions (B3), this implies that

$$(\mathbf{M}_{TT}^{1/2}\vec{v}_k)_a=\frac{c_a(\Omega_L^2-\omega_a^2)}{(\nu_k^2-\omega_a^2)(|c_0|^2+\vec{c}\vec{c})}(\vec{c}\mathbf{M}_{TT}^{1/2}\vec{v}_k). \tag{C13}$$

Since \vec{c} is an eigenvector of \mathbf{M}_{TT} , we can readily show that

$$(\vec{v}_k\mathbf{M}_{TT}^{-1/2}\vec{c})=\frac{1}{\mu}\frac{|c_0|^2}{|c_0|^2+\vec{c}\vec{c}}(\vec{v}_k\mathbf{M}_{TT}^{1/2}\vec{c}). \tag{C14}$$

By combining Eqs. (C13) and (C14), the condition (C11b) is immediately proved. Hence, the transformed classical noise is the same as the noise derived from a straightforward Lagrangian calculation.

This result has immediate implications for the quantum probabilities (6.24). The integrand in the exponent of that expression is proportional to

$$\mathcal{E}'_L(t, A_L(\tau)) \mathbb{M}[\Delta f'(t) \Delta f'(t')]^{\text{inv}} \mathcal{E}'_L(t', A_L(\tau)) \quad (\text{C15})$$

summed over all L . This is all in terms of the equation of motion form (3.22) and noise correlation function (3.26). But since $\mathcal{E}'_L = C(I+G)\mathcal{E}_L$ and $\mathbb{M}[\Delta f'(t) \Delta f'(t')]^{\text{inv}} = C^{-1}(I+G)^{-1} \mathbb{M}[\Delta f(t) \Delta f(t')]^{\text{inv}} C^{-1}(I+G)^{-1}$, we see that the transformation $C(I+G)$ cancels out, and

$$\begin{aligned} \mathcal{E}'_L(t, A_L(\tau)) \mathbb{M}[\Delta f'(t) \Delta f'(t')]^{\text{inv}} \mathcal{E}'_L(t', A_L(\tau)) \\ = \mathcal{E}_L(t, A_L(\tau)) \mathbb{M}[\Delta f(t) \Delta f(t')]^{\text{inv}} \mathcal{E}_L(t', A_L(\tau)); \end{aligned} \quad (\text{C16})$$

i.e., even in the quantum case one can use the simpler form of the classical equation of motion and noise.

-
- [1] R. B. Griffiths, *J. Stat. Phys.* **36**, 219 (1984); *Phys. Rev. A* **54**, 2759 (1996); **57**, 1604 (1998).
- [2] R. Omnès, *Rev. Mod. Phys.* **64**, 339 (1992); *Interpretation of Quantum Mechanics* (Princeton University Press, Princeton, 1994).
- [3] M. Gell-Mann and J.B. Hartle, in *Complexity, Entropy, and the Physics of Information*, edited by W. Zurek, *SFI Studies in the Sciences of Complexity* Vol. VIII (Addison-Wesley, Reading, MA, 1990); in *Proceedings of the 3rd International Symposium on the Foundations of Quantum Mechanics in the Light of New Technology*, edited by S. Kobayashi, H. Ezawa, Y. Murayama, and S. Nomura (Physical Society of Japan, Tokyo, 1990).
- [4] M. Gell-Mann and J. B. Hartle, *Phys. Rev. D* **47**, 3345 (1993).
- [5] T. A. Brun, *Phys. Rev. D* **47**, 3383 (1993).
- [6] T. A. Brun and J. J. Halliwell, *Phys. Rev. D* **54**, 2899 (1996).
- [7] J. J. Halliwell, *Phys. Rev. D* **58**, 105015 (1998).
- [8] J. J. Halliwell, *Phys. Rev. D* **60**, 105031 (1999).
- [9] D. N. Zubarev, *Nonequilibrium Statistical Thermodynamics*, edited by P. Gray and P.J. Shepherd (Consultants Bureau, New York, 1974).
- [10] H. F. Dowker and J. Halliwell, *Phys. Rev. D* **46**, 1580 (1992).
- [11] J. J. Halliwell and A. Zoupas, *Phys. Rev. D* **55**, 4697 (1997).
- [12] See, e.g., W. Zurek, in *Non-Equilibrium Quantum Statistical Physics*, edited by G. Moore and M. Scully (Plenum, New York, 1984); W. Unruh and W. Zurek, *Phys. Rev. D* **40**, 1071 (1989); J. P. Paz and W. Zurek, *ibid.* **48**, 2728 (1993).
- [13] R. P. Feynman and J. R. Vernon, *Ann. Phys. (N.Y.)* **24**, 118 (1963).
- [14] E. Joos and H. D. Zeh, *Z. Phys. B* **59**, 223 (1985).
- [15] W. Zurek, *Phys. Rev. D* **24**, 1516 (1981); **26**, 1862 (1982).
- [16] A. Caldeira and A. Leggett, *Physica A* **121**, 587 (1983).
- [17] R. Omnès, *Phys. Rev. A* **56**, 3383 (1997).
- [18] L. Brillouin, *Wave Propagation in Periodic Structures* (McGraw-Hill, New York, 1946).
- [19] R. Zwanzig, *J. Stat. Phys.* **9**, 215 (1973).
- [20] L. D. Landau and E. M. Lifshitz, *Fluid Mechanics* (Pergamon, London, 1959).
- [21] W. Zurek, in *Non-Equilibrium Quantum Statistical Physics*, edited by G. Moore and M. Scully (Plenum, New York, 1984).
- [22] J. P. Paz and W. Zurek, *Phys. Rev. D* **48**, 2728 (1993).
- [23] C. Anastopoulos, *Phys. Rev. D* **59**, 045001 (1999).