

## FAST TRACK COMMUNICATION

# Fractional dimensions of phase space variables: a tool for varying the degrees of freedom of a system in a multiscale treatment

Matej Praprotnik<sup>1</sup>, Kurt Kremer and Luigi Delle Site

Max-Planck-Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz, Germany

E-mail: [praprot@mpip-mainz.mpg.de](mailto:praprot@mpip-mainz.mpg.de), [kremer@mpip-mainz.mpg.de](mailto:kremer@mpip-mainz.mpg.de) and [dellsite@mpip-mainz.mpg.de](mailto:dellsite@mpip-mainz.mpg.de)

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Online at [stacks.iop.org/JPhysA/40/F281](http://stacks.iop.org/JPhysA/40/F281)**Abstract**

We show how the idea of fractal dimensions of phase space variables can be employed to develop a concept of adaptive resolution treatment of a molecular liquid. The resulting theoretical framework allows for calculation of statistical averages of thermodynamic quantities in multiresolution computer simulation algorithms where the molecular degrees of freedom change on the fly.

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**1. Introduction**

Properties of complex molecular systems can be characterized by interconnected phenomena occurring at different scales. Especially for soft matter this is a key to a better understanding. For instance the properties of small additives in a polymer matrix are determined by both the local interaction parameters and the overall morphology of the matrix, which is determined on a larger scale. In a similar way modern functional materials, of both biological and synthetic origin, can only be understood and quantitatively characterized if the effects of local coupling parameters and the overall fluctuations are taken into account [1, 2]. These interdependences between separate length scales make quantitative theoretical or simulation studies without a well-defined procedure, which takes into account their often rather delicate interplay, very difficult, if not impossible. Thus, it is not sufficient to focus on the different scales separately. On the other hand, one would like to treat a system only at a level of detail, which is necessary. One way to achieve this is to devise a scheme that allows us to locally adapt the level of resolution, which is required for the phenomena considered.

In a previous work, we considered a situation for molecular liquids, where in different spatial regions the system can be viewed with different resolution while the liquid molecules

<sup>1</sup> On leave from the National Institute of Chemistry, Hajdrihova 19, SI-1001 Ljubljana, Slovenia.

move freely between the two regions or ‘phases’. This equilibrium between the two ‘phases’ leads to the problem of ‘molecular representation’, which will be discussed in more detail in the present contribution. Numerically, this has been successfully solved by a robust numerical algorithm. Examples are a simple liquid of tetrahedral molecules, liquid water and a generic solvated macromolecule [3–6].

The general model case we study here is a solvent molecule, which in a ‘high resolution’ region contains atomistic details, and when it crosses an ideal boundary and enters into a domain of ‘lower resolution’ it becomes a simple sphere and the atoms are no longer ‘represented’ (and vice versa). Technically, this change of representation is implemented by introducing a switching region within which the molecules lose (or acquire, if in the opposite direction) resolution and thus some of their degrees of freedom (DOFs). In this region, the change of DOFs can be interpreted as the continuous change of the dimensionality from one to zero (or vice versa) of the phase space related to the particular DOF we want to switch off/on. In this sense, the Hamiltonian preserves its expression for DOFs regardless of the resolution region. Rather it is the dimensionality of the phase space associated with a specific DOF, which tells us how much of this is ‘represented’. In other words, how such a DOF is counted in the calculation of statistical averages of physical quantities? In the limit of dimension equal to one, it is fully counted (the high resolution case), while in the limit of dimension zero (the low resolution case) it is disregarded<sup>2</sup>. We showed that this idea is indeed well founded by applying it to DOFs, which enter quadratically into the Hamiltonian. Then the equipartition theorem applies to fractional dimensions as well [7].

Here, we extend this concept by generalizing the idea of changing the dimensionality beyond the quadratic case, meaning that the equipartition theorem represents only a special case. The robustness of this idea is proven for a class of observables. Next, we discuss the applicability of these concepts for the adaptive resolution molecular dynamics (MD) simulations. Finally, the very idea of adaptive representation is illustrated by the bond length of an ideal diatomic molecule as the statistical observable.

## 2. The statistical average of an observable in fractional phase space

The terms of the problem are the following: we are interested in changing the resolution of a generic DOF  $q$ . For the moment let us assume that this DOF enters the Hamiltonian in the form  $H(q) = |q|^m$ , and that the physical observable we are interested in can be written as  $A(q) = C_n |q|^n$ , where  $C_n$  is a constant. The statistical average of  $A$  in the canonical ensemble is then given by

$$\langle A \rangle = \frac{\int_0^\infty e^{-\beta H(q)} A(q) dq}{\int_0^\infty e^{-\beta H(q)} dq} = \frac{C_n \int_0^\infty e^{-\beta q^m} q^n dq}{\int_0^\infty e^{-\beta q^m} dq}, \quad (1)$$

where  $\beta = 1/k_B T$  and  $T$  is the temperature. Now let us apply the idea, outlined above, to reduce the representation of the DOF  $q$ . This is formally equivalent to a continuous projection from a higher to a lower dimensional phase space (or vice versa) [7]. The phase space associated with  $q$  thus acquires a fractional dimension and the fractional volume element becomes  $d\mu_\alpha(q) = |q|^{\alpha-1} dq / \Gamma(\alpha) = dq^\alpha / \alpha \Gamma(\alpha)$ , where  $\Gamma$  is the gamma function [8–12] and  $\alpha$  is the degree of fractionality. Such a parameter can go from one to zero or vice versa in

<sup>2</sup> This passage from the two limiting cases is nothing else than a coarse-graining procedure whose general scheme and approximations are reported in an example in section 3.

a continuous way producing the effect of switching off/on a DOF. Within this formalism, the statistical average becomes

$$\langle A \rangle_\alpha = \frac{\int_0^\infty e^{-\beta H(q)} q^{\alpha-1} A(q) dq}{\int_0^\infty e^{-\beta H(q)} q^{\alpha-1} dq}. \tag{2}$$

If we take the expression of  $H(q) = |q|^m$ ,  $m > 0$ , and  $A(q) = C_n |q|^n$ ,  $n > 0$ , then equation (2) becomes<sup>3</sup>

$$\langle A \rangle_\alpha = \frac{C_n \int_0^\infty e^{-\beta q^m} q^{\alpha+n-1} dq}{\int_0^\infty e^{-\beta q^m} q^{\alpha-1} dq}. \tag{3}$$

By virtue of the integral [13]

$$\int_0^\infty e^{-\beta q^m} q^k dq = \frac{1}{m} \beta^{-(k+1)/m} \Gamma\left(\frac{k+1}{m}\right), \tag{4}$$

we obtain

$$\langle A \rangle_\alpha = \frac{C_n \Gamma\left(\frac{\alpha+n}{m}\right)}{\Gamma\left(\frac{\alpha}{m}\right)} \beta^{-n/m}. \tag{5}$$

Equation (5) gives the general expression of  $\langle A \rangle_\alpha$ . Interestingly for  $n = m$  we have the case of  $\langle H(q) \rangle_\alpha$ , i.e. the associated energy and the expression is reduced to

$$\langle H(q) \rangle_\alpha = \frac{\alpha}{n} \beta^{-1}. \tag{6}$$

This means  $\langle H \rangle_\alpha = \alpha \langle H \rangle$ , i.e. one obtains the expression for the fractional dimension from the corresponding integer dimension scaled by the parameter of fractionality. The fractional counterpart of the equipartition theorem emerges naturally for  $n = 2$ . In fact, what we found analytically expresses the concept of gradually counting a DOF and its contribution to the statistical properties of the system. For  $n \neq m$  the prefactor  $\frac{\Gamma(\frac{\alpha+n}{m})}{\Gamma(\frac{\alpha}{m})}$  takes care of the switching; however, it is not necessarily linear in  $\alpha$ . Nevertheless  $\langle A \rangle_{\alpha \rightarrow 0} = 0$ , i.e. the contribution of completely switched-off DOF to a statistical average is zero. The approach presented above for switching the DOF  $q$  is valid, in general, for any continuous potential (except the Coulomb or gravitational potential due to their infinite interaction range) and any observable that can be expanded in a Taylor series. Such a potential, e.g., the Lennard–Jones potential, can always be fitted piecewise with polynomials (splines) of positive powers so that the above procedure can be applied.

Note that the virial theorem [16] is also satisfied for this class of potentials. Assume that the potential  $V(q) = aq^{n+1}$  is a power-law function of  $q$ . Then we have  $\langle T \rangle = -\frac{1}{2} \left\langle \frac{\partial V}{\partial q} q \right\rangle = \frac{n+1}{2} \langle V \rangle$  for the integer dimension of  $q$ , where  $T$  is the kinetic energy. For the fractional dimension, using equation (6), we obtain  $\langle T \rangle_\alpha = \alpha \langle T \rangle$  and  $\langle V \rangle_\alpha = \alpha \langle V \rangle$ . Hence, the relation dictated by the virial theorem is preserved also in the switching region.

### 3. Coarse-graining idea in a nutshell

The natural question at this point is whether the concepts shown above can find a practical application. The way we presented the statistical system implies that each generalized coordinate  $\{q\}$ , by which we describe the system, represents its DOFs, i.e. they are all

<sup>3</sup> In the case of the Coulomb (or gravitational) potential ( $m = -1$ ), the statistical average is not defined due to an infinite range of the potential. The potentials with  $m < -1$  that decay faster than the Coulomb potential can be truncated at a certain distance. For this class of potentials, the statistical average can be evaluated either numerically or analytically with some approximations, cf the text.

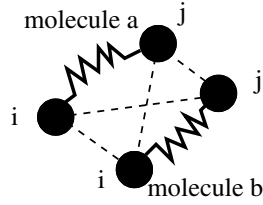


Figure 1. Molecule *a* and molecule *b* interacting at the atomistic level.

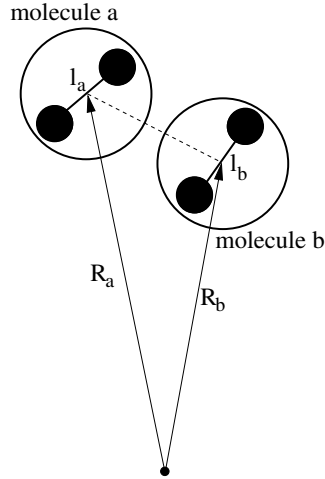


Figure 2. Molecule *a* and molecule *b* interacting via effective inter- and intramolecular potentials. The large circles represent the two molecules in the coarse-grained representation.

independent of each other. Furthermore we require that they are decoupled, i.e. there are no cross terms of these variables in the Hamiltonian of the system. Otherwise the factorization of the Boltzmann factor and the analytical integration of the statistical average is not possible [14]. Given a system of particles, finding such a system of coordinates is generally not a trivial task. In fact, the factorization procedure typically requires some approximations and loss of information<sup>4</sup>. Such a coarse-graining procedure will here be illustrated on the simple example of diatomic molecules where the two atoms *i* and *j* are linked by an elastic potential. Figure 1 shows two such molecules; the inter- and intramolecular potential energies depend on each other. For figure 1, we have

$$\begin{aligned} V(\mathbf{r}_{ia}, \mathbf{r}_{ja}, \mathbf{r}_{ib}, \mathbf{r}_{jb}) &= V_{\text{intra}} + V_{\text{inter}} \\ &= k|\mathbf{r}_{ia} - \mathbf{r}_{ja}|^2 + k|\mathbf{r}_{ib} - \mathbf{r}_{jb}|^2 \\ &\quad + V(\mathbf{r}_{ia}, \mathbf{r}_{ib}) + V(\mathbf{r}_{ia}, \mathbf{r}_{jb}) + V(\mathbf{r}_{ib}, \mathbf{r}_{ja}) + V(\mathbf{r}_{jb}, \mathbf{r}_{ja}), \end{aligned} \quad (7)$$

where  $k$  is the bond-stretching constant. To separate inter- and intramolecular interactions, we use the mapping (see also figure 2)

$$(\mathbf{r}_{ia}, \mathbf{r}_{ja}, \mathbf{r}_{ib}, \mathbf{r}_{jb}) \rightarrow (\mathbf{R}_a, \mathbf{R}_b, l_a, l_b, \theta_{a_1}, \theta_{a_2}, \theta_{b_1}, \theta_{b_2}), \quad (8)$$

<sup>4</sup> In the actual numerical implementation of such a coarse graining, DOFs are not only eliminated, but are also replaced by new interactions between the coarse particles. Thus, the choice of the coarse-graining scheme, which minimizes interdependences of the DOFs, is essential for a successful application [14].

where  $\mathbf{R}$  is the molecular centre of mass,  $l$  is the scalar distance between the atom  $i$  and atom  $j$  in the molecule and  $\theta_{a_1}$  and  $\theta_{a_2}$  are the two orthogonal angles of rotation for the linear molecule  $a$ , respectively. One must note that we did not reduce the number of DOFs by this coordinate transformation. Next, we express the potential as a sum of an ‘effective’ potential plus a correction:

$$V(\mathbf{r}_{ia}, \mathbf{r}_{ja}, \mathbf{r}_{ib}, \mathbf{r}_{jb}) = kl_a^2 + kl_b^2 + V_{\text{eff}}(\theta_{a_1}) + V_{\text{eff}}(\theta_{a_2}) + V_{\text{eff}}(\theta_{b_1}) + V_{\text{eff}}(\theta_{b_2}) \\ + V_{\text{eff}}(\mathbf{R}_a, \mathbf{R}_b) + \Delta V(\mathbf{R}_a, \mathbf{R}_b, l_a, l_b, \theta_{a_1}, \theta_{a_2}, \theta_{b_1}, \theta_{b_2}). \quad (9)$$

If  $\Delta V \approx 0$ , then the potential can be separated exactly into the inter- and intraparts, and the coordinates  $\mathbf{R}_a, \mathbf{R}_b, l_a, l_b, \theta_{a_1}, \theta_{a_2}, \theta_{b_1}, \theta_{b_2}$  are the new set of DOFs. Let us furthermore assume that the effective potentials associated with rotational DOFs are of the form  $V_{\text{eff}}(\theta) = \theta^m$ ,  $m > 0$ . Then, we can write the corresponding Hamiltonian as follows:

$$H = T + V = \alpha_a(T_{\text{intra}_a} + V_{\text{intra}_a}) + \alpha_b(T_{\text{intra}_b} + V_{\text{intra}_b}) + (1 - \alpha_a)(T_{\text{intra}_a} + V_{\text{intra}_a}) \\ + (1 - \alpha_b)(T_{\text{intra}_b} + V_{\text{intra}_b}) + T_{\text{trans}_a} + T_{\text{trans}_b} + V_{\text{eff}}(\mathbf{R}_a, \mathbf{R}_b) \\ = H_{\text{fractal/explicit}} + E_{\text{fractal/internal}} + H_{cg}, \quad (10)$$

where  $T$  and  $V$  are the total kinetic and potential energies, respectively,  $T_{\text{trans}}$  is the translational kinetic energy,  $T_{\text{intra}}$  is the intramolecular kinetic energy corresponding to molecular rotations and vibrations [15],  $V_{\text{intra}} = kl^2 + \theta_1^m + \theta_2^m$  is the associated intramolecular potential energy,  $H_{\text{fractal/explicit}}$  is the total energy of both molecules associated with the fractal explicit DOFs that are switched off/on,  $\alpha$  is the degree of fractionality and  $H_{cg} = T_{\text{trans}_a} + T_{\text{trans}_b} + V_{\text{eff}}(\mathbf{R}_a, \mathbf{R}_b)$  is the total coarse-grained Hamiltonian.  $E_{\text{fractal/internal}}$  is the total internal energy associated with those fractal DOFs that are no longer explicitly considered upon switching. The subscripts  $a$  and  $b$  denote the energy terms corresponding to molecules  $a$  and  $b$ , respectively. At the end we are left only with decoupled  $\mathbf{R}$ ,  $l$  and  $\theta$  terms in the intramolecular energy. These can be treated using equation (6). Note, however, that these terms do not have to be necessarily harmonic as in the normal mode analysis [15]. The equations of motion for those explicit DOFs, which are switched off in the coarse-graining procedure, are in this case decoupled from the equations of motion of the coarse-grained DOFs. Since the total Hamiltonian as given by equation (10) preserves its form regardless of the resolution regime, the equations of motion of the switched-off explicit DOFs in the coarse-grained regime remain the same as in the explicit regime—they are just not considered in the statistical average.

#### 4. Adaptive resolution MD simulation

Recently, we have developed an efficient particle-based MD simulation scheme AdResS [3], which exploits the theoretical concepts described in the previous two sections and allows us to change the molecular resolution on demand. This is done by introducing a switching region where the forces acting on the molecules are obtained as a certain linear combination of explicit and coarse-grained forces. In this section, we shortly review the basic aspects of the method and move further by showing analytically that the intuitively more obvious approach based on the potential rather than the forces, within this scheme, would lead to the violation of Newton’s Third Law. Let us start by considering a system divided into high and low resolution domains in the  $x$  direction. Usually, in complex physical systems, the Hamiltonian cannot be separated into the decoupled terms as in equation (10) because the assumptions that we made in the previous section are only valid to a certain extent. Instead, we use an interpolation formula for the intermolecular force acting between centres of mass of given molecules  $a$  and  $b$ :

$$\mathbf{F}_{ab} = w(x_a)w(x_b)\mathbf{F}_{ab}^{\text{atom}} + [1 - w(x_a)w(x_b)]\mathbf{F}_{ab}^{\text{cg}}, \quad (11)$$

where  $x_a$  and  $x_b$  are the  $x$  centre of mass coordinates of the molecules  $a$  and  $b$  respectively,  $\mathbf{F}_{ab}^{\text{atom}}$  is the sum of all pair atom interactions between explicit atoms of molecule  $a$  and explicit atoms of molecule  $b$  and  $\mathbf{F}_{ab}^{\text{cg}}$  is the total force between the centres of mass of the respective two molecules. The function  $w(x)$  is a weighting function with the properties such that  $w(x) = 1$  in the high resolution domain and  $w(x) = 0$  in the low resolution region. In order to switch on/off the DOFs gradually on-the-fly without extra equilibration when moving between the regions with different resolutions, we introduce the transition regime sandwiched in between the low and high resolution domains. In the transition regime, where  $0 \leq w(x) \leq 1$ , we deal with fractional DOFs. There the definition of the temperature is obtained by considering, for each DOF in the system, the fractional analogue of the equipartition theorem as given by equation (6) for  $n = 2$ :

$$\langle T \rangle_\alpha = \frac{\alpha k_B T}{2}, \quad (12)$$

where  $\langle T \rangle_\alpha$  is the average kinetic energy of a DOF, corresponding to the level  $\alpha$  of resolution. This is now applied to the transition region, defining a local  $\alpha(x) = w(x)$ . While moving through this region, the DOF is continuously switched on or off. The parameter  $\alpha$  has to be considered as the local (constant) value of  $w(x)$  in a given infinitesimal (but still large enough for the equipartition theorem to apply<sup>5</sup>) interval of the switching region. The ansatz (11) satisfies Newton's Third Law and takes into account the transfer of the switched-off explicit DOF onto the molecular centre of mass. To compensate the free energy density gradient due to changing the number of DOFs in the transition regime, we need to supply or remove 'latent' heat corresponding to the internal energy  $E_{\text{fractal/internal}}$  at this 'geometrically induced phase transition' [7] using a thermostat. Hence, our system is not conservative and a potential associated with the force given by equation (11) does not exist [16].

We could, in principle, also define the mixing scheme using the respective potentials instead of forces as

$$V_{ab} = w(x_a)w(x_b)V_{ab}^{\text{atom}} + [1 - w(x_a)w(x_b)]V_{ab}^{\text{cg}}. \quad (13)$$

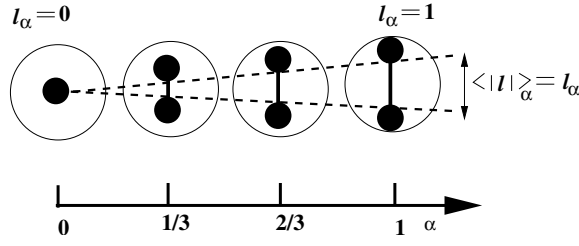
However, this approach leads to the violation of Newton's Third Law. The potential in equation (13) depends on the absolute positions of the particles and not only on their relative distances. The associated conservative force, which is defined as the negative gradient of this potential, acting on the molecule  $a$  is

$$\begin{aligned} \mathbf{F}_{ab} = -\frac{\partial V_{ab}}{\partial \mathbf{r}_a} &= w(x_a)w(x_b)\mathbf{F}_{ab}^{\text{atom}} + [1 - w(x_a)w(x_b)]\mathbf{F}_{ab}^{\text{cg}} \\ &+ \left( \frac{\partial w(x_a)}{\partial x_a} w(x_b) [V_{ab}^{\text{cg}} - V_{ab}^{\text{atom}}], 0, 0 \right), \end{aligned} \quad (14)$$

where  $\frac{\partial}{\partial \mathbf{r}} = \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)$ ,  $\mathbf{F}_{ab}^{\text{atom}} = -\frac{\partial V_{ab}^{\text{atom}}}{\partial \mathbf{r}_a}$  and  $\mathbf{F}_{ab}^{\text{cg}} = -\frac{\partial V_{ab}^{\text{cg}}}{\partial \mathbf{r}_a}$ . Expression (14) for the force differs from the corresponding expression (11) by the additional term  $\frac{\partial w(x_a)}{\partial x_a} w(x_b) [V_{ab}^{\text{cg}} - V_{ab}^{\text{atom}}]$  in the  $x$  component of the force. The respective force acting on the molecule  $b$  is in this case

$$\begin{aligned} \mathbf{F}_{ba} = -\frac{\partial V_{ab}}{\partial \mathbf{r}_b} &= w(x_a)w(x_b)\mathbf{F}_{ba}^{\text{atom}} + [1 - w(x_a)w(x_b)]\mathbf{F}_{ba}^{\text{cg}} \\ &+ \left( \frac{\partial w(x_b)}{\partial x_b} w(x_a) [V_{ab}^{\text{cg}} - V_{ab}^{\text{atom}}], 0, 0 \right). \end{aligned} \quad (15)$$

<sup>5</sup> Large enough means that in the evaluation of equation (12) a locally constant  $\alpha$  can be assumed for the averaging of the velocities, which are associated with the particles in this infinitesimal region. For such a subsystem, the integration scheme of equation (2ff) can be applied.



**Figure 3.** Illustration of the idea of molecular representation. On the vertical axis is reported the average intramolecular bond  $l$  calculated for the fractional dimension, while the horizontal axis reports the degree of fractionality, or equivalently, the switching resolution parameter  $\alpha$ . Note that the circle around the molecules is the same for all values of  $\alpha$ ; this reflects the fact that the molecular excluded volume and consequently the molecular density remain the same regardless of the resolution.

Using  $\mathbf{F}_{ba}^{\text{atom}} = -\mathbf{F}_{ab}^{\text{atom}}$  and  $\mathbf{F}_{ba}^{\text{cg}} = -\mathbf{F}_{ab}^{\text{cg}}$ , we obtain

$$-\mathbf{F}_{ba} = w(x_a)w(x_b)\mathbf{F}_{ab}^{\text{atom}} + [1 - w(x_a)w(x_b)]\mathbf{F}_{ab}^{\text{cg}} - \left( \frac{\partial w(x_b)}{\partial x_b} w(x_a) [V_{ab}^{\text{cg}} - V_{ab}^{\text{atom}}], 0, 0 \right). \quad (16)$$

In order that the force given by equation (14) satisfies Newton's Third Law, i.e.  $\mathbf{F}_{ab} = -\mathbf{F}_{ba}$ , we see from equations (14) and (16) that

$$\frac{\partial w(x_a)}{\partial x_a} w(x_b) = -\frac{\partial w(x_b)}{\partial x_b} w(x_a), \quad (17)$$

implying that

$$\frac{1}{w(x_a)} \frac{\partial w(x_a)}{\partial x_a} = -\frac{1}{w(x_b)} \frac{\partial w(x_b)}{\partial x_b} = \text{const} = 0. \quad (18)$$

From equation (18) it follows that the force defined by equation (14), although it is conservative, can satisfy Newton's Third Law only for a trivial case of  $w(x) = \text{const}$ , corresponding to constant resolution simulations. In order that the diffusion of molecules between regions with different resolution is not perturbed by the resolution change, the conservation of the momentum dictated by Newton's Third Law is crucial in adaptive resolution MD simulations. Starting with equation (13) has thus a clear disadvantage for usage in adaptive resolution MD simulations. Therefore, in AdResS we follow the scheme of equation (11).

### 5. A diatomic molecule: an example of the concept of adaptive representation

In order to complete the view of the approach shown, in this section we demonstrate the meaning of our concept of adaptive representation for the example of the average length of the diatomic molecule:

$$\langle |l| \rangle_\alpha = \frac{\int_0^\infty l^\alpha e^{-\beta l^2} dl}{\int_0^\infty l^{\alpha-1} e^{-\beta l^2} dl}. \quad (19)$$

Exploiting equation (5), we get

$$\langle |l| \rangle_\alpha = \frac{\Gamma(\frac{1}{2})\Gamma(\frac{\alpha+1}{2})}{\Gamma(\frac{\alpha}{2})} \langle |l| \rangle. \quad (20)$$

The meaning of equation (20) is pictorially illustrated in figure 3. It expresses the idea of adaptive representation as outlined so far. The limiting cases  $\alpha = 0$  and  $\alpha = 1$  correspond

to the coarse-grained and atomistic descriptions, respectively. One should imagine to have an optical magnification and move it closer and closer to the molecule. By doing so one goes from the coarse grained to the atomistic description (and of course the same idea is applied for the reverse process).

## 6. Conclusions

The derivation of the statistical properties of a simple system, where the DOFs are slowly changed in a given region via the change of the phase space dimensionality, provides some basic insight into how to define thermodynamic quantities in a fractional phase space. Such a definition can be used as a basis to calculate important quantities, such as the temperature, in simulation schemes where DOFs are switched on or off on demand in a given region. The definition of the temperature, which we obtain via the extension of the equipartition theorem to fractional dimensions, provides a robust and consistent numerical scheme for adaptive resolution simulations [5, 6]. In conclusion, we have shown some basic properties of the idea of changing DOFs on-the-fly in analysing a statistical system. This work lays basic principles for changing of dimensionality of the phase space and the relative implementation in multiresolution numerical simulations.

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