**Ab initio methods for finite temperature two-dimensional Bose gases**

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The stochastic Gross-Pitaevskii equation and modified Popov theory are shown to provide an *ab initio* description of finite temperature, weakly-interacting two-dimensional Bose gas experiments. Using modified Popov theory, a systematic approach is developed in which the momentum cut-off inherent to classical field methods is removed as a free parameter. This is shown to yield excellent agreement with the recent experiment of Hung et al. [Nature, 470 236 (2011)], verifying that the stochastic Gross-Pitaevskii equation captures the observed universality and scale-invariance.

**Introduction** — Ultracold atomic gases represent versatile tools with which to investigate many-body quantum physics [1]. A key tunable property of these systems is their effective dimensionality; increasing the trapping potential, used in experiments to confine and cool atoms, in one or two directions produces gases that are effectively two-dimensional (2D) or one-dimensional (1D), respectively. Low-dimensional geometries in turn lead to richer physics due to the enhanced importance of fluctuations which restrict the onset of long range order [2, 3].

A number of experiments have been performed recently in order to examine the thermodynamic properties of weakly interacting 2D Bose gases [4 — 13]. Due to the high precision now routinely attained in such experiments, a particularly powerful feature is their usefulness in accurately testing microscopic theories. In this respect, the 2D Bose gas is interesting as fluctuations are typically important over a broad critical region [14, 15], meaning the standard mean field approach to weakly interacting Bose gases is not well suited; this breadth was however exploited by Hung et al. [13] to obtain a clear experimental observation of critical phenomena in ultracold atoms near the Berezinskii-Kosterlitz-Thouless (BKT) phase transition [16, 17].

At equilibrium, Monte Carlo (MC) calculations have been successfully applied to the uniform 2D Bose gas [14, 18, 19], notably yielding a microscopic prediction for the BKT transition point [19]. The harmonically trapped case has been studied using quantum MC [20], various mean field theories [21, 22] and classical field calculations [20, 28]. Classical field methods have the advantage of providing a time-dependent description of the gas, which makes them additionally applicable to systems away from equilibrium; nonetheless, a simple yet accurate mean-field theory is also highly desirable to avoid the need for more complicated methods in calculating equilibrium properties. In this work we perform a quantitative comparison between two such complementary methods: (i) the modified Popov (MP) theory of Stoo [21, 22], which is straightforward to solve and provides quick access to equilibrium properties in all dimensions, and (ii) the stochastic Gross-Pitaevskii equation (SGPE) [31, 33] (see also [34]) that has already successfully described several 1D Bose gas experiments [33, 35] and is also applicable in dynamical situations [32, 37]. The experimental *in situ* measurements of Hung et al. [13] offer an ideal test-bed for the theories we wish to consider, free of the complications associated with modelling expansion imaging, thus a primary motivation for this work is to demonstrate the applicability of the SGPE in capturing the universality and scale-invariance of 2D experiments.

A further related aim is to systematically circumvent a standard limitation of classical field calculations, linked to the fact that the Bose gas represented in this way must obey classical statistics. In practical terms, this issue manifests as a sensitivity to the numerical grid (or, equivalently, momentum/energy cutoff) used in solving such models [38, 39], which, as a free parameter, can undermine their use for *ab initio* studies. While calculations based upon classical lattice models have been linked back to their quantum counterparts in the context of Monte Carlo studies [19, 40], the situation is less clear for methods based upon *dynamical* equilibration of classical fields: approaches to date include selecting a cutoff based on the assumption that the classical field temperature should match that of an *ideal* Bose gas with the same condensate fraction [41], specifying a minimum acceptable mode occupation, typically within an energy cutoff somewhere in the range $g_{2\text{D}}n < E_{\text{cut}} \lesssim k_B T$ [39], and a high temperature semi-classical field method valid for $k_B T > \mu$ [42]. Motivated by the desire for a formulaic approach to cut-off choice that is valid also at temperatures $k_B T \lesssim \mu$, and which also includes the effect of interactions, in this work we have devised and tested a strategy by which to specify an ‘optimum’ SGPE grid choice, based upon comparing the classical and quantum limits of MP theory.

**Methodology** — The 2D stochastic Gross-Pitaevskii equation describes the Bose gas via a noisy field $\psi(x,t)$, which satisfies the equation of motion

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \left(1 - i\gamma(x,t)\right) \left[- \frac{\hbar^2}{2m} \nabla^2_{x,y} + V(x) - \mu \right.$$

$$+ g_{2\text{D}} \left(|\psi(x,t)|^2 + 2n_{\text{above}}(x)\right) \bigg] \psi(x,t) + \eta(x,t),$$

where $V(x) = m\omega^2(x^2 + y^2)/2 = m\omega^2 r^2/2$ is the trapping potential in the more weakly confined x-y plane, $g_{2\text{D}} = \sqrt{8\pi(a_0 l_z^2)\hbar^2}/m = g\hbar^2/m$ is the 2D interaction strength (with $a$ the s-wave scattering length), and $\eta$ is a complex Gaussian noise term, with correlations given by the rela-
gas. The MP predictions for the critical chemical potential were in excellent agreement with those obtained from MC simulations \cite{19}. In fact, the MP theory was found only to break down in the region where its equation of state reduces to that of HF, which occurs close to the BKT transition due to the mean field nature of this approach. A renormalization group analysis was subsequently shown to avoid this discontinuity and to match smoothly to the MP equation of state for chemical potentials $\mu > 0.18k_BT$ \cite{23}.

The central object within the MP approach is the quasi-condensate \cite{10} which, in the Thomas-Fermi approximation, obeys $g^{(2)}(n_{qc}+2n) = \mu_{eff}$ where the effective chemical potential may be written as $\mu_{eff} = \mu - V(x)$. The thermal density is calculated from \cite{29,30}

$$n_t = n_{qc} + \frac{1}{V} \sum_{k=0}^{k_{max}} \left\{ \frac{\epsilon_k}{2\hbar \omega_k} \left[ 2N_k + 1 \right] - \frac{1}{2} + \frac{g_{2D}n_{qc}}{2k + 2\mu} \right\},$$

with $\hbar \omega_k = \sqrt{\epsilon_k + 2g_{2D}n_{qc}}$ and $\epsilon_k = \hbar^2 k^2/2m$.

Optimum cutoff selection: Classical vs. quantum statistics.

In the usual formulation of MP, $N_k = N_{BE}^{2D} \equiv 1/(\exp(\beta \hbar \omega_k) - 1)$, since the particles obey Bose-Einstein statistics, and the upper index in the sum in Eq. (2), $k_{max}$, may be straightforwardly taken to infinity. However, setting $N_k = N_{RI}^{2D} \equiv 1/(\beta \hbar \omega_k)$ instead leads to a MP result based upon Rayleigh-Jeans statistics which is therefore analogous to using the classical fluctuation-dissipation result in the SGPE (see e.g. Eqs. (38)-(40) of Ref. \cite{23}). We will use MP$_{RI}$ and MP$_{BE}$ to denote the Rayleigh-Jeans and Bose-Einstein cases, respectively.

Since the MP$_{RI}$ approach gives very good agreement with the SGPE for a given cutoff \cite{47}, this allows us to extract an optimum value for the SGPE grid spacing, as we can examine the accuracy of the classical approximation as $k_{max}$ is varied by directly comparing the MP$_{RI}$ and MP$_{BE}$ results. To measure this difference, we compare predictions for the normalized second-order correlation function, chosen because of the important role played by density fluctuations in quasicondensate. In MP theory, this is given by $g^{(2)} = (n_{qc}^2 + 4n_{qc}n_1 + 2n_1^2)/(n_{qc} + n_1)^2$.

The procedure we adopt then is to first calculate $g^{(2)}(x = 0)$ using the Bose-Einstein distribution in Eq. (2). This value then serves as a target result which we aim to match using MP$_{RI}$ with all other parameters held constant. Once an optimum cutoff is selected in this way, it is then used to calculate the optimum numerical grid spacing for use in the SGPE simulations.

This approach is illustrated in Fig. 4 symbols indicating the $g^{(2)}(0)$ values obtained from MP$_{BE}$ for two temperatures as the energy cutoff, shown on the horizontal axis, is varied. The diagonal dashed lines show the results if we neglect atoms above the cutoff momentum in the MP$_{RI}$ calculations. The symbols asymptote towards these lines for energy cutoffs $\gtrsim k_BT$, as there are then very few atoms in modes above the cutoff energy.

For each temperature, the optimum energy cutoff may be read off from Fig. 1 as the horizontal coordinate of the point at which the classical $g^{(2)}(0)$ data intersects the semi-logarithmic data. We will use $k_{max}$ from these plots unless otherwise specified.

The numerical solution to Eq. (1) introduces an ultra-violet momentum cutoff implemented here by the discretization scheme chosen; this implies that the equilibrium thermal state that is achieved for a given set of physical parameters can differ quite dramatically through variation of the grid spacing alone. There is then clearly some ambiguity as to which cutoff choice provides optimum agreement with nature. To address this point for 2D Bose gases, we choose to make use of the MP theory.

The MP theory \cite{26,30} was formulated specifically to describe low-dimensional Bose gases, taking into account the effects of phase fluctuations to all orders \cite{29}, and has been found to agree well with the SGPE in previous studies \cite{30,44,45}. In Ref. \cite{26}, MP was compared to both Hartree-Fock (HF) and MC results for the 2D Bose gas. The MP predictions for the critical chemical potential and density for the BKT transition were in excellent agreement with those obtained from MC simulations \cite{19}. In fact, the MP theory was found only to break down in the region where its equation of state reduces to that of HF, which occurs close to the BKT transition due to the mean field nature of this approach. A renormalization group analysis was subsequently shown to avoid this discontinuity and to match smoothly to the MP equation of state for chemical potentials $\mu > 0.18k_BT$ \cite{23}.

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For the ideal gas, an expression was derived in Ref. 48 for a cutoff leading to optimum agreement between quantum and classical statistics; in 2D, it was found that this occured at an energy $\beta E \approx 1.6$. Using the method outlined above we typically obtain a value around $\beta E \approx 0.77$, which varies slowly with temperature in the range considered, yet is clearly much lower than the ideal gas prediction, indicating the important role of interactions.

Comparison to Experimental results — In order to validate our scheme, we now directly compare the results to in situ experimental data of Hung et al. 13. We begin with the MP $BE$ method and fix the trap parameters and temperature to those quoted in 13. We then vary the chemical potential until the required density is reached at the trap centre. This provides us with all relevant physical parameters required to solve the SGPE, barring an optimum choice of grid spacing, which is extracted as described; since there are no free parameters, both the MP theory and SGPE provide an ab initio description of the experiment.

Figure 2 shows the SGPE (with an optimum momentum cutoff) and MP results together with the experimental density profiles of Ref. 13. Corresponding data for density fluctuations, obtained from the normalized second order correlation function $g^{(2)}(r)$ via $\langle \delta n^2(r) \rangle = (g^{(2)}(r) - 1)(n(r))^2$, are shown on the bottom row of Fig. 2. By comparing also to HF 49, the trend we observe is that despite matching the experimental density profiles well, the HF results consistently predict density fluctuations that are too large, relative to those observed experimentally. This may be understood since energy reducing correlations which lead to the onset of quasi-condensation are not incorporated in this theory, in accordance with the findings for highly elongated gases presented in Ref. 50. In contrast, the SGPE and MP data agree very well with the experimental findings, thereby confirming the utility of each in describing the physics of 2D Bose gases at finite temperatures. Moreover, these findings highlight that choosing an optimum grid spacing based upon a higher order field correlation such as $g^{(2)}$ is more robust, since the density is a less sensitive measure of the system.

An important feature of Ref. 13 was the experimental demonstration of scale invariance in a 2D Bose gas. Plotting their data against a scaled chemical potential, $\beta(\mu - V(r))$, Hung et al. showed that densities measured at several temperatures collapsed to a single curve when appropriately scaled to the thermal de Broglie wavelength, $\lambda_{dB}$. This was found to be true in both the thermal and superfluid regimes; the fluctuation region may be identified with the crossover from a thermal gas to a superfluid, where the system moves from an enhancement to a suppression of density fluctuations respectively.

Figure 3. Universal behaviour of shifted density profiles $(n - n_c)\lambda_{dB}^2$ versus rescaled chemical potential $\beta(\mu - \mu_c - V(r))/g$. Indicative errorbars are shown for several SGPE data points which originate from the fit used to obtain $\mu_c$. 

Figure 2. Density (top) and density fluctuations (bottom) from the SGPE, modified Popov (Bose-Einstein) and Hartree-Fock calculations versus the experimental data of Ref. 13. The rightmost plots show the SGPE results capture the experimentally observed scale invariance found in Ref. 13, including across the transition region indicated by the grey shaded area.
as may be seen in the lower rightmost plot of Figure 3. An important difference between the MP and SGPE approaches, therefore, is the discontinuity in the density predicted by the former. In contrast, a key strength of the SGPE lies in its applicability across this fluctuation region, as may be seen in the rightmost plots of Figure 2 which show that it also demonstrates scale invariance in good agreement with the experimental data.

To estimate the location of the BKT transition from the SGPE simulations, we employ the fitting function

$$
\langle \delta n^2 \rangle = \lambda^4 \kappa / \beta
$$

as in Ref. [13]. As shown in Figure 4, which once again closely follow the results of experiments of Hung et al., which yields a critical chemical potential, $\mu_c$, and a corresponding critical density, $n_c$. These parameters can then be used to uncover the universal physics of 2D Bose gases, since close to the transition point, the shifted density $(n - n_c) / \nu_f$ should be a universal function of $(\mu - \mu_c) / g$ alone [13, 14]. The universality of 2D Bose gases may then be tested by comparing scaled densities from gases with different interaction strengths, as in Ref. [13].

Conclusions — We have found excellent agreement between ab initio calculations based on the stochastic Gross-Pitaevskii and modified Popov theories with in situ experimental data from the two-dimensional Bose gas experiments of Hung et al.. Combining these two methods, we devised and tested a systematic approach to circumvent the problem of cut-off choice within classical field simulations that could prove crucial in modelling out-of-equilibrium scenarios, which forms a natural extension to this work.

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References:

[1] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. 80, 885 (2008)
[2] N. D. Mermin and H. Wagner, Phys. Rev. Lett. 17, 1133 (1966)
[3] P. C. Hohenberg, Phys. Rev. 158, 383 (1967)
[4] Z. Hadzibabic, P. Krüger, M. Cheneau, B. Battelier, and J. Dalibard, Nature (London) 441, 1118 (2006)
[5] V. Schweikhard, S. Tung, and E. A. Cornell, Phys. Rev. Lett. 99, 030401 (2007)
[6] P. Krüger, Z. Hadzibabic, and J. Dalibard, Phys. Rev. Lett. 99, 040402 (2007)
[7] Z. Hadzibabic, P. Krüger, M. Cheneau, S. P. Rath, and J. Dalibard, New Journal of Physics 10, 045006 (2008)
[8] P. Cladé, C. Ryu, A. Ramanathan, K. Helmerson, and W. D. Phillips, Phys. Rev. Lett. 102, 170401 (2009)
[9] S. Tung, G. Lamporesi, D. Lobser, L. Xia, and E. A. Cornell, Phys. Rev. Lett. 105, 230408 (2010)
[10] S. P. Rath, T. Yefsah, K. J. Günter, M. Cheneau, R. Desbuquois, M. Holzmann, W. Krauth, and J. Dalibard, Phys. Rev. A 82, 013609 (2010)
[11] T. Yefsah, R. Desbuquois, L. Chomaz, K. J. Günter, and J. Dalibard, Phys. Rev. Lett. 107, 130401 (2011)
[12] T. Plisson, B. Allard, M. Holzmann, G. Salomon, A. Aspotech, P. Bouyer, and T. Bourdel, Phys. Rev. A 84, 061606 (2011)
[13] C.-L. Hung, X. Zhang, N. Gemelke, and C. Chin, Nature 470, 236 (2011)
[14] N. Prokof’ev and B. Svistunov, Phys. Rev. A 66, 043608 (2002)
[15] A. Posazhennikova, Rev. Mod. Phys. 78, 1111 (2006)
[16] V. L. Berezinskii, Sov. Phys. JETP 34, 610 (1972)
[17] J. M. Kosterlitz and D. J. Thouless, J. Phys. Chem. 6, 181 (1973)
[18] Y. Kagan, V. A. Kashurnikov, A. V. Krasavin, N. V. Prokof’ev, and B. Svistunov, Phys. Rev. A 61, 043608 (2000)
[19] N. Prokof’ev, O. Ruebenacker, and B. Svistunov, Phys. Rev. Lett. 87, 270402 (2001)
[20] M. Holzmann and W. Krauth, Phys. Rev. Lett. 100, 190402 (2008)
[21] C. Gies, B. P. van Zyl, S. A. Morgan, and D. A. W. Hutchinson, Phys. Rev. A 69, 023616 (2004)
[22] C. Gies and D. A. W. Hutchinson, Phys. Rev. A 70, 043606 (2004)
[23] L.-K. Lim, C. Morais Smith, and H. T. C. Stoof, Phys. Rev. A 78, 013634 (2008)
[24] M. Holzmann, M. Chevallier, and W. Krauth, EPL (Europhysics Letters) 82, 30001 (2008)
[25] R. N. Bisset and P. B. Blakie, Phys. Rev. A 80, 045603 (2009)
[26] T. P. Simula, M. J. Davis, and P. B. Blakie, Phys. Rev. A 77, 023618 (2008)
[27] R. N. Bisset, M. J. Davis, T. P. Simula, and P. B. Blakie, Phys. Rev. A 79, 033626 (2009)
[28] R. N. Bisset and P. B. Blakie, Phys. Rev. A 80, 035602 (2009)
[29] J. Andersen, U. A. Khawaja, and H. Stoof, Phys. Rev. Lett. 88, 070407 (2002)
[30] U. A. Khawaja, J. O. Andersen, N. P. Proukakis, and H. T. C. Stoof, Phys. Rev. A 66, 013615 (2002), erratum: Phys. Rev. A 66, 059902(E) (2002).
[31] H. T. C. Stoof, J. Low Temp. Phys. 114, 11 (1999)
[32] H. T. C. Stoof and M. J. Bijlsma, J. Low Temp. Phys. 124, 431 (2001)
[33] R. A. Duine and H. T. C. Stoof, Phys. Rev. A 65, 013603 (2001)
[34] C. W. Gardiner and M. J. Davis, J. Phys. B 36, 4731 (2003)
[35] S. P. Cockburn, D. Gallucci, and N. P. Proukakis, Phys. Rev. A 84, 023613 (2011)
[36] D. Gallucci, S. P. Cockburn, and N. P. Proukakis, arXiv:1205.6075v1 (2012)
[37] S. P. Cockburn, H. E. Nistazakis, T. P. Horikis, P. G. Kevrekidis, N. P. Proukakis, and D. J. Frantzeskakis, Phys. Rev. Lett. 104, 174101 (2010)
[38] S. P. Cockburn and N. P. Proukakis, Las. Phys. 19, 558 (2009), arXiv:0812.1926v2
[39] P. B. Blakie, A. S. Bradley, M. J. Davis, R. J. Ballagh, and C. W. Gardiner, Adv. Phys. 57, 363 (2008)
[40] P. Arnold and G. Moore, Phys. Rev. Lett. 87, 120401 (2001)
[41] L. Zawitkowski, M. Breveczky, M. Gajda, and K. Rzażewski, Phys. Rev. A 70, 033614 (Sep 2004)
[42] L. Giorgetti, I. Carusotto, and Y. Castin, Phys. Rev. A 76, 013613 (2007)
[43] The density of atoms with momenta greater than the grid cutoff, $n_{above}$, is calculated iteratively, in the Hartee-Fock limit, prior to carrying out the SGPE simulations using the density from MP theory based upon Rayleigh-Jeans statistics.
[44] N. P. Proukakis, Phys. Rev. A 74, 053617 (2006)
[45] S. P. Cockburn, A. Negretti, N. P. Proukakis, and C. Henkel, Phys. Rev. A 83, 043619 (2011)
[46] V. N. Popov, “Functional integrals in quantum field theory and statistical physics,” (Reidel, Dordrecht, 1983)
[47] As in the SGPE, we also include the atoms with momenta above the cutoff in the classical case of MP. For the optimum cutoff, we find this number of atoms to be a small fraction of the total, which we retain mainly for completeness.
[48] E. Witkowska, M. Gajda, and K. Rzażewski, Phys. Rev. A 79, 033631 (2009)
[49] While the chemical potential is fixed between SGPE and modified Popov calculations, we find a different value of $\mu$ must be used in order to match the Hartree-Fock density to the experimental central density. The temperature however remains fixed between all methods.
[50] J.-B. Trebbia, J. Esteve, C. I. Westbrook, and I. Bouchoule, Phys. Rev. Lett. 97, 250403 (2006)