Classical field records of a quantum system: their internal consistency and accuracy

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We quantitatively determine the accuracy and range of validity of the widespread classical field description for quantum Bose gases in 1d, 2d, and 3d by a careful study of the ideal gas limit. The optimum high energy cutoff is shown to depend strongly on the observable in question (e.g. energy, density fluctuations, phase coherence length, condensate fraction). This allows us to place the varying past results in a common context. Above a crossover region near the degeneracy temperature, estimates for different quantities (especially the trio of density fluctuations, energy, and mean density) can no longer be reconciled, explicitly showing the way that the classical field description breaks down. A consistent classical field representation with errors in all typical observables below 10% is possible for temperatures below 0.0072 degeneracy temperature in 1d, and 0.49 critical temperature in 3d. Surprisingly, this is not possible for the 2d ideal gas even at zero temperature.

The quantum mechanics of a wide variety of physical systems can be quite accurately described by an appropriately chosen ensemble of complex fields (also called, classical or c-fields) [1–4]. Examples include quantum gases of ultracold atoms, coherent light fields, and solid state polariton systems. A common feature is the appearance of collective behavior that strongly fluctuates away from the mean field. In quantum many-body systems where this is important, such ensembles of complex fields are often the only practical way to obtain information on fluctuations, single realizations of the system or full distribution functions [1–4]. In the absence of sufficient in situ experimental resolution, the approach is commonly used like a flight recorder to give information on the dynamics of the system before its detection in destructive time-of-flight images.

Though the term “classical” is used, we are talking about the opposite regime to the usual gas of classical particles. Here it is the collective field that has classical properties such that each member of the ensemble could be non-destructively tracked, while the particles lose their individual identity. Examples of such approaches include classical field ensembles [1, 3, 5, 6], Stochastic Gross-Pitaevski equations [2, 7, 8], and the truncated Wigner representation [9–11] for ultracold atoms, and the open stochastic classical field equations for polaritons [12, 13]. Stochastic mean field theory, is a related approach for fermions in e.g. heavy ion collisions [14, 15].

Qualitatively, the condition for the applicability of classical fields to bosons is that the relevant physics can be captured by considering only the highly occupied single-particle modes. Poorly occupied modes above an energy cutoff need to be discarded to avoid pathological behavior such as the UV catastrophe known since late 19th century physics.

However, the matter of just where to draw the line and how accurate the description is, has been a matter of much contention and ambiguity. The history of applying classical fields to ultra cold atomic gases teaches us that accuracy has depended quite strongly on the choice of the high energy cutoff and the observables studied. Past numerical benchmarking [10, 16–24] and also analytical [21, 22] and purely mathematical studies [27] of various single observables have found that it is possible to achieve good to very good agreement, but the details of the recipe vary from study to study.

Here, we intend to make these dependencies clear, and will show that under certain conditions the classical field approximation can be treated as more than just a qualitative guide, but gives predictions that are correct within small error bounds for a wide range of observables.

We will use the case of an ideal gas in the local density approximation (LDA) in the thermodynamic limit. That is, we will consider pieces of the gas cloud having a certain local density. Then it is natural to work in the grand canonical ensemble (GCE), where the rest of the system acts as the particle and thermal reservoir. Such a model underpins more general behavior, and it will be seen that several important conclusions can be reached.

We will first find the temperature dependent “eigen” cutoffs that allow the classical fields to correctly match the density and one other observable. Subsequently, we will determine the resulting errors in other observables, and the cutoff that minimizes the systematic error across the whole range of low order observables. This will tell us about the temperature range over which an accurate complex field description of the system is at all possible.

Classical Field description. The essence of the classical fields method is to replace annihilation (creation) operators $a_k (a_k^\dagger)$ of single particle modes in field operator by complex amplitudes $\xi_k (\xi_k^*)$ which is warranted when occupation is macroscopic. Then we can write:

$$\hat{\Psi}(x) = \sum_k a_k \psi_k(x) \rightarrow \left\{ \sum_{k \in C} \xi_k \psi_k(x) \right\}$$ (1)

where $\psi_k(x)$ is the wave function for the $k$th mode and $C$ is the low energy subspace below the cutoff. In general, it should be understood that $\hat{\Psi}(x)$ corresponds to an ensemble $\{...\}$ of complex field realizations, each with its own set of amplitudes $\xi_k$. Since we will be considering uniform sections of the gas, plane wave modes $k \equiv k_e$ are the most convenient, with momentum cutoff $k_e$ so that only modes $|k| < k_e$ are included in $C$. 


The properties of the uniform dilute gas with contact interaction strength $g$ can be encapsulated by two dimensionless parameters: $\gamma = \frac{mz^2}{\hbar^2 n}$ and reduced temperature:

$$\tau = \frac{T}{T_d} = \frac{1}{\sqrt{2\pi}} \frac{mk_B T}{\hbar^2 n^{2/d}}$$

where $T_d$ is the usual quantum degeneracy temperature in $d$ dimensions with one particle on the thermal de Broglie wavelength $\Lambda_d = \sqrt{\frac{2\hbar^2}{mk_B}}$ scale. It is convenient to define a dimensionless cutoff:

$$f_c = \frac{k_c \Lambda_T}{2\pi}$$

in units of $\Lambda_T$. A value of $f_c = 1$ corresponds to a cutoff at an energy of $\pi k_BT$. We will work in the following units: $\Lambda_T = 1$ and $\hbar = m = 1$, where $m$ is the mass of particles. As result of dealing with an ideal gas ($\gamma \to 0$) there is one physical parameter characterizing the system – the temperature $\tau$, and one technical parameter $f_c$ for the classical fields description. Phase space density equal to one occurs at $\tau = \tau_0 = \{1.539, 1.443, 1.368\}$ in $1d$, $2d$ and $3d$ respectively.

The great majority of experiments concentrate on low order observables such as phase, density or their fluctuations. We will analyze the following:

1. $n$ – density
2. $\varepsilon$ – kinetic energy per particle
3. $l_{pg}$ – phase grain length
It is the size of a coherent region, which we will calculate by $l_{pg} := \frac{1}{n} \int dz \langle \hat{\Psi}(0) \hat{\Psi}(z) \rangle = \int dz g^{(1)}(z)$.

In the quasicondensate regime, when $g^{(1)}(z) \simeq e^{-|z|/l_o}$, $l_{pg}$ equals the phase coherence length $l_o$.

4. $g^{(2)}(0)$ – normalized local density fluctuations
5. $u_G$ – coarse-grained density fluctuations
It is defined as $u_G := \frac{\langle N^2 \rangle - \langle N \rangle^2}{\langle N \rangle} = n \int dz [g^{(2)}(z) - 1] + 1$, where $N$ is the atom number in a region much larger than the density correlation length and $dN = N - \langle N \rangle$. This intensive thermodynamic quantity appears in experimental work [28, 29] and it compares the measured fluctuations in a pixel to Poisson shot noise.

6. $\rho_o$ – condensate fraction
7. $a_r$ – coherence half width
In the presence of the condensate $l_{pg}$ (and $u_G$) diverges, because $g^{(1)}(z \to \infty) = \rho_o$. In light of this we need another measure of the width of phase fluctuations, and will define it by $g^{(1)}(a_r) = \frac{1}{2}(1 + \rho_o)$.

We will compare the predictions of the above observables by classical fields to the exact ideal Bose gas values in the thermodynamic limit. The LDA approximation requires first the density to be correct. A sum over Gibbs factors gives the exact Bose gas density $n(\mu^{(id)})$ and the density estimate $n^{(c)}(\mu^{(c)}, f_c)$ in classical fields as functions of their chemical potentials. We invert these, and with the help of Eq. (2) obtain $\mu^{(id)}(\tau)$ and $\mu^{(c)}(\tau, f_c)$. Other observables e.g. $\varepsilon^{(id)}(\tau)$ and $\varepsilon^{(c)}(\tau, f_c)$ can then be expressed as functions of $\tau$ and $f_c$, as well.

While for the Bose ideal gas, $\tau$ and the choice of units specify all properties of the system, in classical fields choosing $\mu^{(id)}$ and $\mu^{(c)}$ using the same value of $\tau$ only makes the densities agree. The cutoff $f_c$ can be chosen to make one additional observable agree as well, but in general, not all.

The 3d case has an additional feature. The critical temperature in classical fields is cutoff dependent, $T_C^{(c)} = \left[4f_c\right]^{-2/3}$, while in the Bose gas it is $T_C = [\zeta(3/2)]^{-1/3} = \zeta(3/2)$. The critical temperatures are directly related as $\rho^{(id)} = \left[1 - (\tau/T_C^{(id)})^2\right]$ and $\rho^{(c)} = \left[1 - (\tau/T_C^{(c)})^2\right]$. Hence, $f_c^{(c)} = \frac{\zeta(3/2)}{4}$ makes $\rho^{(id)}$ and $\rho^{(c)}$ equal for all $\tau \leq T_C$.

Single observable “eigen” cutoffs: Fig. I shows how such cutoffs matched to different observables (which we will call eigen cutoffs) behave as a function of temperature. We have not shown results for $g^{(2)}(0)$ because it is always correctly predicted to be $g^{(2)}(0) = 2$ for every cutoff (at least in the ideal gas).

The high temperature behavior is qualitatively similar in all dimensions. The eigen cutoffs matched to energy per particle $f_c$ and to coherence half width $f_c^{(c)}$ rise to constant values, while the eigen cutoff matched for density fluctuation $f_c^{(d)}$ drops to zero (take note for this later). The $f_c^{(d)}$ takes intermediate values and is almost constant. An unexpected feature is the similar behavior of cutoffs corresponding to $a_r$ and $\varepsilon$ rather than the $a_r$ and $l_{pg}$ that are more related physically.

The crossover to low temperature behavior is around $\tau = 1$. In the low temperature regime most eigen cutoffs collapse to a common value (0.436 and 0.564, in 1d and 2d, respectively), except for $f_c$ which prefers

![FIG. 1. Matched eigen cutoffs $f_c$ for several observables as a function of temperature $\tau$ (black solid line, $a_r$ – purple line, $l_{pg}$ – green line, $u_G$ – red line, $\rho_o$ – orange line). The top panels (a), (b) show 1d and 2d cases, respectively, and the bottom panels present the 3d situation with (d) a magnification of the critical region. The Bose gas critical temperature $T_C$ is marked as a vertical dashed line, while the black solid line shows the $f_c$ value below which condensation of classical fields occurs.](image-url)
FIG. 2. Variation of the relative errors $\delta_\alpha$ of observables with cutoff $f_c$ at representative high and low temperatures $\tau$. Colors like in Fig. 1 Top row: 1d, second row: 2d, third row: 3d above $\tau_C$, last row: 3d below $\tau_C$.

The higher values 0.653 and 0.724. In 3d, the cutoffs at $\tau \to 0$ are 0.783, 0.753, and 0.653 for $\varepsilon$, $a_r$, and $\rho_o$, respectively.

Noteworthy points: (⋆) in 2d, the eigen cutoff $f_c = 1/\sqrt{\pi}$ that gives the correct phase grain length $l_{pg}$ does not depend on temperature, and (⋆⋆) the wave-like behavior of $f_c^{\tau = 0}$ in 1d (as well as in 2d), that comes from oscillations of $g^{(1)}(z)$ with distance, is caused by the sharp cutoff in momentum space in classical fields.

Relative errors of single observables. Now, how does a non-optimal choice of $f_c$ affect the observables, and their systematic error? This is relevant for practical considerations. For one thing, in a nonuniform system, when the cutoff is matched in one spatial region, it is good to know the sensitivity of results in other regions with a different density on this choice of $f_c$. Furthermore, we need this information to judge how good the classical fields are in describing the system overall.

The relative error $\delta_\alpha$ of an observable $\alpha$ is:

$$\delta_\alpha(\tau, f_c) := \frac{\Delta \alpha}{\alpha} = \left( \frac{\alpha^{(\tau)}(\tau, f_c)}{\alpha^{(\tau, f_c)}(\tau)} - 1 \right)$$

This is shown in Fig. 2. The first observation is that the relative error of energy per particle has an opposite trend to the other quantities. The resulting mismatch is the strongest restriction on the $f_c$ range for which all $\delta_\alpha$ errors are small.

Secondly, in 1d the known fact 2 that $g^{(1)}(z)$ and $g^{(2)}(z)$ do not depend on cutoffs at low $\tau$, is reflected in small errors in $l_{pg}$, $u_G$, and $a_r$. However these errors are no longer small in higher dimensions. As temperature drops, the $\delta_\alpha(\tau, f_c)$ except for $\delta_\varepsilon$, collapse onto curves that stay invariant with $\tau$ and remain steep (the $\tau = 0.08$ and $\tau = 0.05$ panels in Fig. 2. In other words, observables remain sensitive to cutoff all the way down to zero temperature in 2d and 3d.

Global error. What does it take to match all, or at least to be close to all typical observables? Let us consider the global error estimator

$$RMS_{\alpha_1, \alpha_2, ..., \alpha_n}(\tau, f_c) = \sqrt{\left( \delta_{\alpha_1} \right)^2 + \left( \delta_{\alpha_2} \right)^2 + ...}$$

This is a root mean square of the relative errors of chosen observables $\alpha_1, \alpha_2, ...$. Each relative error will, by definition, be less than $RMS$. The main aim of the function $RMS$ will be to catch inaccuracy in any observable.

We have studied the $RMS_{\alpha_1, \alpha_2, ..., \alpha_n}$ with all the observables that we have been considering. Moreover, we also took various combinations of them. It turns out that when we include just $u_G$ and $\varepsilon$, all relevant features that were seen with larger sets of observables are covered. This happens because these quantities are the most “extreme” in terms of the behavior of eigen $f_c$ and of the values and trends of $\delta_\alpha$. This is seen in Figs. 1 and 2. Also, the pair $(\varepsilon, u_G)$ includes observables of 2nd and 4th order in $\Psi$, which are the two main classes measured in experiments. We will use them to define the quantity:

$$RMS(\tau, f_c) = \sqrt{\left( \delta_{\varepsilon} \right)^2 + \left( \delta_{u_G} \right)^2 + ...}$$

that will be our indicator of the overall accuracy and applicability of the classical fields approximation. Below $\tau_C$ in 3d, the condensate fraction $\rho_o$ will be used instead of $u_G$.

Minimizing Eq. 5 at a given temperature will give the optimal cutoff momentum and minimum error indicator $minRMS$. For example, a $minRMS$ value below 0.1 (i.e. < 10% error in observables) is often satisfactory and we will take it as a guideline.

Fig. 3 shows the results for the 1d gas. Global error $RMS$ is very large above the degeneracy temperature $\tau = 1$. For low temperatures it falls to zero, as one would hope. According to our 10% guideline, classical fields should give acceptable results up to $\tau = 0.00716$. The best choice of $f_c$ is fairly invariant with temperature, being in the range (0.655±0.035). In fact, if we choose the average value of $f_c$, we will be close to absolute $minRMS$ regardless of temperature or density. At high $\tau$ an extra second branch appears that is associated with a local minimum of $RMS$ with large errors in $\varepsilon$ and small in $u_G$. It is not of practical importance for us.

Fig. 4 shows the results for the 2d gas. The behavior at low temperature is surprisingly bad. $RMS$ never falls below 0.333. This is a consequence of an inability to satisfy both observables $u_G$ and $\varepsilon$. Their relative errors $\delta_{\varepsilon(u_G)}(\tau, f_c)$ become stuck on the curves shown in the fourth plot of Fig. 2 whenever $\tau \leq 0.08$ and do not cross near zero error. One wonders whether this situation ($minRMS$ well above 10% as $\tau \to 0$) is repeated
for other different sets of observables? It turns out that even the pairs $(\varepsilon, l_{pg})$ or $(\varepsilon, \alpha_r)$ will lead to similar large $\min RMS$ values. In fact, no combination that includes $\varepsilon$ and any other observable will work well, because the $\delta_\alpha(\tau, f_c)$ curves are invariant. The crucial and a priori not so obvious conclusion is that in 2$d$, in the small temperature regime the classical fields description is wrong in the ideal gas.

Fig. 3 shows the results for the 3$d$ gas. The area above critical temperature behaves analogously to low dimensions. However, around the critical temperature, the $RMS$ curve narrows and the accuracy of classical fields becomes very sensitive to the choice of the cutoff $f_c$. This is related to the fluctuations $u_G$ growing to infinity at $\tau_C$. In the condensed regime below $\tau_C$, the $RMS$ curve widens out again while classical fields rapidly become accurate with $RMS < 10\%$ below $\tau = 0.486 \tau_C$.

The case of the uniform GCE is closely related to a trapped canonical ensemble (CE) gas, since the main bulk of the trapped gas is effectively a uniform open system in the $LDA$. Indeed, the low $\tau$ cutoffs for a trapped CE gas [21], whose energies correspond to values of $f_c^{(CE-trap)} = \{0.56, 0.72, 0.84\}$, are fairly close to the GCE values $\omega_{opt}^{CE-box} = \{0.65, 0.64, 0.78\}$ found here (Figs. 4[5]. On the other hand, the uniform CE in a box has much lower $f_c^{(CE-box)} = \{0.30, 0.47, 0.65\}$, and describes very different physics.

The reason for the drop of $f_c^{(id)}$ to zero at high $\tau$ provides an instructive example of how the classical field description breaks down. The root cause lies in the different statistics of particle numbers $N_k$ in the modes: Poissonian for the Bose gas ($\var[N_k^{(id)}] = \langle N_k^{(id)} \rangle$) when $N_k \ll 1$, and exponential for classical fields ($\var[N_k^{(cl)}] = \langle N_k^{(cl)} \rangle^2$). Due to the fact of independent modes, $u_G = \sum_k \var[N_k] / \sum_k \langle N_k \rangle$, and in the Bose gas $u_G \to 1$. To obtain the same with classical fields, occupations $N_k^{(cl)} \sim 1$ are necessary. These are much greater than in the Bose gas, so to also match density the cutoff must be much lower than the Bose gas momentum width $2\pi/\Lambda_T$. From [26], this immediately implies $f_c^{(id)} \ll 1$. With such a great modification to $N(k)$, matching additional observables like $\varepsilon$ becomes out of the question.

A similar breakdown can be expected whenever the physics is captured by low-occupied independent modes. For example, such discrepancies were seen between experiment and classical fields in the quantum Bogoliubov regime of the interacting gas at very low temperatures [28].

The crossover from effectively ideal gases to interacting ones depends on various factors including finite size (see [20] for a detailed discussion). A number of heuristic ways to modify ideal gas expectations and choose the cutoff in the interacting regime have been used in the past [1, 4, 6, 14, 26, 27]. Ongoing studies of how globally optimal cutoffs and $RMS$ values become modified by interactions will be described in a later work.

To conclude, we have judged the goodness of classi-
cal fields for describing the ideal Bose gas in 1\textit{d}, 2\textit{d}, and 3\textit{d} using all the commonly measured observables. The essence of the matter can be captured by the indicator \textit{RMS} based on energy per particle and coarse grained density fluctuations, which are the observables that are the hardest to mutually satisfy. While we can always match density and one other observable with some choice of cutoff momentum \(f_c\), the breakdown of classical fields in the high temperature Boltzmann gas is evidenced by the inability to correctly describe \(\varepsilon\), \(u_G\) and \(n\) simultaneously. Surprisingly, we have found that in the 2\textit{d} gas, classical fields remain incapable of this at any temperature, even \(T \to 0\). On the other hand, we have shown that 10\% or better accuracy in the whole set of usual observables is possible in 1\textit{d} up to temperatures of \(T = 0.0072T_d\) with the prescription \(k_c \approx 0.65\left(\frac{2\pi}{\Lambda T}\right)\) and in 3\textit{d} up to \(T = 0.49T_c\) with \(k_c \approx 0.78\left(\frac{2\pi}{\Lambda T}\right)\).

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