

General continuum approach for dissipative systems of repulsive particles

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We propose a general coarse-graining method to derive a continuity equation that describes any dissipative system of repulsive particles interacting through short-ranged potentials. In our approach, the effect of particle-particle correlations is incorporated to the overall balance of energy, and a nonlinear diffusion equation is obtained to represent the overdamped dynamics. In particular, when the repulsive interaction potential is a short-ranged power law, our approach reveals a distinctive correspondence between particle-particle energy and the generalized thermostatics of Tsallis for any nonpositive value of the entropic index q . Our methodology can also be applied to microscopic models of superconducting vortices and complex plasma, where particle-particle correlations are pronounced at low concentrations. The resulting continuum descriptions provide elucidating and useful insights on the microdynamical behavior of these physical systems. The consistency of our approach is demonstrated by comparison with molecular dynamics simulations.

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Dissipative systems of repulsive particles can be representative of many physical phenomena in nature. For instance, type-II superconductors can be populated by vortices of supercurrents that pierce the system in the direction of the applied magnetic field [1]. These vortices can be considered as single particles, and will dissipate energy as long as they move [2–6]. Another notable example is complex plasma [7,8], where charged microparticles are immersed in an ionized gas. The free charges in the plasma screen the electric repulsion between particles, and electromechanical couplings between particles and media act as a drag force to the movement [7]. Colloidal systems are also well described with such approach [9,10].

A general equation of motion for systems of interacting particles in a dissipative media can be written as

$$m_i \frac{d\mathbf{v}_i}{dt} = \sum_j \mathbf{F}_{ij} + \sum_e \mathbf{F}_e - \gamma \mathbf{v}_i + \sqrt{2\gamma k_B T} \boldsymbol{\eta}_i(t), \quad (1)$$

where \mathbf{v}_i is the velocity of a single particle i . The first summation in Eq. (1) goes over the forces due to other particles. We refer to the effect of the other particles in the system as the internal force $\mathbf{F}_{\text{int}} = \sum_j \mathbf{F}_{ij}$. The second summation in Eq. (1) accounts for the action of external fields on the particle, for instance, the electric and gravitational fields in the case of complex plasma, or applied electric currents in the case of superconducting vortices. We use $\mathbf{F}_{\text{ext}}(\mathbf{r}_i) = \sum_e \mathbf{F}_e$ to represent the external forces acting on the particle. The term $-\gamma \mathbf{v}_i$ describes the dissipative force, and $\sqrt{2\gamma k_B T} \boldsymbol{\eta}_i(t)$ represents the thermal noise. Often in such systems inertial effects can be neglected, when compared to the other terms. In these situations, the system is said to obey an overdamped dynamics. Also, in situations where thermal effects can be neglected, one has the velocity of a particle proportional to the resultant force acting on it,

$$\gamma \mathbf{v}_i = \mathbf{F}_i, \quad (2)$$

where $\mathbf{F}_i \equiv \mathbf{F}_{\text{ext}} + \mathbf{F}_{\text{int}}$.

Solving the equations of motion for a macroscopic system can be unpractical. One possible approach is to describe the system by a “coarse-grained” continuous function $\rho(\mathbf{r}, t)$ such

that $\rho(\mathbf{r}, t)dv$ is the number of particles in the volume dv , at any time t and position \mathbf{r} . Since the number of particles is conserved, continuity holds, $\partial\rho(\mathbf{r}, t)/\partial t = -\nabla \cdot \mathbf{J}(\mathbf{r}, t)$, where $\mathbf{J}(\mathbf{r}, t) \equiv \rho(\mathbf{r}, t)\mathbf{v}(\mathbf{r})$, with the field $\mathbf{v}(\mathbf{r})$ giving the velocity of the particles in dv . The velocity field should be proportional to the resultant force field $\mathbf{f}_1 = \mathbf{f}_{\text{ext}} + \mathbf{f}_{\text{int}}$ acting on each particle near \mathbf{r} . While the external force may depend explicitly on the position, $\mathbf{f}_{\text{ext}} = \mathbf{F}_{\text{ext}}(\mathbf{r})$, in order to determine the force due to particle-particle interactions \mathbf{f}_{int} , it is necessary to know the particle concentration profile. Previous efforts in this direction [11] have considered that the internal force should be proportional to the concentration gradient, $\mathbf{f}_{\text{int}} = -a\nabla\rho$. Here we show that this expression remains valid only if particle-particle correlations are unimportant. We then generalize the approach developed in [11] by disclosing an analytical formalism to account for these correlations in terms of a continuum model, with the only restriction being that the interaction potential decreases fast enough to be considered short range. We demonstrate the usefulness of our approach by comparing its predictions with the results from numerical simulations.

To devise our continuum approach, we note that the potential energy of a particle U_1 should be a function of the local concentration and its derivatives. Under conditions where the interaction has a finite range of action, and $\nabla\rho(\mathbf{r})$ varies slowly enough to be considered constant within this interaction range, it is reasonable to disregard higher derivatives and use a first order expansion to describe the surrounding concentration, $\rho(\mathbf{r}) = \rho(\mathbf{0}, t) + \mathbf{r} \cdot \nabla\rho(\mathbf{r}, t)|_{(\mathbf{r}=\mathbf{0})}$. Moreover, for repulsive interactions, the state of minimum energy is always homogeneous, therefore any contribution of $\nabla\rho$ to the energy U_1 should be in second order. We conclude that, in a first order approximation, the potential energy of a single particle is a function of the local concentration only, $U_1 \equiv U_1(\rho)$.

In our continuum description the total potential energy is

$$U_T = \int \rho(\mathbf{r}, t) U_1[\rho(\mathbf{r}, t)] dv, \quad (3)$$

where the integral is done over the volume of the system. Considering that the single particle potential energy U_1

depends implicitly on time through $\rho(\mathbf{r}, t)$, the time variation of the total potential energy is

$$\frac{dU_T}{dt} = \int \frac{\partial \rho}{\partial t} \left(U_1 + \rho \frac{dU_1}{d\rho} \right) dv. \quad (4)$$

Let us define $W(\mathbf{r})$ as the term between parenthesis in Eq. (4). The continuity equation together with the identity $W \nabla \cdot \mathbf{J} = \nabla \cdot (\mathbf{J}W) - \mathbf{J} \cdot \nabla W$ split Eq. (4) into two integrals. From the Gauss theorem, as long as there is no current \mathbf{J} entering the border of the system, the integral of $\nabla \cdot (\mathbf{J}W)$ vanishes, resulting in

$$\frac{dU_T}{dt} = \int \mathbf{J} \cdot \nabla \left(U_1 + \rho \frac{dU_1}{d\rho} \right) dv. \quad (5)$$

On the other hand, the variation of the potential energy is given by the dissipated power, $dU_T/dt = -\sum_i \mathbf{F}_i \cdot \mathbf{v}_i$, which in the continuum description can be expressed as

$$\frac{dU_T}{dt} = - \int \mathbf{J} \cdot \mathbf{f}_1 dv, \quad (6)$$

where we use $\mathbf{J} = \rho \mathbf{v}$. Comparing Eqs. (5) and (6) we find

$$\mathbf{f}_1 = -\nabla \left(U_1 + \rho \frac{dU_1}{d\rho} \right). \quad (7)$$

Considering $U_1 = U_{\text{ext}}(\mathbf{r}) + U_{\text{int}}(\rho)$, we obtain $\mathbf{f}_1 = \mathbf{f}_{\text{ext}} + \mathbf{f}_{\text{int}}$, with $\mathbf{f}_{\text{ext}} = -\nabla U_{\text{ext}}$, and

$$\mathbf{f}_{\text{int}} = -\nabla U_{\text{int}} = -a(\rho) \nabla \rho, \quad (8)$$

with

$$a(\rho) = 2 \frac{dU_{\text{int}}}{d\rho} + \rho \frac{d^2 U_{\text{int}}}{d\rho^2}. \quad (9)$$

Therefore, the function $a(\rho)$, and consequently the force \mathbf{f}_{int} , are determined from the dependence of the particle-particle potential energy U_{int} on the concentration ρ . Including this in the continuity equation, we obtain

$$\gamma \frac{\partial \rho}{\partial t} = -\nabla \cdot \{ \rho [\mathbf{f}_{\text{ext}} - a(\rho) \nabla \rho] \}, \quad (10)$$

where the nonlinear term $a(\rho) \rho \nabla \rho = -\rho \mathbf{f}_{\text{int}}$ accounts for the contribution of the interparticle forces to the local current.

The particle-particle interaction energy will depend on the concentration around a given particle as

$$U_{\text{int}} = \frac{1}{2} \int \rho'(\mathbf{r}, t) V(r) dv, \quad (11)$$

where $\rho'(\mathbf{r}, t)$ is the expected particle concentration at a point displaced by \mathbf{r} from a central particle, and $V(r)$ is a repulsive radial interaction potential. A simple approximation to the potential energy U_{int} is obtained by disregarding particle-particle correlations and assuming that the concentration

$\rho' \equiv \rho$ is a constant within the range of the potential, leading to

$$U_{\text{int}} = \frac{\rho \Omega_D}{2} \int_0^\infty V(r) r^{D-1} dr, \quad (12)$$

where D is the dimensionality of the system. In two dimensions $\Omega_2 = 2\pi$ is the angle of a circumference, while in three dimensions $\Omega_3 = 4\pi$ is the solid angle of a sphere. Substituting Eq. (12) for U_{int} in Eq. (9), we conclude that a is a constant, and the internal force is proportional to the local gradient as

$$\mathbf{f}_{\text{int}} = -\nabla \rho \Omega_D \int_0^\infty V(r) r^{D-1} dr. \quad (13)$$

For the two-dimensional case, Eq. (13) is consistent with the form proposed in [11, 12]. As already mentioned, this approach disregards particle-particle correlations that could be relevant, and therefore it is a good approximation only under certain conditions.

As a matter of fact, dissipative systems of repulsive particles tend to form structural lattices with at least local order. The effect of the local correlations is especially important for interactions in the fashion of a power law, $V_\lambda(r) = \varepsilon(r/\sigma)^{-\lambda}$. If the exponent λ is large enough, $\lambda > D$, the force is short ranged [i.e., the integral in Eq. (13) does not diverge for large distances, $r \rightarrow \infty$], however, it diverges at $r \rightarrow 0$. It is not likely, however, that two repulsive particles in a dissipative medium will ever collide, therefore this divergence is not physical. A possible way to deal with correlations would be to consider an exclusion region of finite radius r_o around each particle, which becomes smaller as the concentration grows, $r_o = \alpha \rho^{-1/D}$. In this way, the integral (13) can be written as

$$\mathbf{f}_{\text{int}} = -\nabla \rho \Omega_D \int_{\alpha \rho^{-1/D}}^\infty V(r) r^{D-1} dr, \quad (14)$$

where the force \mathbf{f}_{int} is still proportional to the gradient, but now with $a \equiv a(\rho)$, since the exclusion radius r_o depends on ρ . For the case of a power-law potential, $a(\rho)$ becomes finite and is given by

$$a_\lambda(\rho) = \Omega_D \frac{\varepsilon \sigma^\lambda \alpha^{D-\lambda}}{\lambda - D} \rho^{(\lambda/D)-1}, \quad (15)$$

with the condition $\lambda > D$. Although this is just a qualitative correction, it clearly shows that particle-particle correlations affect the resultant force. Moreover, it also indicates that these effects may be accounted for in a continuum model through replacement of the constant a by the function $a(\rho)$. In what follows we propose a general way to obtain an estimate of the function $a(\rho)$.

Due to the dissipative medium, the particles will form configurations of low potential energy. The least-energy state, or ground state, depends on the form of the interaction, and on the particle concentration. However, for repulsive interactions, this ground state should be homogeneous, $\nabla \rho = \mathbf{0}$. Also, often the ground state is a regular lattice. We propose that the structure formed by the particles in the ground state could be used to calculate the single particle energy,

$$U_{\text{int}}(\rho) = \frac{1}{2} \sum_v V(r_v), \quad (16)$$

where $V(r)$ is the pair interaction potential, and the sum is over the vertices v of the homogeneous lattice. Considering the case of a binding potential, where $V(r)$ changes from repulsive to attractive with the distance r , we would have a nonmonotonic U_{int} with a minimum at some value $\rho \neq 0$. This leads to a negative $a(\rho)$ with particles moving from lower to higher concentrations, aggregating in clusters. In this case, our assumption of a slowly varying concentration should not be applicable.

The dependence on ρ is implicit in the positions r_v . To compute the variation $dU_{\text{int}}/d\rho$ it is useful to consider that the lattice parameter of the homogeneous lattice should depend on the concentration $\ell \sim \rho^{-1/D} \Rightarrow (d\ell/d\rho) = -\ell/D\rho$. Note also that the positions of the vertices are proportional to ℓ , that is, $dr_v/d\ell = r_v/\ell$. We can use this to differentiate any function in the form $G(\rho) = \sum_v g(r_v)$, leading to $dG/d\rho = -(1/D\rho) \sum_v r_v [dg(r_v)/dr_v]$. From the derivatives of U_{int} in Eq. (9), we obtain

$$a(\rho) = \frac{1}{2D^2\rho} \sum_v r_v [(D-1)f(r_v) - r_v f'(r_v)]. \quad (17)$$

From Eq. (17), the internal force over a particle is obtained from the surrounding concentration of particles ρ and local gradient concentration $\nabla\rho$. The sum in Eq. (17) goes over all the vertices of a homogeneous lattice of concentration ρ , and includes terms on the magnitude of interaction force $f = -dV/dr$ as well as its derivative $f' = df/dr$. For most interaction potentials, this sum cannot be analytically determined. However, knowing the homogeneous lattice and interaction, it is a simple task to use Eq. (17) to obtain $a(\rho)$ numerically for any concentration.

In the case of a two-dimensional system of particles interacting through a power law, $V_\lambda(r) = \varepsilon\sigma^\lambda r^{-\lambda}$, for all concentrations the homogeneous system rests in a triangular lattice with lattice parameter $\ell = 2^{1/2}/(3^{1/4}\rho^{1/2})$, leading to

$$a_\lambda(\rho) = \rho^{(\lambda/2)-1} \left[\frac{3^{3/4}(2+\lambda)\lambda\varepsilon\sigma^\lambda}{2^{(\lambda/2)+3}} \sum_v \left(\frac{\ell}{r_v} \right)^\lambda \right]. \quad (18)$$

Note that the positions of the vertices r_v are proportional to ℓ , therefore the terms in the sum of Eq. (18) are independent on ρ , which is consistent with our qualitative prediction, Eq. (15).

We now test our approach by comparing its predictions with numerical simulations. In our first test we let N particles interact in a two-dimensional system, confined in the x direction by an external potential $U_{\text{ext}}(x)$, and with periodic boundary conditions in the y direction. We stop our simulation when the system reaches mechanical equilibrium, that is,

$$F_{\text{int}} + F_{\text{ext}} = -a(\rho) \frac{d\rho}{dx} - \frac{dU_{\text{ext}}(x)}{dx} = 0. \quad (19)$$

One can then determine $\rho(x)$ by solving Eq. (19) with the condition $L_y \int \rho dx = N$, where L_y is the transverse dimension of the simulation cell. For the case of a power-law interaction, $V_\lambda(r) = \varepsilon\sigma^\lambda r^{-\lambda}$, $a_\lambda(\rho)$ can be obtained from Eq. (18), and the solution of Eq. (19) is

$$\rho(x) = \left[\rho_0^{\lambda/2} - \frac{\lambda}{2C_\lambda} U_{\text{ext}}(x) \right]^{2/\lambda}, \quad (20)$$

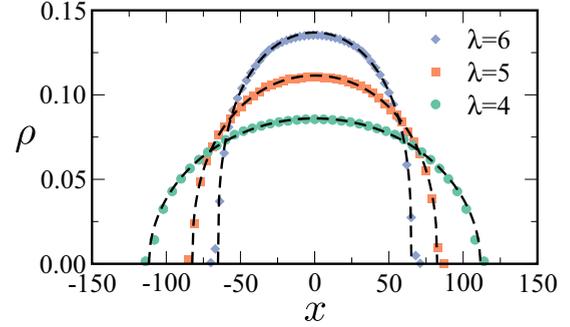


FIG. 1. Density profiles at the stationary state obtained from simulations (symbols). We consider two-dimensional systems of $N = 900$ particles interacting through a power-law repulsive potential $V_\lambda(r) = \varepsilon\sigma^\lambda r^{-\lambda}$. In the x direction, the particles are confined by a quadratic potential $U_{\text{ext}}(x) = kx^2/2$, with $k = 10^{-5}\varepsilon\sigma^{-2}$. In the y direction the simulation cell has a dimension $L_y = 60\sigma$, with periodic boundary conditions. We present results for simulations of this system considering three different values of λ . The dashed lines represent the results of the continuum model via Eq. (20).

where we define the parameter independent on ρ , $C_\lambda = a_\lambda(\rho)\rho^{1-\lambda/2}$. Figure 1 shows that Eq. (20) follows closely the results from numerical simulations for different values of λ . In our results, positions are expressed in units of σ and the concentration ρ is expressed in units of σ^{-D} .

For systems of particles interacting through power-law potentials, the density of energy is a power of the concentration, $\rho U_{\text{int}}(\rho) \sim \rho^{1+\lambda/D}$. In this case, considering $q = 1 - \lambda/D$, the internal energy density, minimized by the overdamped dynamics has a correspondence with the density of entropy in the framework of the generalized Tsallis thermostatics, $s_q(\rho) = (\rho^{2-q} - \rho)/(q-1)$ [13], that should therefore be maximized. In fact, taking the same steps followed in [14], and first introduced in [15], it is possible to show that, as long as $a(\rho) \sim \rho^{(\lambda/D)-1}$, as in Eq. (18), Eq. (10) will drive the system towards an equilibrium state described by Tsallis distribution $P_q(\mathbf{r}) \sim [1 - (1-q)\beta U_{\text{ext}}(\mathbf{r})]^{1/(1-q)}$ [16–18], thus generalizing the previous result of [14,19] for any $q \leq 0$.

Next, we show applications of our approach to models of two physical systems, namely, superconducting vortices and complex plasma. In type-II superconductors the magnetic flux is confined to small regions of the superconductor, each region being a vortex of super-currents carrying one quanta of magnetic flux. Since the vortices cross the sample system in the direction of the applied magnetic field, this corresponds to a quasi-two-dimensional system. Interacting through the so-called London potential [1,5], $V_\lambda(r) = \varepsilon K_0(\frac{r}{\sigma})$, vortices dissipate energy when moving. The least-energy state of this system is a triangular lattice, also called the Abrikosov lattice [20]. Figure 2 shows the function $a(\rho)$, computed through Eq. (17), for this system. For larger concentrations ($\rho > \sigma^{-2}$) one sees that the function saturates at the value predicted by Eq. (13), namely, $a = 2\pi\varepsilon\sigma^2$. However, for smaller concentrations the particle-particle correlations become relevant and $a(\rho)$ goes to zero as ρ decreases. We test this result by simulating systems confined in one direction by a potential $U(x) = kx^2/2$, and with periodic boundary condition in the

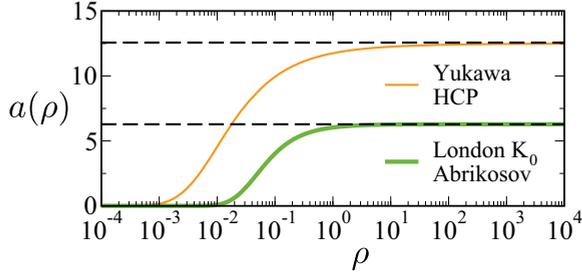


FIG. 2. The function $a(\rho) = |\mathbf{f}_{\text{int}}|/|\nabla\rho|$ as determined through Eq. (17). Two systems are investigated, namely, complex plasma particles interacting through the Yukawa potential, $V_Y = \varepsilon\sigma \exp(-r/\sigma)/r$, and forming hexagonal close-packed (hcp) lattices in three dimensions; superconducting vortices interacting through the London potential, $V_S = \varepsilon K_0(r/\sigma)$, and forming triangular (Abrikosov) lattices. As indicated by the dashed lines, for high enough concentrations, $\rho > \sigma^{-D}$, the curves converge to the value given by Eq. (13), $a = 4\pi\varepsilon\sigma^3$ and $a = 2\pi\varepsilon\sigma^2$, for the three- and two-dimensional systems, respectively.

other direction. Figure 3 displays the solutions of Eq. (19) with the function $a(\rho)$ computed for this particular system, and shows that they closely follow the results from numerical simulations.

The other physical system we investigate is a complex plasma, namely, a colloidal mixture of microscopic charged particles suspended in an ionized gas. The free charges in the gas screen the Coulomb interaction, and the Yukawa potential, $V_Y = \varepsilon\sigma \exp(-r/\sigma)/r$, is a good model for the repulsion between these colloidal particles [21]. Considering that the ground state of this system is an hcp lattice [22,23], we can compute the function $a(\rho)$ as also shown in Fig. 2. Similarly to the case of type-II superconducting vortices, for $\rho > \sigma^{-3}$, the function converges to $a = 4\pi\varepsilon\sigma^3$, in agreement with Eq. (13), while going to zero as the concentration ρ decreases. To test this result, we simulate a three-dimensional system of such particles under the action of an external potential $U_{\text{ext}}(\mathbf{r}) = kr^2/2$ confining the particles in all three dimensions. As before, Eq. (19) is numerically solved, but the normalization must be imposed by $4\pi \int \rho(r)r^2 dr = N$.

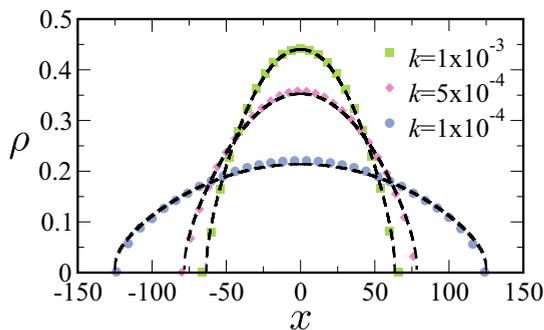


FIG. 3. Density profile at the stationary state obtained from simulations (symbols) for the London potential ($N = 800$, $L_y = 20\sigma$) for three different values of k . The dashed curves represent the predictions of the continuum model.

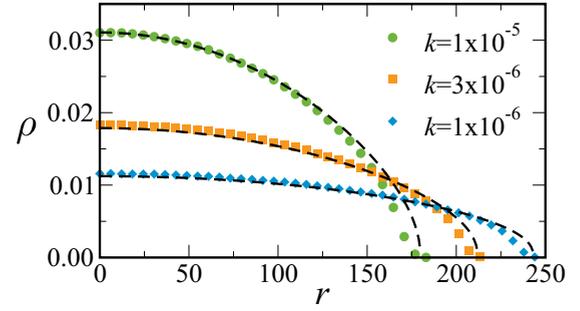


FIG. 4. Density profiles at the stationary state obtained from simulations (symbols). We consider three-dimensional systems of $N = 400\,000$ particles interacting through the Yukawa potential, $V_Y = \varepsilon\sigma \exp(-r/\sigma)/r$. The particles are confined by a quadratic potential, $U_{\text{ext}}(r) = kr^2/2$, with results for three different values of k . The dashed lines represent the predictions of the continuum model.

The comparisons between numerical simulations and the theoretical predictions for the case of complex plasmas are shown in Fig. 4. For the bulk of the system we observe good agreement between theory and simulation, but at the edge of the density profile there is a notable deviation. To understand this deviation, note that we assumed in our approach that the particle concentration gradient varies slowly within the effective range of the interaction potential. Since there is no negative concentration, this assumption fails when the distance to the edge of the profile $\rho/|\nabla\rho|$ is smaller than the characteristic interaction length σ . Thus, at the edge of the profile a continuum description should demand higher orders of approximation. However, this effect becomes negligible in systems where the density profile is not subjected to a strong confinement [24].

In summary, we introduced a general approach to build continuum models for systems of repulsive particles in dissipative media. For the two physical systems investigated here, namely, superconducting vortices and complex plasma, we show how the function $a(\rho)$, relating the gradient of concentration to the force, converges at high concentrations ($\rho > \sigma^{-D}$) to the value predicted by Eq. (13). Therefore, the assumption of a constant ratio of force to gradient represents a good approximation for several cases of interest, especially for highly concentrated systems [11,12]. However, higher concentrations may be a practical impossibility, especially in the case of superconducting vortices, where the critical field imposes a constraint in the maximum concentration of vortices [1]. For systems of low concentration, or for interactions such as power laws, where Eq. (13) diverges, it is necessary to account for the variation of the ratio $a(\rho)$ with concentration, as proposed here. Although we investigated only regular lattices at $T = 0$, this approach could be applied also for disordered cases, such as glassy systems or systems perturbed by thermal effects, by properly computing the average interaction energy per particle $U_{\text{int}}(\rho)$ over the accessible states.

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