

Quantum Criticality

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We investigate the theory of quantum fluctuations in non-equilibrium systems having large critical fluctuations. This allows us to treat the limits imposed by nonlinearities to quantum squeezing and noise reduction, and also to envisage future tests of quantum theory in regions of macroscopic quantum fluctuations. A long-term objective of this research is to identify suitable physical systems in which macroscopic ‘Schrödinger cat’-like behaviour may be observed. We investigate two systems in particular of much current experimental interest, namely the degenerate parametric oscillator near threshold, and the evaporatively cooled (BEC). We compare the results obtained in the positive- P representation, as a fully quantum mechanical calculation, with the truncated Wigner phase space equation, also known as semi-classical theory. We show when these results agree and differ in calculations taken beyond the linearized approximation. In the region where the largest quantum fluctuations and Schrödinger cat-like behaviour might be expected, we find that the quantum predictions correspond very closely to the semi-classical theory. *Nature abhors observing a Schrödinger cat.* – Pacs: 03.65.Bz

Key words: Quantum Fluctuations; Bose-Einstein-Condensate (BEC).

I. Introduction

A question of much current interest in the foundations of quantum theory is the issue of how one can observe a ‘Schrödinger cat’ – namely, a quantum system in a macroscopic superposition state. Apart from philosophical questions, this would test quantum theory in a new and important regime. It is already commonplace to talk of quantum states of the Universe; but before this, one would like to ensure that quantum mechanics is completely valid for, say, the 10^{23} particles in ordinary macroscopic objects.

Currently, the most stringent tests of quantum superpositions or quantum entanglement are restricted to Bell inequality tests involving only one or two particles. This is not macroscopic at all. Nevertheless, quantum Bell inequality tests are not restricted to only two particles, and Bell inequality violations are predicted by quantum mechanics for correlated and entangled systems of arbitrary particle number [1]. Following developments in squeezed-state generation [2] and quantum correlations [3], a consider-

able breakthrough was achieved by Kimble [4] in the observation of the original continuous variable EPR paradox. This followed earlier theoretical predictions about quadrature phase correlations [5], and involves relatively large numbers of photons. It could be extended to a macroscopic EPR test provided certain conditions on causality and local oscillators were utilized.

One must ask how does one generate *entangled* states of macroscopic size, since this is more useful than just a quantum superposition, and could in principle provide a signature for a quantum Schrödinger cat. In order to answer this question, it is essential to find out how to calculate what quantum mechanics predicts! Suitable quantum systems that might generate entanglement are typically nonlinear. Accordingly, we present here some test cases of non-equilibrium quantum fluctuations; in particular the degenerate parametric oscillator near threshold, and the evaporatively cooled BEC. In the region where the largest quantum fluctuations and Schrödinger cat-like behaviour might be expected, we find that the quan-

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tum predictions generally correspond very closely to the semi-classical theory.

This result indicates that it is far from trivial to generate a quantum Schrödinger cat whose properties can be readily distinguished from those predicted by alternate hidden variable theories. This may provide comfort to supporters of quantum mechanics who wish to reconcile its paradoxical view of reality with the usual macroscopic view. On the other hand, it suggests that a test of macroscopic quantum mechanics is a real scientific challenge for the new century.

A) Quantum Dynamics

In order to understand the nature of the problems we face in calculating quantum criticality, it must be realized that these are essentially non-equilibrium many-body problems. Therefore, we face the difficulty that such problems are conventionally regarded as insoluble, and hence not feasible as either analytic or computational problems.

The following quotes can be used to illustrate this:

- “Can a quantum system be probabilistically simulated by a classical universal computer? ... the answer is certainly, No!” (R. P. Feynman [6]).
- “Quantum Molecular Dynamics does not exist in any practical sense... One is forced to either simulate very small systems (i. e. less than five particles) or to make serious approximations.” (D. M. Ceperley [7]).

We take the point of view here that the real world *is* a many-body quantum dynamical problem, and it is necessary to at least try to solve these problems. They are certainly difficult, but not totally insoluble. As evidence for this assertion, results will be given for many-body simulations of the development of Bose-condensation via evaporative cooling of $n = 10,000$ atoms in $m = 32000$ trap modes. This corresponds to a Hilbert space with $(m+n)!/(m!n!) = 10^{10000}$ states, using standard combinatoric theory.

B) +P Representation

The methods used here will rely in the coherent-state positive P -representation [8] of quantum optics, and its extension to functional coherent state representations of fields. We emphasize that other methods may well work better, as the positive P -representation has well-known problems to do with sampling error and boundary terms when the damping is too small. Despite this, it is the only technique yet proven to

work reliably for these types of quantum dynamical problems.

The method consists of the following steps, in the case of a scalar bosonic field ψ :

- Expand the quantum density matrix $\hat{\rho}$ in off-diagonal coherent state projection operators:

$$\hat{\rho} = \int P(\psi_1, \psi_2) \frac{|\psi_1\rangle\langle\psi_2|}{\langle\psi_2|\psi_1\rangle} \mathcal{D}\psi_1 \mathcal{D}\psi_2.$$

- $\mathcal{D}\psi_1, \mathcal{D}\psi_2$ are the functional measures over functional coherent states $|\psi_1\rangle$.
- $P(\psi_1, \psi_2)$ is a positive distribution function which exists for all density matrices.
- When the boundary terms in the integration vanish, P is governed by a Fokker-Planck equation (FPE).
- The FPE leads to two stochastic phase-space equations for each classical phase-space variable.

This method was developed from earlier representation theory methods used in laser theory. It was used, for example, in the first successful prediction of quantum soliton behaviour in optical fibers, which was later verified experimentally [9]. We will also give some comparisons with a truncated version of the Wigner representation, which is equivalent to stochastic electrodynamics – a hidden variable theory. The philosophy here is a very simple one; if the same behaviour can be calculated from both quantum theory and a hidden variable theory, then we must conclude that the quantum state in question is rather classical and shows no extreme quantum paradoxes of a type that has no possible realistic description.

II. Critical Point of a Parametric Amplifier

As a first example of quantum criticality, we investigate the question of how to obtain the most quantum squeezing from that useful tool, the degenerate parametric amplifier. The standard theory predicts that this occurs at the threshold for parametric oscillation, when the quantum fluctuations in one quadrature are zero, while those in the other are infinite. Linearized perturbation theory breaks down at this point, and its predictions are both mathematically unreliable, and completely unphysical.

In the case of pure down-conversion, with just a second-harmonic, the interaction Hamiltonian [10] is the standard one for a non-degenerate, single-mode parametric amplifier or oscillator:

$$H/\hbar = i\mathcal{E}[\hat{a}_2 - \hat{a}_2^\dagger] + \frac{i\chi}{2}[\hat{a}_2\hat{a}_1^{\dagger 2} - \hat{a}_2^\dagger\hat{a}_1^2] \\ + (\text{Reservoirs}).$$

Here \hat{a}_1, \hat{a}_2 represent the fundamental and second-harmonic modes, χ is proportional to the optical non-linearity, while \mathcal{E} is proportional to the coherent driving field at the second-harmonic frequency. In the classical limit, the system has the well-known classical equations of intra-cavity parametric oscillation, where we define $\alpha_i = \langle \hat{a}_i \rangle$, and hence obtain, in the interaction picture:

$$\frac{d\alpha_1}{dt} = -\gamma_1\alpha_1 + \chi\alpha_1^*\alpha_2, \\ \frac{d\alpha_2}{dt} = -\gamma_2\alpha_2 + \mathcal{E} - \frac{1}{2}\chi\alpha_1^2. \quad (2.1)$$

These equations are valid in the limit of large photon number. They are obtained by the use of a classical decorrelation in which all operator products are assumed to factorize, so that $\langle \hat{a}_i^\dagger \hat{a}_j \rangle \simeq \langle \hat{a}_i^\dagger \rangle \langle \hat{a}_j \rangle$, and $\langle \hat{a}_i \hat{a}_j \rangle \simeq \langle \hat{a}_i \rangle \langle \hat{a}_j \rangle$. The solution of these equations is immediate classically and has the property that there is a phase transition at the critical driving field of $\mathcal{E} = \mathcal{E}_c$. For driving fields below this value, one has

$$\alpha_1 = 0, \\ \alpha_2 = \mathcal{E}/\gamma_2, \quad (2.2)$$

while for fields above this value, the signal field α_1 is bistable, with

$$\alpha_1 = \pm \sqrt{\frac{2}{\chi}(\mathcal{E} - \mathcal{E}_c)}, \\ \alpha_2 = \frac{\gamma_1}{\chi}. \quad (2.3)$$

It is the behaviour in the critical region that we are most interested in, as the usual linearized methods break down. Just above the critical region, we see that the quantum system has some of the character of a Schrödinger 'cat'. There are two possible values for the sub-harmonic amplitude α_1 , and the system prior to detection may be in a superposition state of these amplitudes.

A) Positive- P Equations

The following stochastic [11] equations are obtained for any driving field \mathcal{E} :

$$d\alpha_1 = [-\gamma_1\alpha_1 + \chi\alpha_1^*\alpha_2]dt + \sqrt{\chi\alpha_2}dw(t), \\ d\alpha_1^* = [-\gamma_1\alpha_1^* + \chi\alpha_1\alpha_2^*]dt + \sqrt{\chi\alpha_2^*}dw^*(t), \\ d\alpha_2 = [-\gamma_2\alpha_2 + \mathcal{E} - \frac{1}{2}\chi\alpha_1^2]dt, \\ d\alpha_2^* = [-\gamma_2\alpha_2^* + \mathcal{E} - \frac{1}{2}\chi\alpha_1^{*2}]dt.$$

Here the terms γ_k represent the amplitude damping rates. All stochastic means and correlations vanish, except

$$\langle dw(t)dw(t) \rangle = \langle dw^*(t)dw^*(t) \rangle = dt.$$

This means that $dw(t), dw^*(t)$ represent two real Gaussian, uncorrelated stochastic processes.

B) Wigner Representation

The Wigner representation may also be used to treat this problem, but it leads to a Fokker-Planck equation with third-order derivatives, which therefore has no stochastic equivalent. This is just due to the well-known fact that the set of positive Wigner functions is not a complete basis for all quantum mechanical states.

If we truncate the third derivative of the phase space equation we get a genuine Fokker-Planck type equation with positive definite diffusion constant [12]. This can be mapped into the following Itô stochastic differential coupled equations:

$$d\alpha_1 = [-\gamma_1\alpha_1 + \chi\alpha_1^*\alpha_2]dt + \sqrt{\gamma_1}dw_1(t), \\ d\alpha_1^* = [-\gamma_1\alpha_1^* + \chi\alpha_1\alpha_2^*]dt + \sqrt{\gamma_1}dw_1^*(t), \\ d\alpha_2 = [-\gamma_2\alpha_2 - \frac{\chi}{2}\alpha_1^2 + \mathcal{E}]dt + \sqrt{\gamma_2}dw_2(t), \\ d\alpha_2^* = [-\gamma_2\alpha_2^* - \frac{\chi}{2}\alpha_1^{*2} + \mathcal{E}]dt + \sqrt{\gamma_2}dw_2^*(t). \quad (2.4)$$

Here $dw_k(t)$ is now a *complex* Gaussian white noise whose mean and variance are given by

$$\langle dw_k(t) \rangle = 0, \\ \langle dw_k(t)dw_l^*(t) \rangle = \delta_{kl}dt. \quad (2.5)$$

III. Perturbation Theory

The crucial quadrature variables of the system have the definitions

$$\begin{aligned}\hat{x}_j &= (\hat{a}_j + \hat{a}_j^\dagger), \\ \hat{y}_j &= \frac{1}{i}(\hat{a}_j - \hat{a}_j^\dagger).\end{aligned}\quad (3.1)$$

In order to solve these coupled equations systematically, we introduce an expansion parameter g – the ratio of nonlinear to linear rates of change:

$$g = \frac{\chi}{\sqrt{2\gamma_1\gamma_2}}. \quad (3.2)$$

A) Below Threshold Perturbation Theory

Next, we introduce a scaled time $\tau = \gamma_1 t$, a dimensionless driving field $\mu = \chi\mathcal{E}/(\gamma_1\gamma_2)$, and a dimensionless decay ratio $\gamma_r = \gamma_2/\gamma_1$, so that the equations can be expressed in terms of the three dimensionless parameters g, μ, γ_r . Finally, we expand the scaled coordinates in a power series in g , to give

$$\begin{aligned}x_1 &= \sum_{n=0}^{\infty} g^{n-1} x_1^{(n)}, \\ y_1 &= \sum_{n=0}^{\infty} g^{n-1} y_1^{(n)}, \\ x_2 &= \frac{1}{\sqrt{2\gamma_r}} \sum_{n=0}^{\infty} g^{n-1} x_2^{(n)}, \\ y_2 &= \frac{1}{\sqrt{2\gamma_r}} \sum_{n=0}^{\infty} g^{n-1} y_2^{(n)}.\end{aligned}\quad (3.3)$$

The expansion given here has the property that the zero-th order term corresponds to the large classical fields of order $1/g$, while the first order term corresponds to the quantum fluctuations of order 1, and the higher order terms correspond to nonlinear corrections to the quantum fluctuations, of order g and greater.

B) Spectral Correlations

These can be calculated directly from the Fourier transform of the stochastic equations, where Ω is the scaled frequency. The observed squeezing variance is obtained using quantum input/output theory [13, 14] assuming no losses apart from the output coupler. The result, including the lowest nonlinear corrections, is [15]

$$\begin{aligned}V(\Omega) &= 1 - \frac{4\mu}{\Omega^2 + (1 + \mu)^2} + \frac{4g^2\mu^2\gamma_r}{[\Omega^2 + (1 + \mu)^2]^2} \\ &\cdot \left\{ \frac{\Omega^2 + 1 - \mu^2}{2\mu\gamma_r(1 - \mu^2)} + \frac{(1 - \mu + \gamma_r)(1 + \mu) - \Omega^2}{(1 - \mu)[\Omega^2 + (1 - \mu + \gamma_r)^2]} \right. \\ &\quad \left. - \frac{(1 + \mu + \gamma_r)(1 + \mu) - \Omega^2}{(1 + \mu)[\Omega^2 + (1 + \mu + \gamma_r)^2]} \right\}.\end{aligned}$$

C) Optimal Squeezing in Spectrum

Near threshold at $\mu = 1$, we find that the optimal spectral squeezing occurs at zero frequency, with $V(0) = [\delta^2 + 2g^2/\delta]/4$, where $\mu = 1 - \delta$. Minimizing with respect to the driving field provided γ_r is not too small, one finds that

$$V_{\text{opt}}(0) = \frac{3}{4}g^{4/3}.$$

This agrees with an approximate calculation of Pliam and Walls [16], and occurs at a driving field just below threshold, of

$$\mu_{\text{opt}} = 1 - g^{2/3}.$$

D) Critical Squeezing

Integrating over all frequencies gives the total squeezing or quadrature moment. This is a measure related to information, since it includes all possible spectral frequencies. We can calculate this using a different asymptotic perturbation theory [17] which is valid in the critical region, i. e., for $\mu \simeq 1$. Introducing a critical driving parameter $\eta = \delta/g$ to measure how close the driving field is to its value at the bifurcation threshold, one finds that the unsqueezed and squeezed variances are given, respectively, by [15]

$$\langle x_1^2 \rangle = \frac{1}{g} \frac{\int x^2 dx \exp(\eta x^2/2 - x^4/16)}{\int dx \exp(\eta x^2/2 - x^4/16)},$$

$$\langle y_1^2 \rangle_s = \frac{1}{2} - \frac{g\eta}{4} + \frac{g^2(2 + 3\gamma_r)X_1^2}{16(2 + \gamma_r)}.$$

The best total squeezing now occurs slightly above the critical point, due to line-broadening effects which give squeezing over a wider frequency range just above threshold.

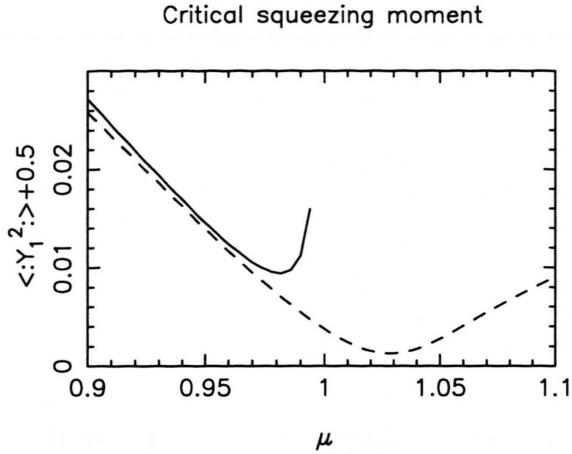


Fig. 1. Critical squeezing moment.

IV. Comparison: Below and Near Threshold

The results in Fig. 1 are for $g^2 = .001$, $\gamma_r = 0.5$. The solid line is the below-threshold perturbation theory which diverges at the critical point; the dashed line is asymptotic method valid in the critical region. Numerical simulation results agree with the dashed line, and have no divergence, as one might expect.

D) Summary of Critical Parametric Fluctuations

In summary, we can readily calculate large nonlinear critical fluctuations in the positive P-representation. These methods provide a test of quantum fluctuations beyond linearized theory. The asymptotic critical expansion agrees with numerical simulations. However, in the critical region, a careful study of the semi-classical equations shows that it gives exactly the same predictions; similar behaviour is known to occur near state-equation turning-points [18]. We have to conclude that in this region the quantum fluctuations, while large, cannot be regarded as having any uniquely quantum properties that we could ascribe to ‘Schrödinger cat-like [19]’ behaviour. In order to reach regimes that might show more differentiation, it seems that we must require lower damping, in order to remove any possible mechanism for turning superpositions into mixtures.

V. BEC Cooling Through the Critical Point

The Bose-Einstein condensate (BEC) that has been produced with trapped atomic samples of neutral atoms [20] is often described as the atomic equivalent

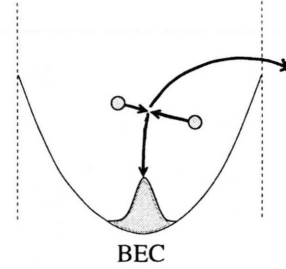


Fig. 2. Actual physics of BEC formation.

to laser light. BECs are a coherent matter waves characterized by what is called the off-diagonal long-range order parameter. Precise measurements of the momentum spread in recent experiments [21] have shown that the long-range order extends over the entire length of the condensate. Other interference experiments [22] have also confirmed the existence of this long-range coherence. But this does not mean that the condensate exists in a coherent state, for which it would have to possess coherence of all orders at all length scales. In fact the presence of inter-particle interactions means that the atom density is anti-correlated at short distances. There have been local measurements that demonstrate the existence of some forms of higher order coherence [23], but a complete description or confirmation of all the coherence properties of the condensate is not yet available.

To address important issues such as these about the nature of the condensate, a quantum mechanical simulation of the evaporative cooling process that leads to condensation must be undertaken. The final ground state of this many-body system is the result of a quantum dynamical process which is far from thermal equilibrium. This problem has been approached by many authors using various approximate methods. But to provide a benchmark for these treatments, and to precisely determine coherence properties, all the quantum effects must be included without approximation.

An illustration of the actual physics of BEC formation is presented in Figure 2.

This is essentially a dynamical problem. Initially we have a hot multi-mode system consisting of interacting particles in a finite trap. The cooling process does not involve phonon reservoirs. Instead, hot atoms collide, and under some circumstances one atom is slowed down to join the condensate, while another is speeded up to the point where it escapes from the

trap. Quantum fluctuations are clearly important near the critical point. We can ask the following questions:

- What state does the evaporation process lead to?
- Is it really in thermal equilibrium?
- What role does symmetry-breaking play?

To answer these questions, we can use quantum phase-space methods (quasi- probabilities) to calculate the quantum time-evolution under the full many-body Hamiltonian. This method retains quantum features and allows a full multi-mode simulation.

A) $+P$ Stochastic Equations

The resulting stochastic equations are very similar in form to the Gross-Pitaevskii equations, except that the phase-space has a doubled dimension, as usual in the positive P -representation:

$$i\hbar \frac{\partial \psi_j}{\partial t} = \left[\frac{-\hbar^2 \nabla^2}{2m} + V - \frac{i\hbar}{2} \Gamma + U \psi_j \psi_{3-j}^* + \sqrt{i\hbar U} \xi_j \right] \psi_j.$$

Here the meaning of the symbols is as follows:

- $j = 1, 2$; m = atomic mass,
- $V(\mathbf{x})$ = trapping potential,
- $\Gamma(\mathbf{x})$ = loss rate,
- U = atom-atom coupling.

The stochastic terms that generate the quantum noise have the following properties:

$$\langle \xi_i(t, \mathbf{x}) \xi_j(t', \mathbf{x}') \rangle = \delta_{ij} \delta(t - t') \delta(\mathbf{x} - \mathbf{x}').$$

The important quantity to calculate corresponds also to the most easily observed quantity – namely the atomic density in either position or momentum space:

$$N = \psi_2^* \psi_1 = \hat{\Psi}_2^+ \hat{\Psi}_1.$$

B) Summary of BEC Critical Fluctuations

We have carried out several first principles quantum simulations of BEC formation[24]. Results were limited by the stochastic sampling error, but were able to be carried to the point of a clear observation of a condensate, provided the simulations were carried out with relatively small condensates, without too strong a coupling. Thus, many-body quantum simulations are (just) feasible with digital computers. We found in this case it was not possible to carry out semi-classical simulations, owing to the ultra-violet divergence

of the multi-mode vacuum noise terms in this representation, causing large sampling errors.

Condensates typically were found to form in excited states, not in the ground state. Frequently, metastable vortices were observed in the numerical simulations. Importantly, we found that all condensates generated had some center-of-mass motion, indicating that the evaporative cooling process is not effective in cooling bulk motion, which therefore has a higher effective temperature than the relative motion internal to the condensate.

VI. Conclusion

Quantum criticality in either a parametric amplifier or evaporatively cooled Bose-Einstein condensate can be treated with stochastic methods in the $+P$ representation. The parametric amplifier, which is damped, is very straightforward. Up to 10,000 bosonic atoms, 32,000 modes, and hence 10^{10000} quantum states can be treated in the BEC case. Excellent results are obtained with this method in the sense that critical point behaviour can be simulated with relatively low sampling error for the parameters used here. In the BEC case, large sampling errors were found if the simulations were carried on for much longer than the initial time-scale required for BEC formation, due to decreasing loss rates. While no evidence was found for quantum paradoxes in either case as yet, it is clear that many-body quantum dynamics can indeed be treated in some cases. This opens up the possibility of new tests of quantum mechanical predictions in areas of macroscopic quantum fluctuations. In future, a promising direction for research is in the development of improved representations able to handle situations of low damping. To optimally test quantum mechanics in new regimes, we need to find ways to generate entangled macroscopic states of massive particles. This is a regime as yet unknown in any tests of quantum entanglement. A possible way to generate such intriguing quantum states is via the use of an atom-molecular coupled BEC [25] as a quantum parametric amplifier for squeezed and entangled matter-waves.

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