

Interaction Potential between Anisotropic Particles: From Measurements to Tailored Design

Yiming Xia,^{1,2,3,*} Mingcheng Yang,^{1,2,†} and Ke Chen^{1,2,‡}

¹*Beijing National Laboratory for Condensed Matter Physics and Laboratory of Soft Matter Physics,
Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

²*School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China*

³*School of Information Technology and Cyber Security, People's Public Security University of China, Beijing 100038, China*



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We extend the classical test particle insertion (TPI) method to anisotropic systems and develop an anisotropic test particle insertion (ATPI) framework that efficiently extracts anisotropic interaction potentials from dense fluids using a small number of equilibrium snapshots. The method leverages the parallelizability of the insertion process, enabling rapid reconstruction of complex anisotropic interactions via high-performance computing. The ATPI method is quantitatively validated for liquids in both simulations and colloidal experiments. With a few modifications, this method is able to extract anisotropic interactions from solid lattices. By exploiting the theoretical equivalence between interaction measurement and design, we further demonstrate that ATPI can be used to construct interaction potentials that drive the system into target structures such as honeycomb lattices, kagome lattices, and dodecagonal quasicrystals. Our approach opens a new avenue for the inverse design of self-assembling systems.

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Introduction—Elemental interactions play a fundamental role in determining the structure, thermodynamics, dynamics, and phase behaviors in statistical systems [1,2]. Precise measurement of the basic interactions in complex systems is of no trivial task and often leads to great advancements in science and technology. Examples include the measurements of charge interactions by Coulomb [3] and the determination of gravitational constant by Cavendish [4]. The challenge primarily arises from isolating pairwise interactions from the inevitable many-body effects and non-negligible noises. Experiments are often complicated by the number of degrees of freedom involved, including distance, orientation, relative velocity, quantum states such as spins, angular momenta, and energy levels or external fields. Even for simple particles such as atoms or small molecules, the exact interaction between them is still difficult to ascertain, and certain approximations have to be employed in theoretical models or computer simulations [5–7]. The interactions between mesoscopic objects such as colloids [8–12] or biological macromolecules [13,14] are even harder to assess due to their complex compositions and structures.

Statistical measurements of interactions between mesoscopic objects are often employed when direct force measurements are not feasible. In thermal equilibrium,

the probability of finding two particles in a certain configuration is directly related to the potential energy of the configuration by the Boltzmann distribution [15]. When the configuration between two particles depends only on the particle separation r , the potential energy $U(r) = -k_B T \ln[g(r)]$ in the dilute limit $\phi \rightarrow 0$, where $g(r)$ is the radial distribution function. In practice, $g(r)$ can be easily obtained from video microscopy images of colloidal suspensions. As the dilute condition is required to avoid interferences from many-body effects, a large number of images is needed to accumulate sufficient statistics for $U(r)$ measurements. The pair potential can also be obtained using optical tweezers by repeatedly trapping and releasing two particles and measuring their trajectories [16]. At higher concentrations, interaction potential can be obtained by comparing the $g(r)$ from experiments and simulations and iteratively correcting the potential function used in simulations [17], by applying machine learning on large scale dataset [18–21], or by iteratively solving the Ornstein-Zernike integral equation with appropriate closure relations [22]. When the configuration between particle pairs depends not only on the particle separation but also on other degrees of freedom such as orientation, the number of snapshots required to adequately map out the pairwise interactions between anisotropic particles increases exponentially with the degrees of freedom, and all the existing statistical methods become experimentally impractical.

Recently, the test particle insertion (TPI) method [23,24] has been developed to measure the interactions between isotropic particles in a disordered fluid environment

*Contact author: ymxia@iphy.ac.cn

†Contact author: mcyang@iphy.ac.cn

‡Contact author: kechen@iphy.ac.cn

[21,25]. Instead of running full-scale simulations, TPI iteratively adjusts the interaction potential to minimize the mismatch in the pair distribution functions between the real system and a virtual system with particle insertions. This method overcomes the limitation of the previous techniques [15,16] by balancing accuracy and computational intensity, and it is validated in colloidal experiments.

In this Letter, we propose an anisotropic test particle insertion (ATPI) approach to extract interaction potentials from structures formed by particles with anisotropic interactions. Using computer simulations, we show that, at 2D, the ATPI scheme can accurately determine the anisotropic interactions from structure snapshots. This method is further validated in video microscopy experiments using magnetic colloidal particles. When accelerated by graphics processing units (GPUs), ATPI is able to obtain the interaction potential between anisotropic particles within a few hours from under 10,000 snapshots, making it a practical method for experimental measurements. Even though the original TPI method is based on the simple liquid theory [26], we find that ATPI can be applied to lattice systems through pre-processing of particle configuration data. This extension enables tailored design of interaction potentials for specific target structures, including honeycomb lattices, kagome lattices, and quasicrystals.

Method—Figure 1 illustrates the basic principles and procedure of ATPI. For a system of 2D anisotropic particles, the pair configuration is determined by particle separation r , azimuth angle θ , and the orientation angle φ relative to the orientation axis of the reference particle; thus, a three-parameter pair correlation function $g(r, \theta, \varphi)$ can be defined for an equilibrium liquid, with $g(r, \theta, \varphi) = n(r, \theta, \varphi) / \bar{\rho}$, where $n(r, \theta, \varphi)$ is the local number density at (r, θ, φ) and $\bar{\rho}$ is the mean number density of the system. To obtain the interaction potential between particle pairs, we first assume a trial interaction potential of $u_0(r, \theta, \varphi) = 0$. Virtual test particles of the same interactions are then inserted on a 40×40 grid, with random orientations (dependences on selected parameters

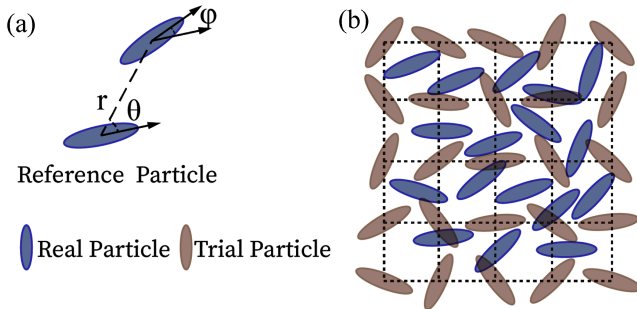


FIG. 1. Principles and procedure of the ATPI method. (a) Diagram for the three variables (r, θ, φ) that determine the configuration of a pair of particles. (b) Illustration of the ATPI method, where a trial particle (red) is independently inserted into each grid point (intersection of dashed lines) with 10 random orientations.

are shown in Supplemental Material [27]). The updated pair correlation function $g^*(r, \theta, \varphi)$ is directly associated with the additional potential energy Ψ by the insertion of test particle, with

$$g^*(r, \theta, \varphi) = \frac{\rho^*(r, \theta, \varphi)}{\bar{\rho}} = \frac{\langle \exp(-\beta\Psi) \rangle_{r, \theta, \varphi}^*}{\langle \exp(-\beta\Psi) \rangle}, \quad (1)$$

where $k_B T$ is the thermal energy and $\rho^*(r, \theta, \varphi)$ is the updated density distribution function. $g^*(r, \theta, \varphi)$ is then compared to the $g(r, \theta, \varphi)$ from the undisturbed real system, and the trial potential function is updated iteratively using

$$u_{n+1}(r, \theta, \varphi) = u_n(r, \theta, \varphi) - \alpha k_B T \ln \frac{g(r, \theta, \varphi)}{g^*(r, \theta, \varphi)}, \quad (2)$$

until $\sum_{i,j,k} |g(r_i, \theta_j, \varphi_k) - g^*(r_i, \theta_j, \varphi_k)|^2$ converges below a prescribed tolerance. Here, α is the iteration step size, and r_i, θ_j , and φ_k are discretized coordinates (see Supplemental Material [27] for the theoretical details).

Results—We first apply ATPI to molecular dynamics simulations in which anisotropic interactions between particles are analytically prescribed. Specifically, anisotropic particles are formed by rigidly bonding multiple smaller particles into dimers or trimers, with the constituent particles interacting through preselected Lennard-Jones potentials. At 2D, an anisotropic particle is characterized by the position of its center of mass and its orientation, which is the vector pointing from the centroid to one of the

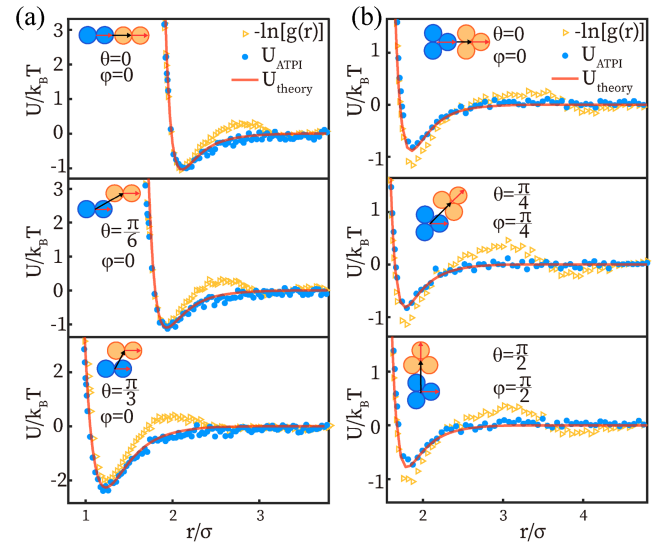


FIG. 2. Interaction potentials between dimers and trimers. The anisotropic interaction potentials (blue circles) of (a) dumbbell-shaped and (b) triangular particles obtained by the ATPI method. Red solid lines are the analytical potentials. Effective potentials directly derived from the radial-angular distribution functions by Boltzmann method (yellow triangles) are shown for comparison. The insets show the relative orientation of the interacting particles.

constituent particles. Figure 2(a) plots the measured potential energy $U(r)$ for different combinations of θ and φ (blue circles) at a packing fraction of 0.38. For comparison, theoretical $U(r)$ (red solid lines) and the $U(r)$ obtained directly from the pair correlation function $g(r)$ (yellow triangles) are also plotted. It is clear that the ATPI accurately recovers the theoretical interactions from snapshots in simulations, while the direct inversion of $g(r)$ significantly deviates from analytical values. Similar results are also obtained in trimer systems. The validation of the interactions for composite particles suggests that the ATPI scheme can be applied to arbitrarily shaped anisotropic particles, as long as the total interaction between a pair of particles is the sum of the pairwise interactions between all subregions of the particles. Since the ATPI algorithm can be deployed in parallel for individual snapshots, the potentials shown in Fig. 2(a) are obtained within 3.4 h from 49,152 frames with 250 particles using four RTX 4090 GPUs, and it can converge after ~ 100 iterations [27].

We then apply the ATPI method in colloidal experiments to measure the anisotropic interactions between superparamagnetic particles under weak external fields. The sample consists of an aqueous suspension of monodisperse superparamagnetic particles ($\sim 1 \mu\text{m}$, Onebead ThermoFisher) confined between two coverslips, forming a quasi-2D configuration. The packing fraction is 0.3, and the particles diffuse freely. The sample is imaged by video microscopy when a weak in-plane magnetic field ($\sim 0.25 \text{ mT}$) is applied using a quadrupole electromagnet. The magnetized particles, each carrying an in-plane magnetic dipole moment, interact through anisotropic dipole-dipole potentials. As the magnetic field is weak, the structure and dynamics of the system are hardly distinguishable visually from those under no external field (see Fig. S2 and the video SV1 in Supplemental Material [27]). Figures 3(a) and 3(b) plot the measured interaction potential for two different orientational configurations (head to tail and side by side) between the particles as a function of particle separation (blue circles) using ATPI from 8000 frames with 1045 particles. The results can be well fitted to the theoretical magnetic dipole interaction function $u(r, \theta) = \mu_0 m^2 (1 - 3 \cos^2 \theta) / (4\pi r^3)$ (solid lines) [32]. The complete two-variable potential is shown in Fig. 3(c). In comparison, the effective interactions from the conventional Boltzmann method [yellow squares in Figs. 3(a) and 3(b)], deviate qualitatively from theoretical functions. This deviation arises from the many-body effect present at the given packing fraction. To avoid many-body interference, experiments need to be performed at extremely low concentrations, which in turn require substantially more snapshots to accumulate sufficient statistics. Figure 3(d) shows the effective potential obtained in a sample at a packing fraction of 0.015 by analyzing 160,000 snapshots using the Boltzmann method. The effective potential is qualitatively similar to the one in Fig. 3(c),

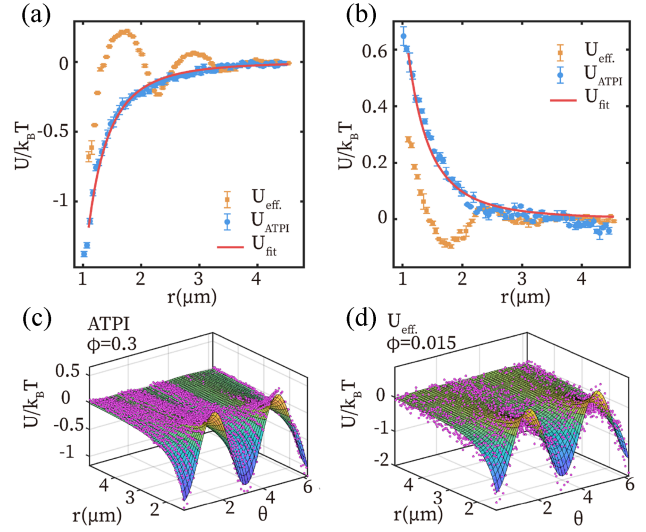


FIG. 3. Interactions between superparamagnetic colloidal particles. Interaction potentials (blue circles) obtained by ATPI for two different configurations, including (a) head to tail and (b) side by side. The solid lines are fit to the dipole interaction function. Yellow squares are the effective potentials extracted from the radial-angular distribution functions by the Boltzmann method. (c) Two-variable interaction potential between magnetic particles by ATPI. (d) Two-variable interaction potential obtained from dilute samples using the Boltzmann method.

but much noisier. The fitted magnetic moments from the results in Figs. 3(c) and 3(d) are $m = 1.87 \pm 0.15 \times 10^{-16} \text{ Am}^2$ and $m = 2.27 \pm 0.26 \times 10^{-16} \text{ Am}^2$, respectively. Further improving the quality of measurements using the Boltzmann method would require tens of millions of snapshots at even lower concentrations, which is impractical for colloidal experiments. We also perform an independent measurement of the attraction dynamics of magnetic particle pairs, and the extrapolated magnetic moment of a particle is $m = 1.65 \pm 0.26 \times 10^{-16} \text{ Am}^2$, in agreement with ATPI results [27].

Finally, we apply the ATPI method to extract anisotropic interactions from solid lattices, which is beyond the original scope of the particle insertion method. For solid lattices, two particular issues need to be addressed. The first issue is the divergence of pair correlation functions for static ideal lattices. The radial-angular distribution functions in these lattices are reduced to a series of Dirac δ functions, causing the iterative update in Eq. (2) to diverge. This problem is solved by introducing random fluctuations to the particles in the snapshots, which mimic the thermal fluctuations in real solids and broaden the peaks in the distribution functions. The second issue is the divergence of potential energy increase from test particle insertions. For a perfect lattice in which all permissible sites are occupied, an attempted insertion almost always results in overlapping with existing particles, thus the rejection of the insertion. To increase the number of successful particle insertions, we

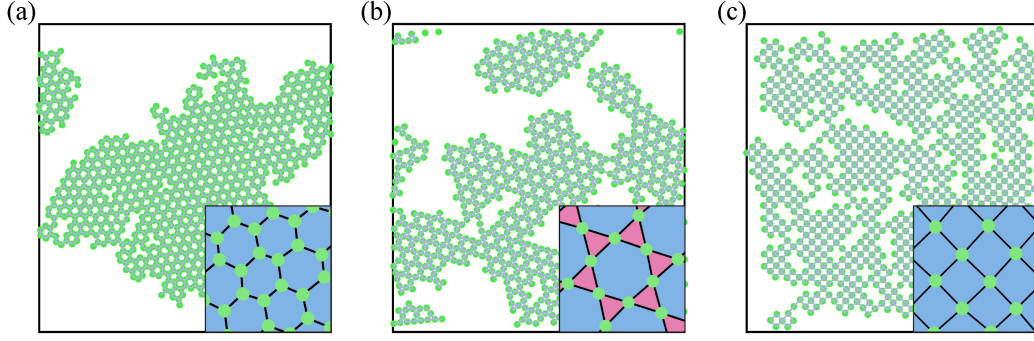


FIG. 4. Self-assembled lattice structures from interaction potentials obtained by ATPI, including the (a) honeycomb lattice, (b) kagome lattice, and (c) square lattice. The insets are the original lattices from which the potential functions are derived.

randomly create a small number of vacancies in the lattices, which provides sufficient space for trial insertions without qualitatively altering the overall lattice structure.

Unlike equilibrium liquids, where the uniqueness of the potential function from the TPI (and ATPI) method is guaranteed by the Henderson theorem [33], the specific potential obtained by ATPI from a solid lattice is no longer unique but depends on the assumed fluctuations and defect distributions, which is consistent with the fact that systems with different interactions may share the same equilibrium structure [27].

The modified ATPI procedure is applied to several typical 2D lattices, including square, honeycomb, and kagome lattices. The details of the obtained potentials, which are expressed by numerical values at discrete coordinates $(r_i, \theta_j, \varphi_k)$, are shown in Supplemental Material [27]. After smoothing and interpolation, these discrete potential functions $U(r_i, \theta_j, \varphi_k)$ are then employed in coarse-grained simulations with initial configurations of liquids. The systems are allowed to evolve to stable structures and recover the same structures from which the potentials are originally derived, as shown in Fig. 4.

The success of the ATPI procedure in simple lattices clearly demonstrates its ability to design interparticle potentials for systems to self-assemble into target structures, which is the inverse problem of finding the equilibrium structure of a system with known interactions. Currently, there are no general methods for designing potentials for arbitrary structural features. As an example, we construct an interaction potential function that can form two-dimensional dodecagonal quasicrystal (DDQC) structures. Figure 5(a) shows the equilibrium structure from the obtained potential, with all the characteristic local features of 2D quasicrystals [Figs. 5(b)–5(d)]. The potential function for DDQC, $U(r, \theta_1, \theta_2)$, which depends on the particle separation r , polar angles of the two particles θ_1 and θ_2 relative to the vector connecting the two particles, can be decomposed into a series of radial and angular components with $U(r, \theta_1, \theta_2) = \sum_i f_i(r) V_i(\theta_1, \theta_2)$ [27,34–36]. Figures 5(e) and 5(f) show the main components $f_0(r)$ and $V_0(\theta_1, \theta_2)$ of the obtained potential. The

minimum of $f_0(r)$ is at $r = \sigma$, corresponding to the characteristic length scale of particles. There are 12 potential minima in $V_0(\theta_1, \theta_2)$, corresponding to different orientational combinations. This specific and relatively complex orientational feature in the interaction potential may explain why it is uncommon to observe 2D quasicrystal structures in systems of a single component [37,38].

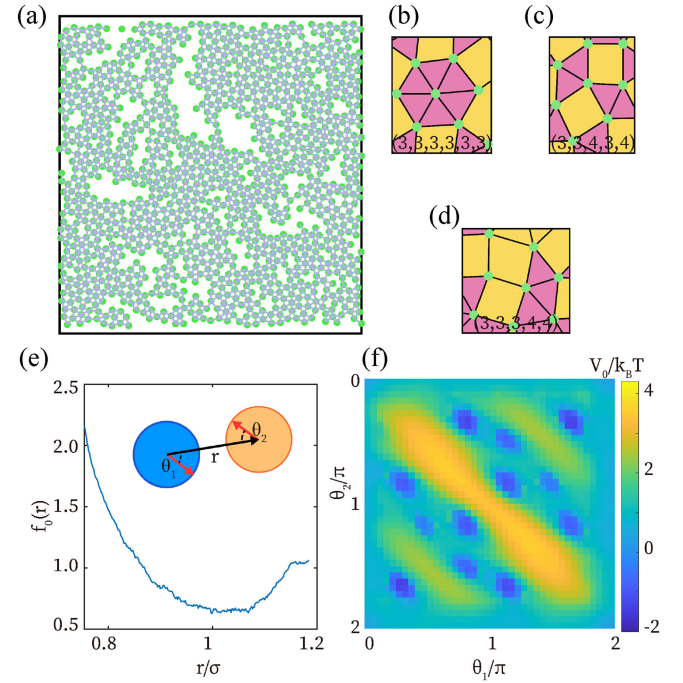


FIG. 5. Design of the interaction potential for dodecagonal quasicrystal structures. (a) The equilibrium structure formed by the particles with the obtained potential. (b)–(d) Three characteristic local structures of the DDQC. The numbers $a_0, a_1, \dots, a_K$, meaning that as we move in a circle around the vertex we encounter a regular a_0 gon, followed by a regular a_1 gon. (e) The main radial component $f_0(r)$ and (f) the main angular component $V_0(\theta_1, \theta_2)$ of the interaction potential function. The inset of (e) shows the definition of polar angles θ_1 and θ_2 .

In summary, our current Letter extends the test particle insertion method to anisotropic systems through the development of the ATPI framework. The ATPI method can accurately measure anisotropic potential between identical particles with pairwise interactions in 2D from a small dataset, and with moderate computational resources. With comparable computational costs to machine learning (ML) methods, the ATPI results are physically more interpretable than ML, while ML is more viable at high densities. The relative efficiency and advantage of ATPI increase significantly with the complexity of the interaction investigated. This approach is particularly useful in systems in which direct measurements are impractical, such as nonspherical colloids, Janus particles, or particles with nonuniform electromagnetic or chemical properties. Compared to the original TPI method for isotropic particles, one advantage of the ATPI method is its ability to design interactions between building blocks that can self-assemble into specific structures, which is useful in both experiments and simulations [39,40]. While our present Letter is limited to equilibrium monodisperse systems, it is worth exploring whether the ATPI method can be further extended to nonpairwise additive interactions [41], polydisperse systems [42], or nonequilibrium systems [43].

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Data availability—The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request. The software will be made available in a public depository after publication [44].

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