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Coulomb crystallites from harmonically confined charged bosons in two dimensions

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Abstract

We exploit rotational-symmetry breaking in the one-body density to examine the formation of structures in systems of N strongly coupled charged bosons with logarithmic repulsions inside isotropic two-dimensional harmonic traps, with N in the range from 2 to 7. The results serve as a map for ordered arrangements of vortices in a trapped Bose–Einstein condensate. Two types of N-body wavefunctions are assumed: (i) a permanent $|\psi_{\rm WM}\rangle$ of N identical Gaussian orbitals centred at variationally determined sites, and (ii) a permanent $|\psi_{\rm SM}\rangle$ of N orthogonal orbitals built from harmonic-oscillator energy eigenstates. With increasing coupling strength, the bosons in the $|\psi_{\rm WM}\rangle$ orbitals localize into polygonal-ringlike crystalline patterns ('Wigner molecules'), whereas the wavefunctions $|\psi_{\rm SM}\rangle$ describe low energy excited states containing delocalized bosons as in supersolid crystallites ('supermolecules'). For $N = 2$ at strong coupling both states describe a Wigner dimer.

1. Introduction

Interest in a two-dimensional (2D) fluid of charged bosons was greatly stimulated by the work of Nelson and Seung [1], who showed that a fluid of flux lines in strongly type-II superconducting materials can be mapped onto this model system in statistical mechanics. The interaction potential law is given by $V(r) = V\ K_0(r/r_0)$, with V a coupling-strength parameter and $K_0(x)$ the modified Bessel function behaving as $-\ln(x)$ at short distances. Following an early variational Monte Carlo study [2], the transition between an Abrikosov lattice and a homogeneous liquid of vortices was studied within this mapping by means of the dislocation mechanism of melting [3] and the density functional theory of freezing [4]. A first-order transition from an Abrikosov lattice to a bosonic superfluid of entangled vortices has also been demonstrated by the path-integral Monte Carlo method [5]. A triangular Abrikosov lattice is, of course, equivalent to the Wigner lattice for a 2D Coulomb system.

More recently, vortices have been created and extensively studied by a variety of experimental techniques [6, 7] in atomic Bose–Einstein condensates confined inside harmonic traps. A vortex created at the centre of a stationary trap corresponds to a maximum of the energy functional and will tend to spiral out of the trap in a finite time [8], but the vortex state can be stabilized by setting the trap into rotation. Upon stirring the condensate at increasing frequency first one vortex and then several vortices are observed to enter the condensate, and such vortex assemblies ultimately form an ordered pattern. These arrangements of vortex lines closely resemble a triangular crystallite almost up to the condensate boundary, even though the gas is subject to the external trapping potential and is therefore inhomogeneous.

In the present work we report theoretical calculations of the structures taken by such arrangements of a small number of vortices. It has been amply demonstrated, by work both on strongly interacting electrons in 2D semiconductor quantum dots [9] and on strongly coupled bosons interacting by either a contact potential or the e^2/r Coulomb law inside 2D harmonic traps [10], that information on the structure of few-particle crystallites can be obtained directly from the one-body density by means of calculations based on the unrestricted Hartree–Fock method, which breaks the rotational symmetry imposed by circular confinement. More generally, an approximate

treatment of a strongly correlated many-body system can in principle lead to states with spontaneously broken rotational symmetry, as discussed for instance by Ring and Schuck [11] and by Reimann and Manninen [12].

In this work we use this very simple theoretical method to evaluate the structure of small crystallites of vortex lines within the Nelson–Seung mapping, by means of self-consistent variational calculations on harmonically trapped bosons with logarithmic interactions using a permanent wavefunction approximation. We consider, in fact, two different types of variational wavefunctions. Whereas the first yields structures that are well known in the literature as 'Wigner molecules', in which the particles are localized within polygonal-ringlike arrangements acting as nuclei for a Wigner crystal, the second type of wavefunction allows for delocalization of the bosons and yields what may be called a 'supermolecule' as the seed for a supersolid. A supersolid [13] is a quantum crystal that exhibits a non-classical moment of inertia, i.e. a type of superfluid response. Interest in this predicted state of quantum matter has been recently revived by reports on the observation of superflow in solid helium inside Vycor [14].

The contents of the paper are briefly described as follows. In section 2 we introduce the model Hamiltonian and the essential formalism for its solution within a self-consistent variational approximation, leading to numerical calculations of vortex structures that are presented and discussed in section 3. Finally, in section 4 we summarize our main conclusions. We refer at this point to recent calculations on the structure and spectrum of classical 2D clusters with a logarithmic interaction potential [15] and on ordered structures formed in rotating ultracold Bose gases [16], as an introduction to a broader view of the field.

2. Formalism

We consider a 2D system of N bosons described by the Hamiltonian

$$\hat{H} = \int \mathrm{d}\boldsymbol{r}\, \psi^\dagger(\boldsymbol{r})\hat{H}_0\psi(\boldsymbol{r}) + \tfrac{1}{2}\int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'\, \psi^\dagger(\boldsymbol{r})\psi^\dagger(\boldsymbol{r}') \times V(|\boldsymbol{r}-\boldsymbol{r}'|)\psi(\boldsymbol{r}')\psi(\boldsymbol{r}) \tag{1}$$

where $\psi(\boldsymbol{r})$ and $\psi^\dagger(\boldsymbol{r})$ are the field operators, $\hat{H}_0 = p^2/(2m) + m\omega^2 r^2/2$ is the single-particle Hamiltonian with m the particle mass, ω is the trap frequency and $V(r)$ is the interparticle repulsive potential taken as the solution of the 2D Poisson equation, $V(r) = -V\ln(r/r_0)$, involving a coupling-strength parameter V and an irrelevant length r_0. In our variational formulation we consider the N-body wavefunction $|\psi\rangle$ that is taken as the totally symmetric product, i.e. the permanent

$$\psi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N) = \frac{1}{N!}\sum_{p=1}^{N!}\phi_{p(1)}(\boldsymbol{r}_1)\phi_{p(2)}(\boldsymbol{r}_2)\ldots\phi_{p(N)}(\boldsymbol{r}_N) \tag{2}$$

where $\phi_i(\boldsymbol{r})$ are single-particle orbitals and the sum runs over all permutations p of indices 1 to N. The energy can be thus written as

$$\begin{aligned} E &= \langle\psi|\hat{H}|\psi\rangle/\langle\psi|\psi\rangle \\ &= \frac{1}{N!}\sum_{p_1,p_2=1}^{N!}\left[\binom{N}{1}H_{0,p1(1)p2(1)}\prod_{i=2}^{N}S_{p1(i)p2(i)} \right. \\ &\quad \left. + \binom{N}{2}V_{p1(1)p1(2)p2(1)p2(2)}\prod_{i=3}^{N}S_{p1(i)p2(i)}\right] \\ &\quad \times\left[\sum_{p_1=1}^{N!}\prod_{i=1}^{N}S_{p1(i)i}\right]^{-1} \end{aligned} \tag{3}$$

where the matrix elements are given by

$$\begin{aligned} H_{0,ii} &= \int \mathrm{d}\boldsymbol{r}\,\phi_i^*(\boldsymbol{r})\hat{H}_0\,\phi_i(\boldsymbol{r}) \\ V_{ijkl} &= \int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'\,\phi_i^*(\boldsymbol{r})\phi_j^*(\boldsymbol{r}')V(|\boldsymbol{r}-\boldsymbol{r}'|)\phi_k(\boldsymbol{r}')\phi_l(\boldsymbol{r}), \end{aligned} \tag{4}$$

and the overlap matrix reads

$$S_{ij} = \int \mathrm{d}\boldsymbol{r}\,\phi_i(\boldsymbol{r})^*\phi_j(\boldsymbol{r}). \tag{5}$$

The energy E in (3) is written to within an irrelevant additive constant and will be given below in units of $\hbar\omega$. Scaling of distances by the harmonic-oscillator length $\ell_0 = \sqrt{\hbar/(m\omega)}$ will also be used.

We introduce at this point two different types of N-body wavefunctions according to the choice of the single-particle orbitals $\phi_i(\boldsymbol{r})$.

2.1. Wigner molecules

The state $|\psi_{\mathrm{WM}}\rangle$ is written as a permanent one of N Gaussian orbitals having the same width σ and centred at positions $\boldsymbol{a}_i$:

$$\phi_i(\boldsymbol{r}) = \frac{1}{\sqrt{\pi}\sigma}\exp\left[-(\boldsymbol{r}-\boldsymbol{a}_i)^2/(2\sigma^2)\right]. \tag{6}$$

The parameters σ and $\boldsymbol{a}_i$ will be determined by minimizing the total energy E for fixed number of particles and allowing the orbitals to overlap. In the limit $V = 0$ we find $\boldsymbol{a}_i = 0$ for all i, i.e. we recover a condensate state $|\psi_{\mathrm{BEC}}\rangle$ in which the N bosons occupy the same Gaussian orbital and create a density peak at the centre of the trap [17].

In our calculations we find that this type of N-particle wavefunction is the lowest-energy state for the N-boson system, owing to the optimization of the overlap between the various orbitals as their peaks move away from the trap centre with increasing repulsive coupling. In fact, the contributions to the total energy coming from the inter-orbital overlaps rapidly decrease as the coupling increases, and become negligible for $V > 4\hbar\omega$, for example. The intra-orbital overlap still continues to decrease through a slow broadening of the single-particle density associated with each Gaussian peak. As we shall see, this leads to a decrease of the total energy E with increasing V at strong coupling.

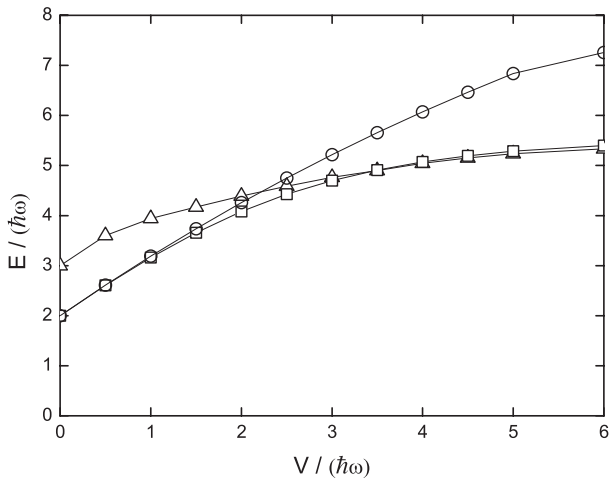

Figure 1. Total energy E (in units of $\hbar\omega$) as a function of $V/(\hbar\omega)$ for $N = 2$ bosons interacting via a logarithmic potential law inside an isotropic two-dimensional harmonic well, as calculated by the unrestricted Bose–Hartree–Fock approximation for the states $|\psi_{\rm BEC}\rangle$ (circles), and $|\psi_{\rm SM}\rangle$ (triangles) and the Gaussian approximation for $|\psi_{\rm WM}\rangle$ (squares).

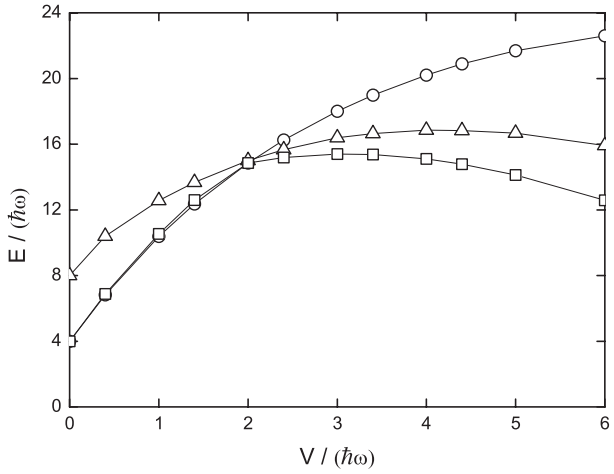

Figure 2. Same as in figure 1, but for $N = 4$ bosons.

2.2. Supermolecules

The state $|\psi_{\rm SM}\rangle$ is built as a permanent of N orthogonal orbitals, which corresponds to the unrestricted Bose–Hartree–Fock (UBHF) approximation for the N-body wavefunction [18]. In this case, the energy equation (3) reduces to

$$E = \sum_i n_i\, H_{0,ii} + \tfrac{1}{2}\sum_{i,j} n_i n_j (V_{ijij} + V_{ijji}) - \tfrac{1}{2}\sum_i n_i(n_i+1)V_{iiii} \tag{7}$$

where n_i are the orbital occupation numbers.

In our calculations we take $n_i = 1$ for the N orbitals of lowest energy and express the single-particle orbitals through expansions in an orthonormal basis $\{\varphi_n\}$ provided by the

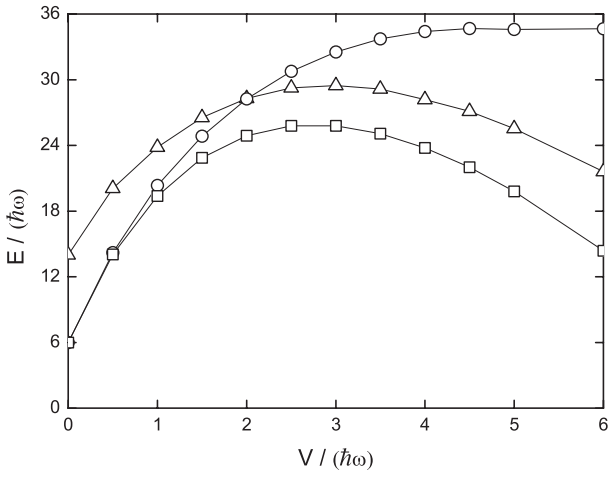

Figure 3. Same as in figure 1, but for $N = 6$ bosons. The energy difference between the (0, 6) and (1, 5) configurations in states of the $|\psi_{\rm WM}\rangle$ type cannot be seen on this energy scale.

eigenstates of the harmonic oscillator. That is, we write

$$\phi_i(\boldsymbol{r}) = \sum_n C_{i,n}\varphi_n(\boldsymbol{r}). \tag{8}$$

The expansion parameters $C_{i,n}$ are the variational parameters subject to the normalization and orthogonality conditions. In practice, for numerical reasons we have had to limit the expansion in equation (8) to a maximum of 120 harmonic-oscillator eigenstates, corresponding to 14 oscillator energy levels. We have checked for $N = 6$ at strong coupling that restricting the expansion to include only six oscillator levels yields a topologically identical density profile.

The form (8) for the orbitals allows the formation of more elaborated structures than the Gaussian ansatz used in the previous section. Indeed, we show below that some of the orbitals may delocalize for strong interactions giving rise to what we have termed a supermolecule.

3. Results and discussion

Figures 1–3 report plots of the total energy E of various states in the self-consistent variational approximation, as a function of the coupling $V/(\hbar\omega)$ for $N = 2, 4$ and 6, respectively (entirely similar plots are obtained in the cases $N = 3$ and 5). Figures 4–6 illustrate instead the density profiles associated with some of these states in the strong-coupling case $V = 4\hbar\omega$. The left-hand panels in figures 4–6 refer to a state of the type $|\psi_{\rm WM}\rangle$, whereas the right-hand panels refer to states of the type $|\psi_{\rm SM}\rangle$.

As anticipated, the state $|\psi_{\rm WM}\rangle$ always corresponds to the lowest total energy: it reduces to the state $|\psi_{\rm BEC}\rangle$ in the limit $V = 0$, and decreases with increasing V for $N \geqslant 3$ at strong coupling. The energy of the state $|\psi_{\rm BEC}\rangle$ is instead continuously increasing with V, thus indicating that condensation becomes progressively unfavoured. The wavefunction $\psi_{\rm SM}$ describes an excited state at all values of the coupling for $N \geqslant 3$, but its energy soon crosses the energy of the condensed state $|\psi_{\rm BEC}\rangle$ and ultimately bends over with

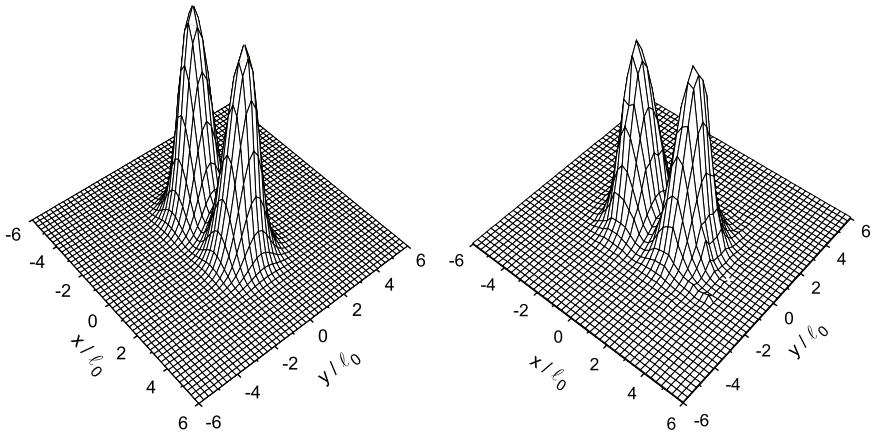

Figure 4. Density profile (in arbitrary units) at $V = 4\hbar\omega$ as a function of position in the (x, y) plane (in units of the harmonic-oscillator length $\ell_0 = \sqrt{\hbar/(m\omega)}$ and with the origin taken at the centre of the well) for $N = 2$ bosons interacting via a logarithmic potential law inside an isotropic two-dimensional harmonic well, as calculated by the Gaussian approximation in the state $|\psi_{\rm WM}\rangle$ (left panel) and the unrestricted Bose–Hartree–Fock in the state $|\psi_{\rm SM}\rangle$ (right panel).

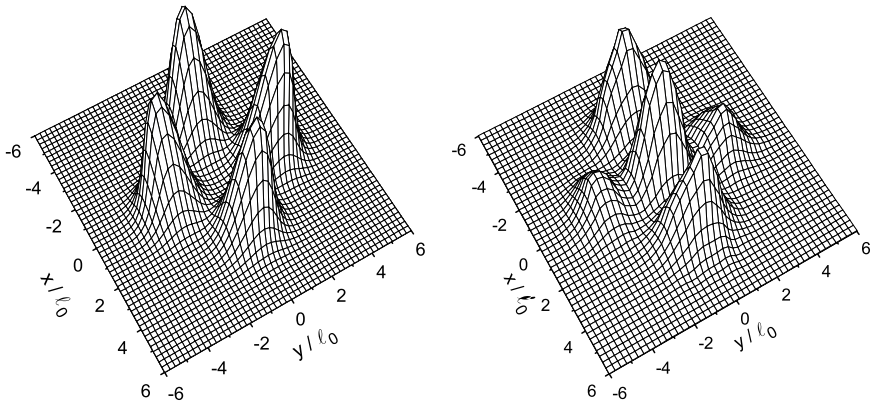

Figure 5. Same as in figure 4, but for $N = 4$ bosons.

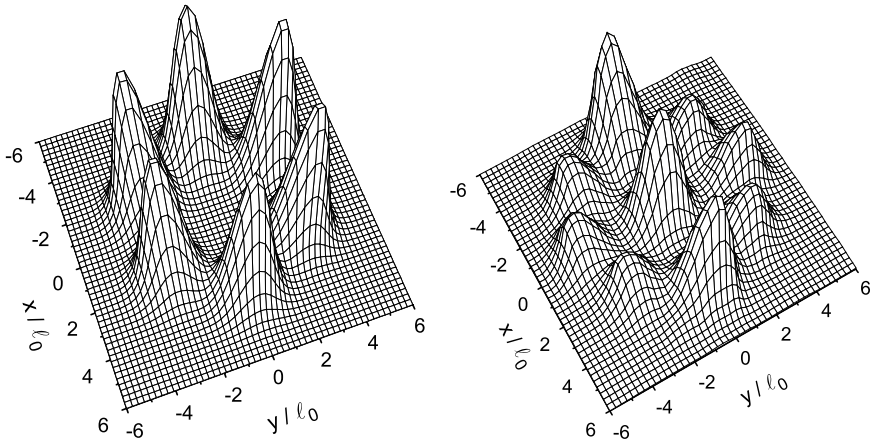

Figure 6. Same as in figure 4, but for $N = 6$ bosons and showing the density profile of the (0, 6) configuration in the left panel.

increasing V. We have checked that these trends continue over a range of coupling strength about double that illustrated in the figures. Due to the possibility of overlapping orbitals, this form of the wavefunction correctly describes the crossover from the $|\psi_{\rm BEC}\rangle$ to the $|\psi_{\rm WM}\rangle$ state.

In more detail, we see from figure 1 that the states $|\psi_{\rm WM}\rangle$ and $|\psi_{\rm SM}\rangle$ attain the same total energy for $N = 2$ at strong coupling, within the inaccuracies of our calculations that are due on one hand to the use of a Gaussian approximation and on the other to a truncated-basis expansion. As is seen from the

density profiles reported in figure 4 for $V = 4\hbar\omega$, both states describe a Wigner dimer—although the details of the density distributions associated with these two wavefunctions appear to be somewhat different.

In the case $N = 6$ we have actually found two different Wigner-molecule states that lie at very nearly the same energy over the range of coupling covered in figure 3. These correspond to different configurations of the density distribution, which are (i) a (0, 6) configuration consisting of six peaks located at the corners of a hexagon, and (ii) a (1, 5) configuration consisting of a central peak surrounded by five peaks located at the corners of a pentagon. In the left-hand panel in figure 6 we show the density profile of the (0, 6) state, which is slightly deeper in energy at $V = 4\hbar\omega$. For increasing V the energy curves of the (1, 5) and (0, 6) configurations clearly separate, showing that at strong coupling the lower energy state still corresponds to the (0, 6) configuration. This is in contrast to what has been found by Romanovsky *et al* [10] for the $1/r$ potential for which the transition from a single polygon to a polygon with a central peak already occurs for six particles. For the logarithmic interaction potential the second configuration is favoured for $N = 7$, where the density profile consists of a central peak surrounded by six peaks at the corners of a hexagon. This difference can be attributed to the relative weakness of the logarithmic potential as compared to the $1/r$ one, which in turn allows for more particles to be arranged on a single ring.

Comparison between the left-hand and right-hand panels in figures 5 and 6 illustrates the difference between Wigner molecules and supermolecules. Whereas in a Wigner molecule the bosons are localized into polygonal-ringlike crystalline patterns, in a supermolecule they are at least partly delocalized within an ordered pattern by being allowed to move in a correlated fashion between a higher multiplicity of sites including 'interstitial' sites. For a supermolecule made of $N = 3$ and 5 bosons (not shown), we find, respectively, four and seven peaks in the density profile. For the case $N = 6$ we have checked that the topology of the profile associated with the state $|\psi_{\rm SM}\rangle$ persists up to $V = 10\hbar\omega$. Finally, the state $|\psi_{\rm SM}\rangle$ yields 10 density peaks for $N = 7$.

4. Conclusions

In summary, we have used the Nelson–Seung mapping and the permanent wavefunction approximation to illustrate the ordered patterns that may be formed by an assembly of a limited number of vortices in a superfluid. In the lowest-energy state the vortices are localized at the sites of a polygonal-ringlike crystallite, which can act as a seed for the formation of a triangular Abrikosov lattice as is observed in numerous experiments on trapped Bose–Einstein condensates of ultracold bosonic atoms. Our results for these arrangements of bosons interacting with a logarithmic potential law inside a 2D harmonic well are analogous to those reported by Romanovsky *et al* [10] for bosons interacting with other types of force laws, except for six particles which we find to be arranged in an hexagon instead of a (1, 5) configuration as a result of the more realistic logarithmic potential. We have also shown, however, that at slightly higher energy the vortices can form a second type of ordered pattern, in which they can move in a correlated fashion on a variety of regular sites having different values of the average occupation number. Such 'supermolecules' could be viewed as being the seeds for a supersolid.

As a final comment, we should explicitly point out that the rotational symmetry imposed by an isotropic trap on the one-body density will be restored in a more refined treatment of these systems. Theoretical methods using projection techniques to transcend the symmetry-breaking Hartree–Fock approximation have been proposed and applied by Yannouleas and Landman [19, 10], and from their results we can expect that the energy of the various ordered patterns will drop—possibly decreasing or even cancelling out the energy difference between the two types of states that we have assumed in the permanent approximation when each set of radial peaks goes into a circular annulus. However, we feel that such a refinement lies outside the main thrust of our work. In a refined theory the formation of ordered patterns would then have to be revealed by means of much heavier calculations concerning two-body and higher correlation functions. Developments in this direction have so far been limited to instantaneous pair correlations [20].

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