

Maxwell relation between entropy and atom-atom pair correlation

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For many-particle systems with short range interactions the local (same point) particle-particle pair correlation function represents a thermodynamic quantity that can be calculated using the Hellmann-Feynman theorem. Here we exploit this property to derive a thermodynamic Maxwell relation between the local pair correlation and the entropy of an ultracold Bose gas in one dimension (1D). To demonstrate the utility of this Maxwell relation, we apply it to the computational formalism of the stochastic projected Gross-Pitaevski equation (SPGPE) to determine the entropy of a finite-temperature 1D Bose gas from its atom-atom pair correlation function. Such a correlation function is easy to compute numerically within the SPGPE and other formalisms, which is unlike computing the entropy itself. Our calculations can be viewed as a numerical experiment that serves as a proof-of-principle demonstration of an experimental method to deduce the entropy of a quantum gas from the measured atom-atom correlations.

Introduction.—Entropy plays a fundamental role in thermodynamics, statistical mechanics, and quantum information theory. However, measuring it directly or calculating it from the defining multiplicity function or the density matrix of an interacting many-body system often represents a formidable challenge. Instead, the entropy is often deduced from other thermodynamic quantities (such as the heat capacity or the free energy) using the relevant thermodynamic relations [1, 2]. Here, we derive and discuss a thermodynamic Maxwell relation by which the entropy of a quantum many-body system with short-range interactions can instead be related to, and hence deduced from, the local particle-particle correlation function. Such a pair correlation function characterizes the probability of two particles to be found in the same position compared to uncorrelated particles and can often be computed using methods of many-body and quantum field theory either analytically or numerically [3, 4]. It can also be measured experimentally in, e.g., ultracold quantum gas experiments using photoassociation [5].

The surprising aspect of the Maxwell relation between the pair correlation and the entropy that we discuss here is that the pair correlation function is usually viewed and treated as a typical two-body observable, whereas the entropy is a thermodynamic quantity. However, what promotes the pair correlation into a thermodynamic quantity as well is the fact that we are only considering many-body systems with short-range interactions that can be characterized by the s -wave scattering length [6, 7]. In this case, the inter-particle interactions can be approximated by a simple contact interaction, meaning that the two-body correlation function at zero inter-particle separation indeed becomes a thermodynamic quantity. This was first demonstrated by Lieb and Liniger in their seminal work on the exact Bethe ansatz treatment of a uniform one-dimensional (1D) Bose gas with repulsive contact (delta-function) interactions [8]. By using the Hellmann-Feynman theorem and differentiating the total ground state (zero-temperature, $T=0$) energy of the gas

with respect to the interaction strength, Lieb and Liniger were able to calculate the mean interaction energy component, which itself is proportional to the unnormalized pair correlation function (see below).

The extension of the Hellmann-Feynman theorem to finite temperature systems [4, 9], together with the exact Yang-Yang thermodynamic Bethe ansatz (TBA) solution for the 1D Bose at finite temperature [10], was later utilized to calculate the local pair correlation at any temperature and interaction strength. In this case, the pair correlation function is related to the partial derivative of the Helmholtz free energy with respect to the interaction strength [4, 9, 11]. In this work, we take this relationship a step further by combining it with the fact that the partial derivative of the same Helmholtz free energy with respect to the temperature, on the other hand, gives the entropy of the system according to the canonical ensemble formalism of statistical mechanics. Therefore, by using the commutative property of mixed second derivatives of the Helmholtz free energy (with respect to the interaction strength and temperature) one obtains the Maxwell relation between the pair correlation and the entropy that we discuss here.

As a practical application of this Maxwell relation, we utilize it for computing the entropy of a weakly interacting 1D Bose gas in the quasicondensate regime in the context of the classical c -field approach of the stochastic projected Gross-Pitaevskii equation (SPGPE) [12–15]. The SPGPE is a well established and widely used numerical approach for computing thermal equilibrium and dynamical properties of finite temperature Bose gases, such as partially condensed Bose-Einstein condensates in 2D and 3D, or phase-fluctuating quasicondensates in 1D [16]. Despite its wide applicability to ultracold quantum gas systems, computing the entropy of such systems within the SPGPE has not been accomplished prior to this work. Here, we compute the entropy of a 1D quasicondensate within the SPGPE approach; we restrict ourselves to the 1D Bose gas because of the

availability of the exact TBA solution for both the entropy and the pair correlation function, to which we compare, and hence validate, our numerical SPGPE results. However, we point out that the Maxwell relation derived and discussed here is equally applicable to 2D and 3D systems, as well as to Fermi gas systems with similar contact interactions.

Lieb-Liniger model and two-particle correlation.—We start by considering the Lieb-Liniger model describing a uniform 1D gas of N bosons of mass m interacting via a pair-wise delta-function potential on a line of length L with periodic boundary conditions and of linear density of $n = N/L$. In second-quantized form, the Hamiltonian of such a system is given by

$$\hat{H} = -\frac{\hbar^2}{2m} \int dx \hat{\Psi}^\dagger \frac{\partial^2 \hat{\Psi}}{\partial x^2} + \frac{\chi}{2} \int dx \hat{\Psi}^\dagger \hat{\Psi}^\dagger \hat{\Psi} \hat{\Psi}. \quad (1)$$

Here, $\hat{\Psi}^\dagger(x)$ and $\hat{\Psi}(x)$ are the bosonic field creation and annihilation operators, whereas χ quantifies the strength of boson-boson interactions, assumed to be repulsive ($\chi > 0$). This interaction strength can be expressed in terms of the 3D s -wave scattering length a via $\chi \approx 2\hbar\omega_\perp a$ [17], away from a confinement induced resonance, where $\omega_\perp$ is the frequency of the harmonic potential in the transverse (tightly confined) dimension.

The normalized two-point particle-particle correlation is defined in terms of the field operators as the expectation value of a normally-ordered product of two density operators, $\hat{n}(x) = \hat{\Psi}^\dagger(x)\hat{\Psi}(x)$ and $\hat{n}(x') = \hat{\Psi}^\dagger(x')\hat{\Psi}(x')$:

$$g^{(2)}(x, x') = \frac{\langle \hat{\Psi}^\dagger(x)\hat{\Psi}^\dagger(x')\hat{\Psi}(x')\hat{\Psi}(x) \rangle}{n(x)n(x')}. \quad (2)$$

In other words, the pair correlation $g^{(2)}(x, x')$ is a normalized and normally-ordered density-density correlation function. It is normalized to the product of mean densities $n(x) = \langle \hat{n}(x) \rangle$ and $n(x') = \langle \hat{n}(x') \rangle$ at points x and x' so that for uncorrelated particles (with $\langle \hat{\Psi}^\dagger(x)\hat{\Psi}^\dagger(x')\hat{\Psi}(x')\hat{\Psi}(x) \rangle = \langle \hat{\Psi}^\dagger(x)\hat{\Psi}(x) \rangle \langle \hat{\Psi}^\dagger(x')\hat{\Psi}(x') \rangle$), one has $g^{(2)}(x, x') = 1$. For values of $g^{(2)}(x, x') \neq 1$, the pair correlation characterizes an enhanced ($g^{(2)}(x, x') > 1$) or suppressed ($g^{(2)}(x, x') < 1$) probability of finding two particles at positions x and x' , respectively, compared to uncorrelated particles.

Due to the translational invariance of the uniform system that we are considering, where $n(x') = n(x) = n$, the above pair correlation $g^{(2)}(x, x')$ can only depend on the relative distance $|x - x'|$ between the two particles, i.e., $g^{(2)}(x, x') = g^{(2)}(|x - x'|)$. The local or the same-point ($x = x'$) correlation then corresponds to

$$g^{(2)} \equiv g^{(2)}(0) = \frac{\langle \hat{\Psi}^\dagger(x)\hat{\Psi}^\dagger(x)\hat{\Psi}(x)\hat{\Psi}(x) \rangle}{n^2}. \quad (3)$$

In the canonical formalism, the partition function $Z(T, N, L, \chi)$ can be written in terms of either the

Helmholtz free energy F or the Hamiltonian $\hat{H}$ via $Z = \exp(-F/k_B T) = \text{Tr} \exp(-\hat{H}/k_B T)$. By differentiating the Helmholtz free energy $F(T, N, L, \chi) = -k_B T \ln Z$ with respect to the interaction strength χ , at constant N , L , and T , one finds that [4]

$$\left(\frac{\partial F}{\partial \chi} \right)_{T, N, L} = \frac{1}{Z} \text{Tr} \left(e^{-\hat{H}/k_B T} \frac{\partial \hat{H}}{\partial \chi} \right) = \frac{L}{2} \langle \hat{\Psi}^\dagger \hat{\Psi}^\dagger \hat{\Psi} \hat{\Psi} \rangle, \quad (4)$$

and hence

$$g^{(2)} = \frac{2}{Ln^2} \left(\frac{\partial F}{\partial \chi} \right)_{T, N, L}. \quad (5)$$

This relationship between the local pair correlation and the Helmholtz free energy is what was used in Ref. [4] to calculate the $g^{(2)}$ function using the exact Yang-Yang TBA [10] solution for F , as a function of the dimensionless interaction strength γ and the dimensionless temperature τ , defined via

$$\gamma = \frac{m\chi}{\hbar^2 n}, \quad \tau = \frac{2mk_B T}{\hbar^2 n^2}. \quad (6)$$

We note here that these two dimensionless parameters completely characterize the thermodynamic properties of a uniform 1D Bose gas [4, 10].

Maxwell relation.—We now recall that the partial derivative of the same Helmholtz free energy with respect to temperature T gives the entropy S of the system:

$$S = - \left(\frac{\partial F}{\partial T} \right)_{\chi, L, N}. \quad (7)$$

Combining Eqs. (5) and (7) with the commutative property of mixed second derivatives of F , i.e. $\frac{\partial}{\partial \chi} \left(\frac{\partial F}{\partial T} \right)_{L, N} = \frac{\partial}{\partial T} \left(\frac{\partial F}{\partial \chi} \right)_{L, N}$, leads to the following Maxwell relation:

$$\boxed{\left(\frac{\partial S}{\partial \chi} \right)_{T, L, N} = -\frac{Ln^2}{2} \left(\frac{\partial g^{(2)}}{\partial T} \right)_{\chi, L, N}}. \quad (8)$$

Equation (8) is one of this paper's key results and implies that the entropy of the gas can be calculated by integrating the partial derivative of the pair correlation function $g^{(2)}$ with respect to T over the interaction strength χ . More specifically, the entropy of the uniform 1D Bose at a specific value of χ (and some fixed values of T , L , and N) can be evaluated via

$$\boxed{S(\chi, T, L, N) = S(\chi_0, T, L, N) - \frac{Ln^2}{2} \int_{\chi_0}^{\chi} \left(\frac{\partial g^{(2)}(\chi', T, L, N)}{\partial T} \right)_{\chi', L, N} d\chi'}. \quad (9)$$

where $S(\chi_0, T, L, N)$ serves the role of the integration constant and is assumed to be known for the method

to work. In practice, $S(\chi_0, T, L, N)$ can be chosen to correspond to the entropy of an ideal ($\chi_0 = 0$) 1D Bose gas, $S(0, T, L, N)$, which can indeed be calculated for any T using standard methods of statistical mechanics [1, 18].

As a simple analytic illustration of the utility of Eq. (9), we calculate the entropy of a 1D Bose gas in highly degenerate, nearly ideal Bose gas regime that can be treated using perturbation theory with respect to γ (see the results for the so-called decoherent quantum regime in Ref. [4, 18], valid in the region $2\sqrt{\gamma} \ll \tau \ll 1$). In this regime, the pair correlation function $g^{(2)}$, which was calculated in Ref. [4] without resorting to the Helmholtz free energy, is given by

$$g^{(2)} = 2 - 4\gamma/\tau^2. \quad (10)$$

Therefore, Eq. (9) yields the following result for the corresponding entropy:

$$S = S_{\text{IBG}} - 4k_B N \gamma^2 / \tau^3. \quad (11)$$

where $S_{\text{IBG}} = S(0, T, L, N)$ is entropy of the ideal 1D Bose gas at the same temperature [18].

Application to the SPGPE approach.—We now illustrate the utility of Eq. (9) using a numerically computed pair correlation function within the SPGPE approach. This itself can be viewed as a numerical experiment demonstrating how one can deduce the entropy of a quantum gas from the measured atom-atom correlations.

The SPGPE approach (see Appendix) is a classical or c -field method for computing thermal equilibrium and dynamical properties of degenerate Bose gases at finite temperatures [12, 13, 16, 19–29]. Evolving the SPGPE from an arbitrary initial state, for sufficiently long time (such that the memory of the initial state is lost), samples thermal equilibrium configurations of the system from the grand-canonical ensemble. These configurations are represented by stochastic realizations of the complex c -fields $\Psi_{\mathbf{C}}(x, t)$, which we will denote as $\Psi_{\mathbf{C}}(x)$ for thermal equilibrium states. In the SPGPE approach, the pair correlation function $g^{(2)}$ is computed according to:

$$g^{(2)} = \frac{\langle \Psi_{\mathbf{C}}^*(x) \Psi_{\mathbf{C}}^*(x) \Psi_{\mathbf{C}}(x) \Psi_{\mathbf{C}}(x) \rangle}{\langle \Psi_{\mathbf{C}}^*(x) \Psi_{\mathbf{C}}(x) \rangle^2}, \quad (12)$$

where the expectation values are over a large number of stochastic realisations.

In this work, we are interested in the pair correlation function, $g^{(2)}$, of a 1D quasicondensate at thermal equilibrium, in the parameter range $\sqrt{\gamma} \ll \tau \ll 1$, where the c -field approach is valid [19, 29]. In Fig. 1 we show the dependence of this correlation function over a range of the dimensionless interaction strength $\gamma \in [10^{-4}, 10^{-2}]$, for a fixed value of the dimensionless temperature $\tau = 0.2$, obtained from the SPGPE approach. For comparison, we also show the exact TBA result (squares) and the approximate analytic result of Eq. (10) (dashed line).

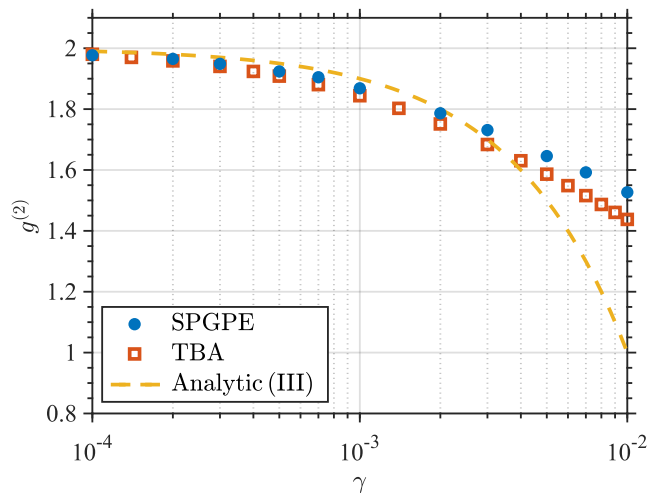


FIG. 1. Local pair correlation $g^{(2)}$ for a 1D quasicondensate as a function of the dimensionless interaction strength γ , for a fixed dimensionless temperature $\tau = 0.2$. The numerically computed data from the SPGPE simulations are shown as circles and are compared to the exact TBA result (squares), and the analytic approximation of Eq. (10) (dashes).

As we see, in the limit of an ideal Bose gas ($\gamma \rightarrow 0$) at finite temperature, the pair correlation approaches the value of $g^{(2)} = 2$, which is the Hanbury Brown–Twiss effect of bosonic bunching ($g^{(2)} > 1$) first observed for photons from a chaotic (thermal) light source [30] and more recently for an ultracold atomic gas above the transition to a Bose-Einstein condensate [31–33]. It corresponds to large density fluctuations and an enhanced probability of detecting two indistinguishable bosons in the same position due to the constructive interference of the respective probability amplitudes. As the strength of the repulsive interaction increases, the said probability decreases and manifests itself in the reduction of the value of $g^{(2)}$ below 2 [4, 5]. At some finite, but still weak ($\gamma \ll 1$) interaction strength, the pair correlation crosses the coherent level of $g^{(2)} = 1$ characteristic of a phase-fluctuating quasicondensate with suppressed density fluctuations, which itself shares the properties of a weakly interacting Bose-Einstein condensate in the mean-field description [31, 32].

As the interaction strength increases further and approaches the regime of very strong or hard-core repulsion ($\gamma \rightarrow \infty$), also known as the Tonks-Girardeau limit of fermionization, the pair correlation reduces further down to $g^{(2)} \rightarrow 0$ (see Ref. [4, 5]). This reduction reflects the fact that the bosons are now strongly (anti)correlated and behave effectively as fermions, wherein the bosonic hard-core repulsion mimics the fermionic Pauli blocking. In the pair correlation function, such repulsion manifests itself as antibunching ($g^{(2)} < 1$), which itself is due to the destructive interference of probability amplitudes for detecting two indistinguishable fermions in the same position [33]. This regime, however, is beyond the applicabil-

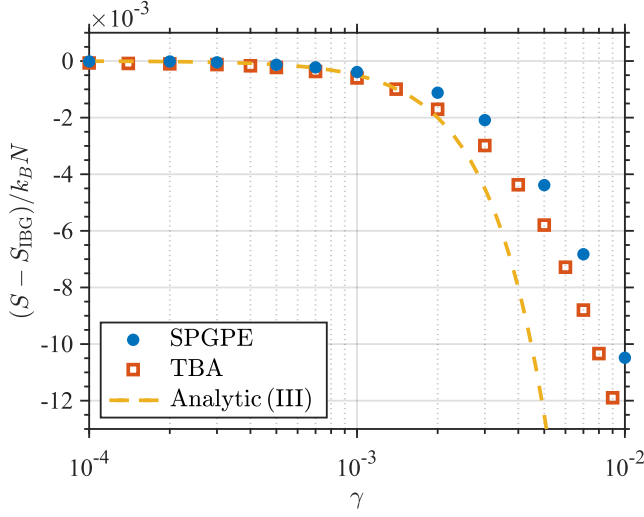


FIG. 2. Entropy of a 1D quasicondensate as a function of the dimensionless interaction strength γ , relative to that of an ideal Bose gas at the same temperature, $S(\gamma, \tau) - S_{\text{IBG}}(\tau)$, for $\tau = 0.2$. The SPGPE data computed using Eq. (9) is shown as circles and is compared to the exact TBA data (squares), and the analytic approximation of Eq. (11) (dashes).

ity of the SPGPE approximation ($\gamma \ll 1$, $2\gamma \ll \tau \ll 1$; see, e.g., Ref. [18, 29], and references therein), and this is why in Fig. 1 we do not show the behaviour of the $g^{(2)}$ beyond the weakly interacting regime of $\gamma \ll 1$. Because of the same approximate nature of the SPGPE approach, we see that the SPGPE data for $g^{(2)}$, while agreeing well with the exact TBA results at small γ , starts to deviate from the TBA results as γ increases and approaches its upper bound of $\gamma = 0.01$, where the condition $2\gamma \ll \tau$ is not well satisfied. Similarly, the analytic result of Eq. (10) deviates from TBA to a larger extent as γ is increased, because it is applicable in an even more restricted region of $2\sqrt{\gamma} \ll \tau \ll 1$ [4, 18].

We next deduce the entropy of the 1D quasicondensate using Eq. (9) and the SPGPE data for $g^{(2)}$, except that now the integration in Eq. (9) is done numerically. To obtain the dependence of $S(\chi, T, L, N)$ on χ at a fixed T , or rather on the dimensionless γ at a fixed τ , we convert Eq. (9) to the dimensionless units and first evaluate the derivative $(\partial g^{(2)}(\gamma', \tau)/\partial \tau)_{\gamma'}$ using the central difference scheme, for a range of values of γ' . We next evaluate the integral over γ' numerically, as a function of the upper bound. The upper bound is scanned within $\gamma \in [10^{-4}, 10^{-2}]$, while fixing the lower bound at $\gamma_0 = 10^{-6}$, which is sufficiently low for the SPGPE results to be nearly identical to the IBG results at finite T , for which $g^{(2)} = 2$ and $S(\gamma_0, T, L, N) \simeq S_{\text{IBG}}(T, L, N)$. In Fig. 2 we show the SPGPE result for the entropy difference per particle, $(S - S_{\text{IBG}})/k_B N$ obtained from the SPGPE approach as a function of γ , for a fixed value of the dimensionless temperature τ . We again compare

these data with the exact TBA result (squares) and the analytic result of Eq. (11) (dashed line). As we see, the entropy is maximal in the ideal Bose gas limit ($\gamma \rightarrow 0$), where $g^{(2)} = 2$ is also maximal, reflecting the large density fluctuations and excess randomness (bunching) in the probability of finding two indistinguishable bosons in the same position. As the strength of repulsive interactions increases, the random density fluctuations become more and more suppressed, which is also evident in the decrease of the entropy of the gas, as expected. Overall, we see a good agreement between the SPGPE and TBA results, particularly at small values of γ , where the condition of validity of the SPGPE approximation is better satisfied; the agreement becomes worse as γ is increased, for the same reason as the discrepancy in the behaviour of $g^{(2)}$ discussed earlier.

Summary and outlook.—We have derived and discussed a new Maxwell relation by which the entropy of a quantum many-body system with contact two-body interactions can be related to, and deduced from, the local two-particle correlation function. We have validated this method through a numerical experiment based on the c -field SPGPE simulations and computed—for the first time (to the best of our knowledge) within the SPGPE formalism—the thermodynamic entropy of a weakly interacting 1D Bose gas in the quasicondensate regime.

The Maxwell relation derived here may find immediate applications, such as measuring the entropy and deducing the thermodynamic equation of state, in quantum gas experiments that take advantage of tuneable interparticle interactions and measurements of atom-atom correlations using photoassociation or in-situ imaging techniques in quantum gas microscope setups. It can also be applied to other computational approaches, such as DMRG and phase space stochastic gauge methods [34, 35], that are capable of computing particle-particle correlations from the many-body wave-function or density matrix formalisms, but struggle to compute the entropy from, e.g., the multiplicity or the free energy.

Beyond quantum gas systems, the main results discussed here, Eqs. (8) and (9), can aid the study of traditional condensed matter systems that are often characterized through the static structure factor that describes scattering experiments. Indeed, the static structure factor $S(\mathbf{k})$ is related to the nonlocal pair correlation $g^{(2)}(\mathbf{r})$ via a Fourier transform, $S(\mathbf{k}) = 1 + n \int d\mathbf{r} g^{(2)}(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}}$. Therefore, measurements or theoretical knowledge of $S(\mathbf{k})$ can be used to deduce the local pair correlation $g^{(2)}(0) \equiv g^{(2)}$ by an inverse Fourier transform, which can then be used for determining the thermodynamic entropy from Eq. (9). Finally, one can envisage derivation of related Maxwell relations for a large class of spin Hamiltonians in which: (a) the spin-spin interaction term can be similarly calculated using the Hellmann-Feynman theorem; and (b) the relevant spin-spin correlation function can be experimentally measured.

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Appendix: The Stochastic Projected Gross-Pitaevskii approach.—In the SPGPE approach [13, 19, 21], the quantum field operator $\hat{\Psi}(x, t)$ is decomposed into two regions, a c -field region and an incoherent thermal region. The c -field region contains highly occupied low-energy modes and is described by a single complex-valued classical field $\Psi_{\mathbf{C}}(x, t)$. The incoherent region, on the other hand, contains sparsely occupied high-energy modes that act as an effective thermal bath, treated as static, with temperature T and chemical potential μ that governs the thermal average number of particles in the system (in the c -field region). The boundary between these two regions is defined by an appropriately chosen energy cutoff ϵ_{cut} [36].

In this approach, the thermal equilibrium state of the system is prepared by evolving the simple growth stochastic projected Gross-Pitaevskii equation (SPGPE) for the complex c -field $\Psi_{\mathbf{C}}(x, t)$ [13, 21],

$$d\Psi_{\mathbf{C}}(x, t) = \mathcal{P}^{(\mathbf{C})} \left\{ -\frac{i}{\hbar} \mathcal{L}_0^{(\mathbf{C})} \Psi_{\mathbf{C}}(x, t) dt + \frac{\Gamma}{k_B T} (\mu - \mathcal{L}_0^{(\mathbf{C})}) \Psi_{\mathbf{C}}(x, t) dt + dW_{\Gamma}(x, t) \right\}. \quad (13)$$

Here, the projection operator $\mathcal{P}^{(\mathbf{C})}\{\cdot\}$ sets up the high-energy cutoff ϵ_{cut} , whereas Γ is the so-called growth rate responsible for the coupling between the c -field and the effective reservoir (served by the incoherent region). In addition, $\mathcal{L}_0^{(\mathbf{C})}$ is the Gross-Pitaevskii operator defined by

$$\mathcal{L}_0^{(\mathbf{C})} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) + \chi |\Psi_{\mathbf{C}}(x, t)|^2, \quad (14)$$

where $V(x, t)$ is the external trapping potential, if any. The last term, $dW_{\Gamma}(x, t)$, in Eq. (13) is a complex-valued stochastic white noise term with the following nonzero correlation:

$$\langle dW_{\Gamma}^*(x, t) dW_{\Gamma}(x', t) \rangle = 2\Gamma \delta(x - x') dt. \quad (15)$$

As we mentioned in the main text, the stochastic realisations of the c -field $\Psi_{\mathbf{C}}(x, t)$ prepared via the SPGPE after a sufficiently long evolution time sample the grand-canonical ensemble of thermal equilibrium states of the system. These stochastic realisations can then be evolved in real time according to the mean-field projected Gross-Pitaevskii equation [21], following a certain out-of-equilibrium protocol. This would then represent real-time dynamical evolution of the system starting from an initial thermal equilibrium state. In this work, however, we do not simulate any real-time dynamics; instead, we are interested in the pair correlation function, $g^{(2)}$, of a 1D quasicondensate at thermal equilibrium. Accordingly, our simulations involve only the SPGPE stage.

Denoting the SPGPE realizations of the complex c -field $\Psi_{\mathbf{C}}(x, t)$ after a sufficiently long evolution time via $\Psi_{\mathbf{C}}(x)$, the thermal equilibrium values of physical observables are then calculated in terms expectation values of products of $\Psi_{\mathbf{C}}(x)$ and its complex conjugate $\Psi_{\mathbf{C}}^*(x)$ over a large number of stochastic realizations. This is much in the same way as calculating the same observables in terms of expectation values over normally-ordered products of quantum field operators $\hat{\Psi}(x)$ and $\hat{\Psi}^\dagger(x)$, except that their non-commuting nature is ignored. As an example, the particle number density $n(x) = \langle \hat{\Psi}^\dagger(x) \hat{\Psi}(x) \rangle$ in the SPGPE approach is calculated as $n(x) = \langle \Psi_{\mathbf{C}}^*(x) \Psi_{\mathbf{C}}(x) \rangle$, where the brackets $\langle \dots \rangle$ refer to ensemble averaging over a large number of stochastic trajectories; similarly the pair correlation function $g^{(2)}$ can be computed via Eq. (12) of the main text.

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