Significance of the nature of disorder on the universal features of the spatio-temporal correlations of two-dimensional Coulomb-clusters

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Abstract. We comprehend the role of imperfections arising from different origins on the universal features in materials consisting of interacting particles. Specifically, we report the static and dynamic responses in a cluster of Coulomb particles in two dimensions. Properties associated with melting in confined systems with pinned impurities are studied, and results are compared with those from irregularly trapped system of particles. While the disorder of first type leads to diffusive single-particle dynamics, the motion of a particle in an irregular trap remains chaotic but ballistic. The many-particle system does not differentiate between these two models of disorder insofar as their qualitative properties are concerned—particularly for describing the thermal melting of the underlying Coulomb-"solid". However, quantitative differences persist and could be observed—the relaxation time scales differ significantly by tuning impurity concentration.

1 Introduction

The effect of quenched disorder on the properties of systems, which would be otherwise ordered, has been a subject of extensive study [1–9]. A particular example that draws special attention is a two-dimension (2D) system of classical particles undergoing melting, because the translational order and bond-orientational order set in the system at different threshold temperatures. This results in a hexatic phase between the solid and liquid states in clean 2D systems [10–15]. The role of disorder on such a melting, as well as the fate of the hexatic phase under the influence of disorder has generated significant research interest [16,17]. Such studies are relevant to physical systems under common investigations [18–22]. These include randomly pinned Abrikosov vortex lattice in type-II superconductors [23], Wigner crystals [24–26], dusty plasma [20,27–30], ion traps [31], electronic solid on Helium bubbles [32], among others. Disorder realized in physical system arises from different origins, and often times its microscopic details remain unknown. Still, it is a conventional wisdom that there are universal features of disordered systems which are not sensitive to the microscopic details of the underlying impurities.

The complex interplay of inter-particle interactions and disorder has generated important research ideas in the broad area of condensed matter physics. Unraveling such interplay in small systems with finite number of particles is significant from both technological and fundamental perspectives [28,33–36]. While a sharp phase transition cannot be expected in a confined system [37], a thermal crossover from a ‘solid’-like to a ‘liquid’-like phase still occurs [38].

How significant are the microscopic details of disorder for properties of complex system? For example, disorder can arise from the randomness of the pinning centers in a system [39]. In such a model of disorder, a single test particle travels diffusively. On the other hand, an irregularity in the trapping potential can also make the trajectory of the test particle unpredictable, leading to a ballistic yet chaotic motion. Is this fundamental difference in the motional signature of a single particle of any relevance for describing the universal properties of a disordered system composed of many interacting particles? We address this question in this article considering (long-range) Coulomb-interacting particles in confined geometries.

Transport in small grains realizes exciting physics of interference and correlations [25,33]. When the confinement of the grain breaks all spatial symmetries, it behaves like a disordered system. Such systems are expected to show universal statistics of energy levels and energy functions [40]. An interesting comparison of chaotic versus diffusive dynamics has been carried out
in experiment using microwave studies [41]. An important difference between them, however, is the following: A strong pinning disorder can lead to localization [42] defying the applicability of random matrix theory [43], but a ballistic motion is extended across the whole system [44]. Nevertheless, for weaker disorder strengths, a comparison between the motions of interacting many-particles in different environments is an intriguing point to explore [45,46].

Addressing these issues, our key results are the following: The systems with pinned impurities possess a more robust positional order than in irregular confinements, while the bond-orientational order responds in a similar manner in both systems. The details of the disorder have little role on the ‘melting’ of the Coulomb ‘crystal’ [38]. Both the systems show qualitatively similar motional signatures. However, they differ in notable quantitative details. The pinning disorder increases the relaxation time considerably, in agreement with existing literature [47].

The rest of this article is organized as follows. Section 2 explains our model and its parameters and the details of our numerical simulations. Section 3 discusses different static properties in different subsections. We also estimate the thermal crossover from a solid-like to a liquid-type behavior from the temperature (T) dependence of the positional and bond-orientational orders. In Sect. 4, we calculate the dynamic observables focusing on the temporal evolution of these two differently disordered systems. Finally, Sect. 5 describes the one- and two-particle dynamics in terms of our analysis of Poincaré sections in the disordered systems. We conclude our results in Sect. 6.

2 Model and methods

As mentioned, our primary goal is to compare the universal physics of the two models of disorder which generate chaotic and diffusive dynamics of a single particle in confined geometries. The most commonly studied confined systems use a parabolic trap. We thus consider a system of N classical particles in a confining potential. These particles interact with Coulomb repulsion and are restricted in a two-dimensional (2D) xy-plane. We neglect screening in our small finite clusters [48]. The Hamiltonian for a circular confinement can be given by,

$$H = \sum_{i,j=1}^{N} \frac{1}{|r_i - r_j|} + \sum_{i} V_{Cr}(r_i), \quad (1)$$

where,

$$V_{Cr}(r) = r^2, \quad (2)$$

Here, $r_i = |r_i| = \sqrt{x_i^2 + y_i^2}$ is the distance of i-th particle from the center of the confinement. The first term describes the Coulomb repulsion of particles. The second term represents the confinement potential. In writing the Hamiltonian in Eq. (1), we used a rescaled position variables $\tilde{r}$, in accordance with Refs. [25,49].

In order to represent a “clean” and regular system in 2D, we choose the $V_{Cr}(r)$, in which the classical motion of a single particle is integrable. [25] The “cleanliness” of the regular circular potential is best understood when we compare our results with those for disordered traps.

As the first example of disordered system, we introduced “pinning” in the aforementioned $V_{Cr}(r)$. Pinning is introduced by adding a fraction ($n_{imp}$) of N constituent particles in the system at random location within this trap. Disorder averaging [50] is performed by taking 12 independent realizations of impurity configurations for each $n_{imp}$. Such a pinning disordered system is expected to show a universal features of diffusive dynamics of particles in the trap. Note that here $n_{imp}$ controls the strength of disorder.

On the other hand, for the study of chaotic and ballistic motion in a trap, we require a disorder realization which shows a nearly fully chaotic motion [51] of a single particle in it, where all spatial symmetries are broken, and still confined by a soft potential akin to experiments with electrostatic trapping. Therefore, we considered the following model of irregular trap as a disordered system.

$$V_{Ir}(r) = a \left[ \frac{x^4}{b} + by^4 - 2\lambda x^2 y^2 + \gamma(x-y)xyr \right]. \quad (3)$$

$V_{Ir}(r)$ breaks all spatial symmetries and is also generates ballistic and chaotic motion of a single particle [48,51].

In order to appreciate the units of our scaled variables (length, energy, and time), in terms of standard units, we consider the example of an electron in a GaAs heterostructure with typical confinement energy of $\hbar \omega = 1 \text{ meV}$, for which our units become: $r' = 630 \text{ Å}$, $E' = 1.7 \text{ meV}$ and $t' = 376 \text{ fs}$ [52].

Together with the lack of spatial symmetries, the chaotic motion of the single particle is taken to be a signature of disorder in the irregular trap. This system is characterized by four parameters $a$, $b$, $\lambda$, and $\gamma$ [53], which could be tuned to adjust the disorder strength. The overall multiplicative factor $a (> 0)$ controls the average density of particles in the system without effecting the trajectory of a single particle in the confinement. Trajectory of a single particle in the irregular trap extends over the whole system, and hence they cannot be considered as a strongly disordered, like in the case of our pinned circular trap where a large “strength” of disorder, i.e., $n_{imp}$, can even localize the motion of a particle. For the purpose of a fair comparison, we considered $n_{imp} \leq 0.1$. The values of other parameters used are $b = \pi/4$, $\lambda = [0.565, 0.635]$ and $\gamma = [0.10, 0.20]$ [54]. We generate up to 7 independent realizations of the irregular confinement. In order to explore the universal features of disordered systems, we aim to compare the role of the diffusive dynamics in the pinned system versus the chaotic and ballistic motion of Coulomb par-
particles in the irregular trap. In a confined geometry at \( T = 0 \), the ground state will be the one that is consistent with the symmetry (or the lack of it) of the underlying trap. Upon increasing \( T \), the constituent particles of the Coulomb cluster execute random excursions from their equilibrium position, and beyond a threshold temperature, \( T_c \), the crystal “melts”.\(^1\) Such melting in the bulk systems are tuned by the dimensionless parameter \( \Gamma = \sqrt{\pi} \cdot T / \pi \) [55]. For our comparative study of clean and disordered traps, we induce melting by tuning \( T \) alone, and we consider systems which are composed of the same total number of particles \( N \), and have the same density \( n \) of particles. When we increase (or decrease) the total particle number \( N \), we simultaneously relax (or squeeze) the soft confining potential, such that the traps become shallower (or narrower). This allows us to keep the density of particles same for all cases of our study.

To study the physical observables, we carried out classical molecular dynamics (MD) [56] with \( N = 150 \) particles (plus pinned particles for the system with impurities). Note that in our study, we kept the number of degrees of freedom (i.e., the mobile particles) the same while comparing the two models of disorder. Thus, our pinned circular system has \( n_{\text{imp}} \times N \) number of extra particles compared to our irregular trap. We performed MD runs for up to \( 10^7 \) MD steps with a time step size of \( \delta t = 0.005 \) in our dimensionless unit. Solidity in a clean 2D system in the thermodynamic limit is associated with long-range orientational order and quasi long-range positional order [57]. In what follows, we explore the pair correlation function and 6-fold BOO in order to gain insight into the thermal melting of Coulomb clusters in traps.

### 3 Static properties

#### 3.1 Bond orientational order

The Bond orientational order (BOO) of a system, a crucial characterization of a system of classical particles in 2D undergoing melting, is defined for a crystal having 6-fold symmetry (e.g., a triangular lattice) as [58],

\[
\psi_b(r_k) = \frac{1}{N_b} \sum_{l=1}^{N_b} \exp(i \theta_{kl}).
\]

Here, the angle \( \theta_{kl} \) is the bond angle between the particle \( k \) and with its nearest neighbors \( l \) about an arbitrary (but fixed for all nearest neighbors) axis. We identify the nearest neighbors of particles using the Voronoi construction [59]. For the purpose of a fair comparison, we wish to find \( n_{\text{imp}} \) that typifies the strength of disorder in aforementioned system. This is implemented by studying the distribution of \( |\psi_b| \) from the pinned circular trap with different \( n_{\text{imp}} \)'s and then identifying the one that produces a \( P(|\psi_b|) \) closest to the one generated from the \( V_{\text{IR}}(r) \) for the same number of particles participating in the dynamics at the same \( T \).

![Fig. 1](image)

**Fig. 1** a The distribution \( P(|\psi_b|) \) at \( T = 0.002 \) is shown by color traces for different \( n_{\text{imp}} \). The dotted line represents the \( P(|\psi_b|) \) for irregular confinement at the same \( T \). Evidently, the dotted line matches best with the results in pinned system for \( n_{\text{imp}} = 0.02 \). b The thermal evaluation of \( P(|\psi_b|) \) in both the pinned circular system \( (n_{\text{imp}} = 0.02, \) solid lines) and irregular (dotted lines) indicates that the \( T \)-dependence of \( P(|\psi_b|) \) is nearly identical.

Subsequently, we study the effect of \( T \) on \( P(|\psi_b|) \) for \( n_{\text{imp}} = 0.02 \) in Fig. 1b. Our results demonstrate that the temperature evolution of \( P(|\psi_b|) \) in the range \( T = 0.002-0.05 \) for the pinned and irregular confinements is nearly identical. Note that the increase of \( n_{\text{imp}} \) weakens BOO in a system, trapping particles into an arrested state [47]. In contrast, thermal evolution drives a solid into a liquid-like phase.

In the limit \( T \to 0 \), a perfect triangular lattice in the bulk system yields \( P(|\psi_b|) = \delta \)-function at \( \psi_b = 1 \). A confined system develops a tail in \( P(|\psi_b|) \) for \( |\psi_b| \leq 1 \) even at \( T = 0 \), [60,61] but the strong peak at \( \psi_b = 1 \) persists. \( P(|\psi_b|) \) changes from a sharply peaked distribution at low \( T \) to a broad, and nearly symmetric distribution for a high \( T \) melted state in confinements [48]. Thus, we conclude that the diffusive versus chaotic-ballistic dynamics of single particles in the respective traps have little effect on the thermal evolution of the

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\(^1\) A bulk system shows diverging susceptibility at a transition which turns into a broad peak at \( T_X \) at the thermal crossover in finite systems.
3.1.1 Orientational susceptibility

While the $T$-dependence of $P(\langle |\psi_0| \rangle)$ depicts the thermal crossover from a solid-like phase to a liquid-like phase at a quantitative level, it is the study of orientational susceptibility which estimates the crossover temperature scale $T_X$ which we discuss in the following. The orientational susceptibility $\chi_6$ is defined as,

$$\chi_6 = N[\langle |\psi_0|^2 \rangle - \langle |\psi_0|^2 \rangle].$$  \hspace{1cm} (5)

Here, the angular brackets $\langle \cdots \rangle$ imply average over all particles, as well as over MD configurations at a given $T$.

The temperature dependence of $\chi_6$ for pinned and irregular traps is shown in Fig. 2. The broad hump in $\chi_6(T)$ centered around $T_X \approx 0.02$ is discernible in both the traces. Though both the models of disorder share same $T_X$, as expected, and more or less a similar thermal evolution, the pinned system shows a sharper peak in $\chi_6$, as evident from Fig. 2. Note that the actual values of $\chi_6$ are different in the two different models of disorders, though the location of the hump at $T_X$ is very similar. This emphasizes our earlier conclusion that the diffusive versus chaotic-ballistic dynamics of particles in the respective traps has a minor role on the melting of Coulomb-interacting particles in these confinements. While the $T_C$ in a 2D-bulk system [55] depends only on the average density, it is interesting to note here that such a finding holds for finite and inhomogeneous system, irrespective of the nature of disorder.

Having studied the thermal evolution of the orientational ordering on different traps, we next proceed to explore the positional order in these systems.

3.2 Pair correlation function

Positional order in a system is tracked by the pair correlation function $g(r)$, which yields the probability of finding a particle at a distance $r$ on an average, from a reference particle, and is defined as [63]

$$g(r) = \frac{1}{2\pi r N} \sum_{i=1}^{N} \sum_{j \neq i=1}^{N} \langle \delta(r - |\vec{r}_i - \vec{r}_j|) \rangle.$$  \hspace{1cm} (6)

In Fig. 3a–d, we demonstrate the dependence of $g(r)$ at low $T$ for $n_{\text{imp}} = 0.02, 0.033, 0.06$ and $0.10$ respectively using solid lines. The distances are rescaled by the average distance between particles in the system, $r_0$ (see Fig. 3).

The dashed line represents $g(r)$ calculated for $V_{Ir}(r)$. The long-range nature of the decaying envelope of oscillations in $g(r)$ measures the positional order in the systems. With the increase of $n_{\text{imp}}$, such oscillation becomes progressively damped, yet, it is evident that the pinned system displays a robust positional order compared to the irregular system. It is also interesting to note that unlike for the case of $P(\langle |\psi_0| \rangle)$, the nature of $g(r)$ in the system with pinning disorder does not find a reasonable match with that for $V_{Ir}(r)$ in the entire range of $n_{\text{imp}} \in [0.02-0.10]$. Thus, the diffusive versus chaotic-ballistic motion of single particles in the respective traps indeed differ in displaying positional order. In the following, we proceed to comprehend the origin of this difference.

In pinned system, the symmetry of a six-coordinated neighborhood (just the existence, and not the quantitative measure) gets disturbed only in a small local region around the pinning centers, leaving out the configuration of other particles largely unaltered elsewhere in a circular trap. On the other hand, the spatial undulations of $V_{Ir}(r)$ persist over the entire region of the trap, which causes distortions of the lattice lines everywhere in the system of the underlying triangular lattice. As a result, positional order weakens without disturbing the
orientational order in $V_{t}(r)$. To illustrate this further, we present the distribution of the nearest neighbor’s distances in the two confinements in Fig. 4 which supports the aforementioned argument in the following manner. Figure 4 presents the distribution of the nearest neighbor distances in the pinned system ($n_{\text{imp}} = 0.02$) and for irregular trap at $T = 0.002$. The nearest neighbors of a particle are identified using Voronoi construction [59]. The distribution makes it evident that the nearest neighbor distances occur over a wider range of values in $V_{t}(r)$, which washes out the periodic oscillations in $g(r)$ and thus weakens the positional order, compared to the pinned circular trap.

Having established the weaker dependence of positional order on $n_{\text{imp}}$, at least in the range of $n_{\text{imp}}$ studied, we proceed to explore the thermal evolution of $g(r)$ which is shown in Fig. 5. With increasing $T$, the initial peaks and the oscillations of $g(r)$ start fading away from its tail.

The irregular system (dashed line) shows only a strong first peak followed by a few feeble humps in the $g(r)$, indicating depleted positional order even at the lowest $T$—a characteristic of a liquid-like state [49]. Upon increasing $T$, the height of the initial peaks decreases, and all higher-order modulations disappear beyond $T > 0.020$. Note that in our study, $g(r)$ vanishes for large $r$, e.g., for $r \geq 10$, reflecting the finite size of our system. This is unlike the bulk system for which $g(r \rightarrow \infty) = 1$ [64].

While $g(r)$ evolves smoothly with $T$, and does not signal a sharp thermal crossover, we propose to estimate $T_X$ for our confined systems from $g(r)$ using the following procedure.

First, we amplify the effect of the modulations of $g(r)$ by eliminating the smoothly falling part of it. This resolves its oscillatory part and also allows it to saturate to the unit value at large $r$ like in bulk system, as shown in Fig. 6. Finally, the solid to liquid crossover is quantified by the total area $A_g$ under the modulating part of $g(r)$. As expected, the solid will have a larger $A_g$ form stronger and long-range oscillations, and $A_g$ must decrease with increasing $T$. The inset of Fig. 6 shows that the nature of the fall of $A_g(T)$ has two near-linear branches, and we identify $T_X$ where the change of the slope takes place. Analyzing our data, we obtain $T_X \approx 0.0195$. This is consistent with the previously estimated $T_X = 0.019 \pm 0.002$ [53] from orientational susceptibility in an irregular trap. This is interesting to note that even though the pinned system has a more robust positional order, the estimate of $T_X$ remains insensitive.

Having performed the comparative analysis between the thermal crossover between a solid-like to a liquid-like state in different confinements, we conclude that the nature of the disorder and hence the underlying single particle dynamics has no significant role on the universal physics of disorder on ‘melting’, though differences exist in the details. Next, we turn to analyze dynamical characteristics associated with melting of Coulomb clusters in these confinements.

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Footnote 2 continued

oscillatory falling part of $g(r)$ with the obtained averaged curve.

Footnote 3 continued

Note that the area under $g(r)$ calculates the coordination number of the particles, and its deviation from the value in a crystal signals the thermal crossover.

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Fig. 4 The distribution of the nearest neighboring distances of pinned circular (pink) and irregular (blue) traps illustrate that the such distances are more inhomogeneous in irregular trap and thereby weaken the positional order more easily compared to that in pinned system, as found in Fig. 3a.
show two nearly linear branches for small- and large-$T$. The magnitude of the total area $A_n$ under each trace (disregarding their sign) decreases with $T$. The decrease of $A_n$ with $T$ is shown in the inset, which show two nearly linear branches for small- and large-$T$. The change of slope occurs at $T_X \approx 0.02$

4 Dynamic properties

In an earlier study [53], it was shown that the Coulomb particles in irregular confinements generate intriguing motional signatures akin to glassy dynamics. Here we carry out studies of the time evolution of particles in the pinned circular trap to investigate if and how the nature of disorder affects the temporal properties.

4.1 Mean square displacement

We discuss below our results by considering dynamical mean squared displacement (dMSD), which is a measure of the deviation of the position of a particle with respect to a reference position over time $t$:  

$$\langle \Delta r^2(t) \rangle = \frac{1}{N} \sum_{i=1}^{N} \langle (\vec{r}_i(t) - \vec{r}_i(0))^2 \rangle. \quad (7)$$

We present in Fig. 7 the trace of $\langle \Delta r^2(t) \rangle$ at low $T$ in solid-like phase ($T = 0.006$) for $n_{imp} = 0.02, 0.033, 0.06$ and 0.10. The trace of $\langle \Delta r^2(t) \rangle$ obtained for $V_E(r)$ is also shown by the dashed line for reference. For a very short time, the particles exhibit ballistic motion until they move appreciably to sense the presence of other particles. At large times, the particles show diffusive motion for all $n_{imp}$. Between these two temporal regimes, the dMSD shows plateaus, and the plateau becomes well resolved and wider with increasing $n_{imp}$.

The result from the irregular confinement has a similarity with the pinned systems for smaller $n_{imp}$. These plateaus originate from the ‘caging effects’ [65–67] in which at low $T$, most of the particles remain localized for a long time in the cage formed by the repulsive neighbors.

The cage breaking occurs sporadically, giving rise to dynamic heterogeneity and glassiness [53]. It is evident from Fig. 7 that with the increase of $n_{imp}$, the relaxation gets progressively slower in pinned system compared to that in irregular confinements. This is expected because the pinned particles prohibit cooperative rearrangements [47], and thereby increasing the relaxation time. The localized nature of the particles with pinning disorder is also evident from the fact that the particles diffuse up to a smaller distances at large times with increasing $n_{imp}$, as seen from Fig. 7.

4.2 Van Hove correlation function

The most convenient way to explore the spatio-temporal evolution of a system is the study of the self part of the van Hove correlation function [63,68], defined as  

$$G_s(r,t) = \langle \frac{1}{N} \sum_{i=1}^{N} \delta (\vec{r} - (\vec{r}_i(t) - \vec{r}_i(0))) \rangle. \quad (8)$$

Physically, $G_s(r,t)$ gives the probability that a particle has moved by a distance $r$ in time $t$, on an average. Our results for $G_s(r,t)$ for low temperature ($T = 0.006$) are presented in Fig. 8, where panels (a–d) describe results for $n_{imp} = 0.02, 0.033, 0.06$ and 0.10. The results for $G_s(r,t)$ on the irregular trap is also shown in panel (e) for comparison.

As noted earlier [49], $G_s(r,t)$ data can be broadly classified into three temporal regions—a small $t$ where $G_s(r)$ is Gaussian, an intermediate temporal region where $G_s(r)$ shows no appreciable change as a function of $t$, and a third, where $G_s(r)$ features multiple peaks. Does a pinned trap show similar qualitative behavior? Our results in Fig. 8a–d for random pinned system are qualitatively similar to above findings; however, the
represents the results from irregular trap. The behavior of \( t \) is similar to dMSD results in Fig. 7. For each \( n \) irregular trap are comparable only to the weak motion in microscopic nature of disorder, e.g., ballistic yet chaotic.

Panel (e) shows non-Gaussian behavior for large \( r \), which is consistent with the Poincaré section shown in Fig. 9a where we analyze the trajectory of a single particle with pinning disorder in \( V_{\text{fr}}(r) \). While \( V_{\text{fr}}(r) \) is a homogeneous function, the intersection coordinates \((x, p_x)\) are considered to sample the Poincaré section. After a large number of intersections with the given plane, the resulting structure of the Poincaré section allows us to understand the nature of the trajectory of the particle under consideration. For chaotic motion, Poincaré section consists of a two-dimensional region with randomly scattered points.

In the following, we proceed to report our results of Poincaré section analysis of the dynamics of single and two particles in our disordered confinements.

5 Poincaré section analysis

As discussed already, the nature of motion a single particle in disordered traps could differ depending on the microscopic nature of disorder, e.g., ballistic yet chaotic motion in \( V_{\text{fr}}(r) \), while diffusive \([41]\) in \( V_{\text{Cr}}(r) \) with pinning centers. It is interesting to ask how the nature of the dynamics of a single particle in a disordered environment gets affected in the presence of other interacting particles? Can the presence of interaction among the particles make the motional signatures broadly equivalent in two differently disordered environments? In the subsequent sections, we address these questions by analyzing the structure of the phase space for a single particle in the two confinements. We also study the phase space structure of one particle in the presence of another Coulomb interacting particle in the above two cases. To understand the phase space structure for different cases, we focus on analyzing the Poincaré section \([69, 70]\) of the trajectory of a particle obtained by integrating the Hamilton equation of motion for a given initial condition. Each time the trajectory crosses a given plane, in our case, \( y = 0 \) plane, with positive momentum \( p_y \), the intersection coordinates \((x, p_x)\) are considered to sample the Poincaré section. After a large number of intersections with the given plane, the resulting structure of the Poincaré section allows us to understand the nature of the trajectory of the particle under consideration. For chaotic motion, Poincaré section consists of a two-dimensional region \([51, 69, 70]\) with randomly scattered points.

In the following, we proceed to report our results of Poincaré section analysis of the dynamics of single and two particles in our disordered confinements.

5.1 Poincaré section analysis for single-particle

First, we study the motion of a single particle in the irregular trap. Since \( V_{\text{fr}}(r) \) is a homogeneous function, we can scale the associated Hamiltonian, and thus study a single energy surface is sufficient to explore the dynamical features of the single particle in the system. Hence the only case of unit energy of the test particle \((E = 1)\) is investigated. Previous studies had shown that for \( \lambda \in [0.565, 0.635] \) and \( \gamma \in [0.10, 0.20] \), the dynamics of a single particle is chaotic \([51, 54]\), which is consistent with the Poincaré section shown in Fig. 9a where we analyze the trajectory of a single particle in \( V_{\text{fr}}(r) \) for \( \lambda = 0.635 \) and \( \gamma = 0.1 \). As we see from Fig. 9a, the Poincaré section consists of a two-dimensional region nearly uniformly filled with randomly placed points (different colors represent points obtained for different initial conditions); a typical signature of a chaotic motion.

Next, we study the Poincaré section for a single particle with pinning disorder in \( V_{\text{Cr}}(r) \). While \( V_{\text{Cr}}(r) \) is a homogeneous function, the presence of the Coulomb interaction between the test particle and the pinning centers breaks the homogeneity condition for the total Hamiltonian. As a result, the motional signature depends on the value of the total energy of the system. Thus, for the pinned system (with the number of pinning centers denoted as \( n_{\text{pin}} \)), we consider Poincaré section for different energy surfaces. We carried out the Poincaré section analysis only for systems with one or two mobile particles, with \( n_{\text{pin}} \), number of pinning particles frozen in the system.\(^4\) Note that the dynamics of a single particle in \( V_{\text{Cr}}(r) \) \((n_{\text{pin}} = 0)\) is periodic at any

\(^4\) With such small numbers of mobile particles, the notation \( n_{\text{imp}} \) loses its relevance.
value of $E$. For $E = 10$, we analyze the Poincaré section with $n_{\text{pin}} = 1, 10,$ and 15 in Fig. 9b–d. For $n_{\text{pin}} = 1$, Poincaré section consists of closed orbits implying regularity of the dynamics of the particle (see Fig. 9b). With increasing $n_{\text{pin}}$ such closed orbits start to deform, and for $n_{\text{pin}} = 10$, we find that the most parts of the Poincaré section get filled up uniformly with some elliptical orbits as shown in Fig. 9c. Such smooth curves (Kolmogorov–Arnold–Moser (KAM) tori [71]) in the Poincaré section correspond to regular, quasi-periodic motion while the clouds correspond to chaotic motion [69,70]. Thus, for $n_{\text{pin}} = 10$, the system exhibits mixture of chaos and order. With increasing $n_{\text{pin}}$, the proportion of phase space occupied by such regular regions diminishes continually, and for $n_{\text{pin}} = 15$, the Poincaré section gets filled up almost uniformly representing a fully chaotic dynamics of the particle for all initial conditions (see Fig. 9d). We have not noticed any invariant tori within our numerical accuracy for $n_{\text{pin}} = 15$. Thus, for a fixed $E (= 10)$, we find that the nature of the dynamics depends on the number of pinned particles in the system. Next, we analyze the effect of $E$ on the nature of the dynamics for fixed $n_{\text{pin}}$. The Poincaré section for $n_{\text{pin}} = 15$ with $E = 5.7$ is shown in Fig. 10a. It consists of elliptic and hyperbolic orbits indicating regular, quasi-periodic motion of the particle at this energy level. A generic feature of quasi-periodic dynamics is the appearance of hyperbolic and elliptic points in the Poincaré section. Interestingly, when the energy is further increased by a significant amount, here $E = 120$ (Fig. 10c), the Poincaré section gets divided into small islands along with a large chaotic sea. Therefore, the classical motion of the particle in circular confinement

with $n_{\text{pin}} = 15$ remains chaotic in nature for a certain range of energy. Beyond this energy range, it goes into a mixed state. We also analyze the Poincaré section with $n_{\text{pin}} = 100$ for $E = 5.7, 18.9$, and 120. Similar to the circular system with $n_{\text{pin}} = 15$, $n_{\text{pin}} = 100$ system also passes from regular to chaotic and chaotic to mixed with an increase in energy (see Fig. 10d–f). Thus, we find that while the nature of the dynamics of a single particle depends on the details of the disorder, there exists a broad parameter regime where a single particle exhibits qualitatively similar motional signatures in an irregular confinement and a circular confinement with pinned particles. How does structure of the Poincaré section get altered in the presence of inter-particle interaction? To address this question, we next study the Poincaré section for the irregular and pinned system with two Coulomb-interacting particles.

5.2 Poincaré section analysis for two-particle system

To understand the effect of interaction on the dynamics of the particles, we first analyze the Poincaré section resulting from the dynamics of two Coulomb-interacting particles in the irregular confinement. To obtain the Poincaré section, we focus on the trajectory of any one particle and follow the same procedure as we did for a single particle. The Poincaré section associated with the system of two Coulomb-interacting par-
Fig. 11 The Poincaré section for motion of 2 particles. Panels (a–c) shows results for an irregular confinement with $E = 1.5, 9$ and 100. Panel (d–f) represents the Poincaré plane for circular trap with $n_{\text{pin}} = 1$ and for $E = 16.3, 30$ and 100 respectively. The 2-Coulomb particles in the $V_{\text{Ir}} (r)$ continues its chaotic motion independent of $E$. In comparison, the 2 particles in pinned system lifts the higher threshold energy to exhibit chaotic motion.

Interestingly, at low energy ($E = 16.3$) where Coulomb interaction dominates the kinetic energy, the presence of pinned particle, which interacts strongly with the two other particles, divides the Poincaré section into two disjoint parts as shown in Fig. 11d. With increasing energy particles start to overcome the Coulomb energy barrier, and at sufficiently high energy we get a uniformly filled Poincaré section representing chaotic dynamics as shown in Fig. 11e–f.

6 Conclusion

While there are universal features of disorder associated with the thermal crossover of a confined Coulomb crystal, the details of disorder bring in notable differences in observables typically accessed in experiments. We demonstrated this for systems with Coulomb-interacting particles in environments which generate qualitatively different single-particle dynamics, e.g., chaotic ballistic versus diffusive motion. Analysis of the static properties shows that while the two systems possess different spatial ordering, the thermal crossover temperature $T_X$ remains the same. This is established from the study of orientational susceptibility and thermal evolution of area under the modulations of normalized pair correlation function—a novel quantity capturing the thermal crossover in finite systems. While the description of a uniform bulk system suggests that the phase transition temperature depends only on the average density of the constituent particles, it is interesting to note that such a conclusion also applies to finite and inhomogeneous systems, irrespective of the nature of the disorder. Analysis of the dynamical properties, such as mean square displacement and Van Hove correlation function, depicts the presence of glassiness in both disordered systems. A careful analysis of the Poincaré section under different conditions reveals the subtleties of the nature of the dynamics in two types of disordered systems. The microscopic origin of disorder varies depending on materials and an experimental setup, and the two types of disorders addressed in our study are relevant for understanding, for example, the thermal properties of quantum dots, melting of electronic crystals on Helium bubble, ion traps, and dusty plasma, among others. Our study will guide such experiments in identifying the quantitative effects of the underlying disorder. Extending the scope of our research to encompass the consequences of quantum fluctuations will be a fascinating and worthwhile endeavor.

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Author contributions

JP: Implemented the project, analyzed the results and developed numerical codes specific to the project. BA: Contributed in code developments of the numerical formalism and helped in analyzing results. AG: Conceived the problem, planned the methodology and supervised the project. All authors contributed in writing and refining the manuscript.

Data Availability Statement
This manuscript has no associated data or the data will not be deposited. [Author’s comment: This is a theoretical study and there are no experimental data. The datasets generated during the study are displayed as figures, and can be made available upon request.]

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