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Dissipative particle dynamics for a harmonic chain: A first-principles derivation

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The equations of dissipative particle dynamics for a linear harmonic chain are deduced from first principles. From the original chain, a coarse-grained chain is constructed by grouping the particles in clusters; the equations of motion for the position and momenta of these clusters are derived. The clusters interact with their neighbors with elastic springs and Brownian dashpots. We provide explicit expressions for the renormalized elastic constant, the friction coefficient, and the amplitude of the random forces.

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I. INTRODUCTION

The technique of dissipative particle dynamics (DPD) has been introduced by Hoogerbrugge and Koelman in order to simulate hydrodynamic behavior in complex systems such as, e.g., colloidal suspensions [1,2]. The aim of the technique is to reduce the computational effort required by molecular dynamics (MD) simulations [3–6] by coarse graining the description of the fluid. From a numerical point of view, DPD might represent an alternative to other techniques such as, for example, lattice gas cellular automata [7], lattice Boltzmann automata [8], or the direct simulation Monte Carlo method for dilute gases [9]. All these techniques try successfully to reduce the computational burden of MD when addressing hydrodynamic problems.

In DPD the fluid is modeled with point particles that interact through conservative, dissipative, and random forces. These point particles are not regarded as the molecules of the fluid but rather as droplets or clusters of molecules. During the interaction of these clusters, energy is not conserved and this is taken into account by the dissipative and random forces. Nevertheless, these forces are required to satisfy Newton's third law and therefore they conserve the momentum of the interacting clusters. This crucial point makes the technique suitable for simulating hydrodynamic processes because it implies that there exists a transport equation for the hydrodynamic momentum density field [1]. This clever insight has been put in a firm theoretical basis recently [10,11].

The success of DPD in fluid systems with complex boundary conditions encourages us to apply it also to solid systems. The computational requirements in the solution of elasticity problems with boundary conditions as complex as those arising in, for example, fracture dynamics are formidable. Molecular dynamics simulations of crack dynamics are currently performed with a number of particles of the order of 10^6 [12]. The general idea of DPD, that of using coarse-grained particles in order to reduce the computational burden, can also be applied to the simulation of solids. In an analogous way as in fluid systems, now a point particle is regarded as representing a portion of a solid made of many atoms. These coarse-grained particles interact through conservative, dissipative, and random forces with their neighboring particles. The main question that arises is what sort of dissipative and random forces should we introduce in a solid system? In a fluid system, the structure of the equations of motion for the dissipative particles was dictated from symmetry considerations (rotational, translational, and Galilean invariance) and simplicity (linear forces). In this way, it was proposed that the dissipative forces are like those produced by a dashpot between a given pair of particles. This means that the dissipative force on a given particle due to another particle is proportional to the *relative* approaching velocity. Note that this type of force is completely different from a viscous frictional force applied to each particle (which depends on its absolute velocity). This last type of dissipative force does not conserve momentum and the resulting macroscopic description is not hydrodynamic but diffusive, i.e., we have a Brownian dynamics simulation [13].

In a solid elastic system dissipation can also be introduced according to symmetry requirements [14]. For example, Langer has considered dissipation in a continuous medium by using a term proportional to $\partial^2\dot{u}/\partial x^2$, where u is the displacement field [15]. This is in agreement with Landau and Lifschitz [14]. Note that the finite difference discrete version of such a term corresponds to a dissipation proportional to relative velocities of the nodes (or particles). Another form of dissipation has been introduced in lattice models where a viscous friction proportional to the absolute velocity of the particles has been considered [16]. This simpler form was adopted for mathematical convenience but it turned out to have a physical effect on the morphology of the cracks.

The aim of this paper is to derive the algorithm of DPD for the simplest model of an elastic solid, the 1D

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harmonic chain. The simplicity of the model allows for an explicit analysis and furnishes valuable insight into the general problem of relating the model parameters of DPD and the microscopic dynamics of the underlying system that is being modeled. In this respect, we expect to gain some insight in the structure of DPD that can be useful to other nontrivial systems such as fluids, multidimensional lattices, and polymers.

The essential idea consists on coarse graining the original model and deducing the equations of motion for the coarse-grained variables. In this spirit, the particles of the chain are grouped in bunches of a given size (see Fig. 1) in a way reminiscent of the renormalization group procedure as applied in polymer physics [17]. The "mesoscopic" state of the system is now described by the position of the center of mass and the momentum of these clusters of particles. These mesoscopic variables instead of the conventional "macroscopic" field variables (densities of particle number, momentum, energy, and displacement) were selected due to our intention of developing molecular-dynamics-like simulation (i.e., off-lattice simulations) instead of finite-difference methods where the effect of complex moving boundary conditions are more difficult to treat. By using a standard technique of projection operators we deduce the equations of motion for the mesoscopic variables [18–20].

The paper is organized as follows. In Sec. II we present the model and its coarse graining. In Sec. III we recall the standard technique of projection operators and we particularize it to the model presented in Sec. IV. Finally, some conclusions are presented.

II. THE HARMONIC CHAIN AND THE COARSE-GRAINED CHAIN

Let us consider a set of N particles moving in one dimension and connected through Hookean springs. The equations of motion are

$$\begin{aligned} \dot{x_i} &= \frac{p_i}{m}, \\ \dot{p_i} &= \kappa(x_{i+1} - 2x_i + x_{i-1}), \end{aligned} \tag{1}$$

where x_i is the deviation from the equilibrium position $\overline{x}_i = ia$ of particle i (a is the lattice spacing), p_i is its momentum, κ is the elastic constant, and m the mass of the particles. We assume fixed ends, i.e.,

$$\begin{aligned} \dot{p_1} &= \kappa(x_2 - 2x_1), \\ \dot{p_N} &= \kappa(x_{N-1} - 2x_N), \end{aligned} \tag{2}$$

Note that these linear microscopic dynamic equations can be written as

$$\dot{p_i} = -\kappa A_{ij} x_j, \tag{3}$$

where A_{ij} is the Rouse matrix [21]

$$A_{ij} = \begin{cases} 2 & \text{if } i = j, \\ 1 & \text{if } i = j \pm 1, \\ 0 & \text{otherwise.} \end{cases} \tag{4}$$

The Hamiltonian of the system is given by $H = T + V$, where the kinetic and potential contributions are, respectively,

$$\begin{aligned} T &= \sum_{I}^{N} \frac{p_i^2}{2m}, \\ V &= \frac{\kappa}{2} \mathbf{x}^T \mathbf{A} \mathbf{x}, \end{aligned} \tag{5}$$

and $\mathbf{x} = (x_1, \ldots, x_N)$.

Now we define a set of mesoscopic variables by grouping the particles in bunches of size n. The position of the center of mass of the bunch and its momentum are taken as the set of mesoscopic variables that describe the chain in a coarse-grained way. The mesoscopic variables are

$$\begin{aligned} X_\mu &= \frac{1}{n} \sum_{i_\mu \in \mathcal{R}_\mu}^{n} x_{i_\mu}, \\ P_\mu &= \sum_{i_\mu \in \mathcal{R}_\mu}^{n} p_{i_\mu}, \end{aligned} \tag{6}$$

where $\mathcal{R}_\mu$ is the list of indices of particles that constitute the μth group. Note that the equilibrium average of the microscopic and mesoscopic variables vanishes.

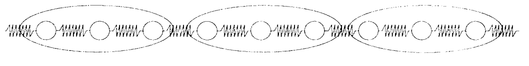

FIG. 1. The original 1D harmonic chain is coarse-grained by grouping several particles into clusters. In the coarse-grained level the chain is described by the position and momenta of the center of mass of the clusters. The resulting 1D coarse-grained chain consists of "particles" that interact with their neighbors through elastic springs and Brownian dashpots.

III. MORI THEORY

Our aim is to deduce theoretically the equations of motion for the set of mesoscopic variables (6), given the microscopic dynamics (2). The technique of projection operators is very useful in this respect. For completeness and in order to fix the notation, we recall in this section the technique.

Following Ref. [22], we first introduce a scalar product defined by

$$(\phi, \psi) \equiv \int \rho^{eq}(z) \phi(z) \psi(z) dz \equiv \mathrm{tr}[\rho^{eq} \phi \psi], \tag{7}$$

where the equilibrium ensemble is $\rho^{eq}(z) = \frac{1}{Z} \exp\{-\beta H(z)\}$, Z is the partition function, and

$\beta = 1/k_BT$. The Liouville operator is self-adjoint with respect to this scalar product. Next, we introduce a relevant ensemble by

$$\bar{\rho}_t(z) \equiv \frac{1}{Z}\exp\{-\beta H(z) + \beta\lambda_i(t)A_i(z)\}, \tag{8}$$

where summation over repeated indices is understood, A_i denotes the set of relevant mesoscopic variables, and $\lambda_i(t)$ are a set of thermodynamic parameters that depend on time. The relevant variables are selected in such a way that their equilibrium average vanishes. The average of A_i performed with the relevant ensemble coincides with the actual average performed with the solution of the Liouville equation, that is,

$$\langle A_i\rangle_t = \mathrm{tr}[\rho_t A_i] = \mathrm{tr}[\bar{\rho}_t A_i]. \tag{9}$$

We will assume in the following that the system is in a state near equilibrium. Near equilibrium the relevant ensemble must be similar to the canonical ensemble and therefore the parameters $\lambda_i(t)$ are small, allowing for an expansion of the form

$$\bar{\rho}_t(z) = \rho^{eq}(z)[1 + \beta\lambda_i(t)A_i(z)]. \tag{10}$$

We further define the deviations from equilibrium:

$$\begin{aligned} \rho_t &= \rho^{eq}[1 + \Psi_t], \\ \bar{\rho}_t &= \rho^{eq}[1 + \overline{\Psi}_t], \end{aligned} \tag{11}$$

in such a way that $\overline{\Psi}_t = \beta\lambda_i(t)A_i$. In terms of the deviations from equilibrium Eq. (9) becomes

$$\langle A_i\rangle_t = (A_i, \Psi_t) = (A_i, \overline{\Psi}_t) \tag{12}$$

which implies

$$\beta\lambda_i(t) = (A_i, A_j)^{-1}(A_j, \Psi_t), \tag{13}$$

and therefore

$$\overline{\Psi}_t = A_i(A_i, A_j)^{-1}(A_j, \Psi_t) \equiv \mathcal{P}\Psi_t, \tag{14}$$

where $\mathcal{P}$ is a projection operator that extracts the relevant part of the actual ensemble.

By applying the following mathematical identity,

$$\begin{aligned} \exp\{iLt\} = {} & \exp\{iLt\}\mathcal{P} \\ & + \int_0^t \exp\{iLu\}\mathcal{P}iL\mathcal{Q}\exp\{iL\mathcal{Q}(t-u)\} \\ & + \mathcal{Q}\exp\{iL\mathcal{Q}t\}, \end{aligned} \tag{15}$$

to $\dot{A}_i(t) = \exp\{iLt\}iLA_i$ and using the form (14) of the projector, an exact equation of motion for $A_i(t)$ is obtained,

$$\dot{A}_i(t) = \Omega_{ij}A_j(t) - \int_0^t K_{ij}(t-u)A_j(u)du + F_i(t), \tag{16}$$

where the drift term Ω, the dissipative kernel K, and the random force F_i are given, respectively, by

$$\begin{aligned} \Omega_{ij} &= (A_j, A_k)^{-1}(A_k, iLA_i), \\ K_{ij}(t) &= (A_j, A_k)^{-1}(F_k(0), F_i(t)), \\ F_i(t) &= \mathcal{Q}\exp\{iL\mathcal{Q}t\}iLA_i. \end{aligned} \tag{17}$$

The random forces satisfy the following properties:

$$\begin{aligned} \langle F_i(t)\rangle &= 0, \\ \langle F_k(0)F_i(t)\rangle &= K_{ij}(t)(A_j, A_k), \\ \langle A_kF_i(t)\rangle &= 0. \end{aligned} \tag{18}$$

IV. MORI THEORY APPLIED TO THE HARMONIC CHAIN

We now particularize the formalism of the preceding section to the case that the relevant variables A_i are X_μ, P_μ. The relevant ensemble (10) now takes the form

$$\bar{\rho}_t(z) = \rho^{eq}(z)[1 + \beta\lambda^X_\mu(t)X_\mu(z) + \beta\lambda^P_\mu(t)P_\mu(z)]. \tag{19}$$

The physical meaning of the Lagrange multipliers $\lambda^X_\mu(t), \lambda^P_\mu(t)$ is obtained from (13), which can be written in the form

$$\begin{aligned} \langle X_\mu\rangle_t &= \langle X_\mu X_\nu\rangle\beta\lambda^X_\nu(t) + \langle X_\mu P_\nu\rangle\beta\lambda^P_\nu(t), \\ \langle P_\mu\rangle_t &= \langle P_\mu X_\nu\rangle\beta\lambda^X_\nu(t) + \langle P_\mu P_\nu\rangle\beta\lambda^P_\nu(t). \end{aligned} \tag{20}$$

We have then to compute the equilibrium second moments. We will need first to compute the equilibrium second moments of the microscopic variables. For example,

$$\langle \mathbf{x}\mathbf{x}^T\rangle = \int \mathbf{x}\mathbf{x}^T\frac{1}{Z}\exp\left\{-\beta\frac{\kappa}{2}\mathbf{x}^T\mathbf{A}\mathbf{x}\right\}d^N\mathbf{x}. \tag{21}$$

By introducing $\mathbf{x} = \Lambda\mathbf{y}$, where Λ is an orthonormal matrix that diagonalizes the Rouse matrix $\mathbf{A}$, i.e., $\Lambda^T\mathbf{A}\Lambda = \mathbf{D}$, $\mathbf{D}$ a diagonal matrix and $\Lambda^T\Lambda = \mathbf{1}$, we have

$$\begin{aligned} \langle \mathbf{x}\mathbf{x}^T\rangle &= \Lambda\left[\int \mathbf{y}\mathbf{y}^T\frac{1}{Z}\exp\left\{-\beta\frac{\kappa}{2}\mathbf{y}^T\mathbf{D}\mathbf{y}\right\}d^N\mathbf{y}\right]\Lambda^T \\ &= \frac{k_BT}{\kappa}\Lambda\mathbf{D}^{-1}\Lambda^T = \frac{k_BT}{\kappa}\mathbf{A}^{-1}, \end{aligned} \tag{22}$$

where we have used

$$\frac{\int_{-\infty}^{\infty} x^2\exp\{-ax^2\}dx}{\int_{-\infty}^{\infty}\exp\{-ax^2\}dx} = \frac{1}{2a}. \tag{23}$$

The inverse of the Rouse matrix is given by [21]

$$A^{-1}_{ij} = \begin{cases} i[(N+1)-j]/(N+1) & \text{if } i \le j, \\ j[(N+1)-i]/(N+1) & \text{if } i \ge j, \end{cases} \tag{24}$$

and therefore if $i_\mu \le i_\nu$

$$\frac{1}{N}\langle x_{i_\mu}x_{i_\nu}\rangle = \frac{k_BT}{\kappa}\frac{i_\mu}{(N+1)}\left(1 - \frac{j_\nu}{(N+1)}\right). \tag{25}$$

For $\mu \le \nu$ let us compute

$$\begin{aligned}\frac{1}{N}\langle X_\mu X_\nu\rangle &= \frac{1}{n^2}\sum_{i_\mu i_\nu}\langle x_{i_\mu}x_{i_\nu}\rangle = \frac{k_BT}{\kappa}\frac{1}{n^2}\sum_{i_\mu i_\nu}\frac{i_\mu}{(N+1)}\left(1-\frac{i_\nu}{(N+1)}\right)\\ &= \frac{k_BT}{\kappa}\left[\frac{1}{n}\sum_{i_\mu}\frac{i_\mu}{(N+1)}\right]\left[\frac{1}{n}\sum_{i_\nu}\left(1-\frac{i_\nu}{(N+1)}\right)\right]\\ &= \frac{k_BT}{\kappa}\left[\frac{\mu}{N'}-\frac{n-1}{2(N+1)}\right]\left[1-\frac{\nu}{N'}+\frac{n-1}{2(N+1)}\right],\end{aligned} \tag{26}$$

where $N' = N/n$ is the number of groups of size n in the chain. The inverse of this matrix is difficult to obtain, but we note that in the limit of very large chains $N, N' \to \infty$ and $(n-1)/2(N+1) \to 0$. The resulting matrix is proportional to the inverse of the Rouse matrix (24), that is,

$$\langle X_\mu X_\nu\rangle = \frac{k_BTn}{\kappa}A^{-1}_{\mu\nu}, \tag{27}$$

where $A_{\mu\nu}$ is an $N' \times N'$ Rouse matrix. Therefore,

$$\langle X_\mu X_\nu\rangle^{-1} = \frac{\kappa}{k_BTn}A_{\mu\nu}. \tag{28}$$

Next, because of the statistical independence of position and momentum for the microscopic variables it follows that the mesoscopic position and momentum are also statistically independent, that is, $\langle X_\mu P_\nu\rangle = \langle P_\mu X_\nu\rangle = 0$. Finally, the second moments of the mesoscopic momentum are

$$\langle P_\mu P_\nu\rangle = nmk_BT\delta_{\mu\nu}. \tag{29}$$

Substitution of these results into (20) leads finally to the desired physical meaning for the Lagrange multipliers, i.e.,

$$\lambda^X_\mu(t) = \kappa A_{\mu\nu}\langle X_\nu\rangle_t \tag{30}$$

which is the negative of the average elastic force on group μ. Also,

$$\lambda^P_\mu(t) = \frac{1}{mn}\langle P_\mu\rangle_t \tag{31}$$

which is the average velocity of group μ.

We consider now the equation of motion (16) for the position X_μ. One can compute the drift and irreversible terms, but it is simpler to just take the derivative and, obviously, one obtains $\dot{X}_\mu = \frac{P_\mu}{m}$. On the other hand, the equation for the momentum is nontrivial. The reversible part is given by

$$\begin{aligned}\Omega_{ij}A_j(t) \to X_\nu(t)&\left[\sum_\sigma\langle X_\nu X_\sigma\rangle^{-1}\langle X_\sigma iLP_\mu\rangle + \sum_\sigma\langle X_\nu P_\sigma\rangle^{-1}\langle P_\sigma iLP_\mu\rangle\right]\\ +P_\nu(t)&\left[\sum_\sigma\langle P_\nu X_\sigma\rangle^{-1}\langle X_\sigma iLP_\mu\rangle + \sum_\sigma\langle P_\nu P_\sigma\rangle^{-1}\langle P_\sigma iLP_\mu\rangle\right]\\ =& -\frac{\kappa}{n}A_{\mu\nu}X_\nu,\end{aligned} \tag{32}$$

where we have used that $\langle X_\sigma iLP_\mu\rangle = -\langle iLX_\sigma P_\mu\rangle = -\langle P_\sigma P_\mu\rangle/nm$ and $\langle P_\sigma iLP_\mu\rangle = 0$. We note that the reversible term gives rise to an elastic contribution to the force. For the irreversible part, we first note that because $iLX_\mu = P_\mu/m$, proportional to a relevant variable, the corresponding random force (17) will be zero. On the other hand, the nonzero random force corresponding to the momentum variable will be $F^P_\mu(t) \equiv \mathcal{Q}\exp\{iL\mathcal{Q}t\}iLP_\mu$. The irreversible term will become simply

$$\begin{aligned}&\int_0^t K_{ij}(t-u)A_j(u)du\\ &\quad\to \int_0^t K_{\mu\nu}(t-u)P_\nu(u)du\\ &\quad= \int_0^t duP_\nu(u)\sum_\sigma\langle P_\nu P_\sigma\rangle^{-1}\langle F^P_\sigma F^P_\mu(t-u)\rangle\\ &\quad= \frac{1}{nmk_BT}\int_0^t duP_\nu(u)\langle F^P_\nu F^P_\mu(t-u)\rangle.\end{aligned} \tag{33}$$

Our aim is to study in more detail the correlation matrix $\langle F^P_\nu F^P_\mu(t)\rangle$ of the projected force. We first note that the total force acting on the group μ is due only to the springs that connect this group to its nearest neighbors, that is,

$$F_\mu = iLP_\mu = -(x_{i_\mu} - x_{j_{\mu-1}}) + (x_{i_{\mu+1}} - x_{j_\mu}), \tag{34}$$

where $i_\mu, i_{\mu+1}$ represent the leftmost particle of the groups $\mu, \mu+1$ and $j_\mu, j_{\mu+1}$ represent the rightmost particle of the groups $\mu-1, \mu$. For compactness, we will denote the length of the left spring of group μ (which connects the group μ with the group $\mu-1$) by l_μ and the length of the right spring of group μ (which connects the group μ with the group $\mu+1$) by r_μ. Obviously, $r_\mu = l_{\mu+1}$, $l_\mu = r_{\mu-1}$ and

$$F_\mu = -l_\mu + r_\mu. \tag{35}$$

We next introduce the projected spring lengths

$$\begin{aligned}\delta l_\mu &= \mathcal{Q} l_\mu = l_\mu - (l_\mu, X_\sigma)A_{\sigma\nu}X_\nu,\\ \delta r_\mu &= \mathcal{Q} r_\mu = r_\mu - (r_\mu, X_\sigma)A_{\sigma\nu}X_\nu.\end{aligned} \tag{36}$$

In this way, the projected force can be written as

$$F^P_\mu(t) = -\delta l_\mu(t) + \delta r_\mu(t), \tag{37}$$

where $\delta l_\mu(t) \equiv \mathcal{Q}\exp\{iL\mathcal{Q}u\}\delta l_\mu$. Therefore, the correlation of projected forces will become

$$\begin{aligned}\langle F^P_\nu F^P_\mu(t)\rangle = {}&\langle \delta l_\nu \delta l_\mu(t)\rangle - \langle \delta l_\nu \delta r_\mu(t)\rangle - \langle \delta r_\nu \delta l_\mu(t)\rangle\\ &+\langle \delta r_\nu \delta r_\mu(t)\rangle\end{aligned} \tag{38}$$

Now, when the size n of the groups is large enough, the different springs will be far apart and their length will become uncorrelated. This means that the correlation matrix will have the form

$$\begin{aligned}\langle F^P_\mu F^P_\mu(t)\rangle &= \langle \delta l_\mu \delta l_\mu(t)\rangle + \langle \delta r_\mu \delta r_\mu(t)\rangle\\ &= \langle \delta r_{\mu-1}\delta r_{\mu-1}(t)\rangle + \langle \delta r_\mu \delta r_\mu(t)\rangle\\ &\equiv \gamma_{\mu-1}(t) + \gamma_\mu(t),\\ \langle F^P_\mu F^P_{\mu+1}(t)\rangle &= -\langle \delta r_\mu \delta l_{\mu+1}(t)\rangle = -\gamma_\mu(t),\\ \langle F^P_\mu F^P_{\mu-1}(t)\rangle &= -\langle \delta l_\mu \delta r_{\mu-1}(t)\rangle = -\gamma_{\mu-1}(t),\end{aligned} \tag{39}$$

and zero if $|\mu-\nu| > 1$. We expect that the autocorrelation of the spring length will be the same for all groups so that $\gamma_\mu(t) = \gamma(t)$. Actually, it is possible to compute $\gamma_\mu(0)$ explicitly and it is seen that $\gamma_\mu(0) = \gamma(0)$. Therefore, we arrive at the following expression:

$$\langle F^P_\mu F^P_\nu(t)\rangle = \gamma(t)A_{\mu\nu}. \tag{40}$$

Now, let us note that the typical time scale of $\gamma(t)$ will be of the order of the period $(m/\kappa)^{1/2}$ of a connecting spring. On the other hand, the typical time scale of variation of the momentum of each group will be much larger if the groups are large enough. This allows for a Markovian approximation of the form

$$\frac{1}{nmk_BT}\int_0^t du P_\nu(u)\langle F^P_\nu F^P_\mu(t-u)\rangle = \frac{\gamma}{nm}A_{\mu\nu}P_\nu(t), \tag{41}$$

where the friction coefficient γ is defined in terms of a Green-Kubo formula, i.e.,

$$\gamma = \frac{1}{k_BT}\int_0^\infty du\gamma(u) = \frac{1}{k_BT}\int_0^\infty du\langle \delta r_\mu \delta r_\mu(u)\rangle. \tag{42}$$

The Markovian approximation is equivalent to assuming the following form for the kernel:

$$K_{\mu\nu}(t-u) = \frac{\gamma}{nm}A_{\mu\nu}\delta(t-u) \tag{43}$$

or equivalently [see Eq. (41)] the following correlation for the random forces:

$$\langle F^P_\mu(t)F^P_\nu(t')\rangle = k_BT\gamma A_{\mu\nu}\delta(t-t'). \tag{44}$$

The final equations of motion for the mesoscopic variables are then

$$\begin{aligned}\dot X_\mu &= \frac{P_\mu}{m},\\ \dot P_\mu &= -\frac{\kappa}{n}A_{\mu\nu}X_\nu - \frac{\gamma}{nm}A_{\mu\nu}P_\nu + F^P_\mu(t),\end{aligned} \tag{45}$$

or, more explicitly,

$$\begin{aligned}\dot X_\mu &= \frac{P_\mu}{m},\\ \dot P_\mu &= \frac{\kappa}{n}(X_{\mu+1} - 2X_\mu + X_{\mu-1}),\\ &\quad -\frac{\gamma}{nm}[P_\mu(t) - P_{\mu-1}(t)] + \frac{\gamma}{nm}[P_{\mu+1}(t) - P_\mu(t)]\\ &\quad +F^P_\mu(t).\end{aligned} \tag{46}$$

These are Langevin equations for the motion of the mesoscopic variables. From a mathematical point of view, these equations are ill-defined and the rigorous expression for these kind of equations is in the form of stochastic differential equations (SDE) [23]. We will formulate below the SDE corresponding to the Langevin equations (46). This is not only a matter of taste but also a requirement in order to formulate well-defined numerical algorithms. The SDE's corresponding to (46) are

$$\begin{aligned}dX_\mu(t) &= \frac{P_\mu(t)}{m}dt,\\ dP_\mu(t) &= -\left[\frac{\kappa}{n}A_{\mu\nu}X_\nu(t) + \frac{\gamma}{nm}A_{\mu\nu}P_\nu(t)\right]dt\\ &\quad + (k_BT\gamma)^{1/2}\left[dW_{\mu+1\mu}(t) - dW_{\mu\mu-1}(t)\right],\end{aligned} \tag{47}$$

where $dW_{\mu\nu} = dW_{\nu\mu}$ are independent increments of the Wiener process which satisfy

$$dW_{\mu\nu}(t)dW_{\mu'\nu'}(t) = (\delta_{\mu\mu'}\delta_{\nu\nu'} + \delta_{\mu\nu'}\delta_{\nu\mu'})dt, \tag{48}$$

i.e., $dW_{\mu\nu}(t)$ is an infinitesimal of order 1/2 [23]. The heuristic connection between the Langevin equations (46) and the SDE's (47) is through the nonrigorous equation

$$F_\mu^P(t) = (k_B T\gamma)^{1/2}\left[\frac{dW_{\mu+1\mu}}{dt}(t) - \frac{dW_{\mu\mu-1}}{dt}(t)\right] \quad (49)$$

which is not correct from a mathematical point of view as it suggests the existence of the derivative of the Wienner process [23]. Nevertheless, using the rule (48) one arrives at the correct expression for the correlation of the random force, i.e., $\langle F_\mu^P(t)F_\nu^P(t')\rangle \approx k_B T\gamma A_{\mu\nu}1/dt$ if $t = t'$ and zero otherwise. The term $1/dt$ (which is infinity in the continuum limit) can be assimilated to $\delta(t-t) = \delta(0)$.

A final word on the explicit calculation of the friction coefficient γ in (42) is in order. This calculation is very difficult in view of the presence of the projected dynamics represented by the operator $\exp\{iL\mathcal{Q}\}$. It should be noted though that $\gamma > 0$ because otherwise the system would have the unphysical property of being "self-accelerated." On the other hand, the dependence of the friction coefficient on the microscopic parameters of the original harmonic chain can be obtained by dimensional analysis,

$$\gamma = (m\kappa)^{1/2}\gamma^*, \quad (50)$$

where the dimensionless friction coefficient γ^* is obtained from an expression like (42) but using dimensionless microscopic variables to begin with. It should be emphasized that γ^* is a number intrinsic for the 1D chain and cannot be given an arbitrary value for modeling purposes.

V. SUMMARY AND CONCLUSION

Starting from a microscopic description of a harmonic chain in terms of the positions and momenta of the atoms of the chain we have deduced the equations of motion for a coarse-grained chain constructed from the original one by grouping the atoms in clusters of definite size n. The chain is assumed to be in a statistical state near equilibrium. In the limit of very long chains and for large groupings of particles, the clusters interact elastically and dissipatively, with a friction force that depends on the relative velocity of neighboring particles. Moreover, the clusters are subject to thermal random δ-correlated forces that take into account the eliminated degrees of freedom and which depend on the temperature of the equilibrium state. The structure of the equations of the renormalized chain is thus identical to that of dissipative particle dynamics as applied to fluid systems. More precisely, the particularization of the equations of DPD as given in Ref. [10] to the harmonic chain produces exactly the Eqs. (47). Therefore, we have derived for this particular system the equations of DPD from first principles.

The elastic constant and the friction coefficient of the coarse-grained chain are defined in terms of microscopic variables. Worth noting is the fact that they are inversely proportional to the size of the clusters. This corresponds to the intuitive idea that the time scales of the coarse-grained variables grow as the size of the cluster and it is consistent with the Markovian approximation taken in the deduction of the equations.

The appearance of noise and dissipation in the renormalized chain is simply a matter of describing the system at a coarse-grained level. For if we imagine a microscopic motion of a pulse in the atomic chain, due to the intrinsic dispersion of the discrete chain (i.e., each normal mode of the chain has a different frequency) this pulse will spread out. Therefore, the motion of the microscopic pulse will affect as time proceeds more and more clusters which will move more and more slowly. However, there is no dissipation in the original atomic chain and there will always be a remanent motion of the atoms. This incoherent motion is captured by the random noise in the renormalized chain.

The extension of the formalism to not only linear chains but also multidimensional lattices is cumbersome but we expect that the general features of the equations are retained, that is, the coarse-grained portions interact elastically, dissipatively, and with a random force. The potential use of DPD for solids as a way of solving complex elasticity problems where the complexity may appear as in the case of fluid systems as a consequence of boundary conditions remains to be explored. Our particular interest in DPD for solids arose from our attempt to simulate crack dynamics in brittle materials. It has been found that a phenomenological Stokes dissipation (proportional to the *absolute* velocity of the particles) has an effect in the morphology of cracks propagating in lattices [16]. The results of this paper suggest that dissipation is proportional to the *relative* velocities between particles. In the continuum limit, the dissipative term in the equations of motion for the displacement becomes $\partial^2\dot{u}/\partial x^2$, as proposed by Langer [15] and in agreement with Landau and Lifschitz [14]. It would be very interesting to explore the consequences of this form of dissipation in the formalism developed by Marder *et al.* in order to consider instabilities in the steady state velocity of propagating cracks in lattice models [16].

The fact that the friction coefficient is defined in terms of microscopic dynamics shows that in order to model a lattice crystal in a coarse-grained level not any value of γ is allowed but only a precise value, characteristic of the geometry and dynamics of the lattice, will represent faithfully the crystal. This also has relevance in DPD for fluids, where a general connection of the dissipative friction coefficient with the microscopic dynamics is still lacking. Work is in progress in that direction.

Finally, the results presented in this paper are relevant in polymer dynamics also. Usually, a polymer molecule is modeled as a linear chain of particles interacting through elastic springs. It is apparent from the results of this paper that in order to be consistent with the coarse-graining procedure implicit in this modeling, the dissipation due to the inner motion of the monomers within the chain has to be taken into account. Such models with "internal viscosity" have been considered and analyzed in the past [24].

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