Non-ideal Boson system in the Gaussian approximation

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Abstract

We investigate ground-state and thermal properties of a system of non-relativistic bosons interacting through repulsive, two-body interactions in a self-consistent gaussian mean-field approximation which consists in writing the variationally determined density operator as the most general gaussian functional of the quantized field operators. Finite temperature results are obtained in a grand canonical framework. Contact is made with the results of Lee, Yang and Huang in terms of particular truncations of the gaussian approximation. The full gaussian approximation supports a free phase or a thermodynamically unstable phase when contact forces and a standard renormalization scheme are used. When applied to a Hamiltonian with zero range forces interpreted as an effective theory with a high momentum cut-off, the full gaussian approximation generates a quasi-particle spectrum having an energy gap, in conflict with perturbation theory results.
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1 Introduction

The non-relativistic interacting Bose gas is certainly among the most extensively investigated problems of many-body physics. Early interest in this problem has been strongly motivated by the low temperature properties of helium [1]. It has been sustained, on the theoretical side, by a persisting elusiveness of the deeper nature of the condensation process [2] and, on the experimental side, by developments which led to the recent observation of the more artificial Bose condensates [3]–[5].

Much of the persisting uneasiness about the condensation process of a nonideal boson gas hinges on the fact that the body of available results relies mainly on perturbative methods, a circumstance which tends to be considered as a liability. Nonperturbative approximation schemes have been developed, on the other hand, in connection with the problem of self-interacting, relativistic Bose fields which became relevant e.g. for inflationary models of the universe [6]. This problem has also been used as a testing ground for nonperturbative methods which could then be applied to more complicated systems of interacting fields. In this context, the gaussian variational approach [7] has received considerable attention, also in view of its relation to extended mean field methods traditionally employed in nonrelativistic many-body physics [8, 9, 10, 11].

The purpose of this paper is to describe an application of the gaussian variational approximation to the much studied problem of interacting nonrelativistic bosons in order to bring about a direct confrontation of this approach with at least part of the available results for this problem. We use a formulation [9] which is very close to the standard language of nonrelativistic, extended mean field approaches of the Hartree-Fock-Bogolyubov type, which can on the other hand be directly related to the methods adopted in connection with the Schrödinger representation of quantum field theory [10]. Although for simplicity we
restrict ourselves to the case of uniform systems, extending the formulation to finite, inhomo-
geneous systems such as those actually realized in the recent alkeli atom experiments is completely straightforward [8] using well known many-body techniques [12]. The inclusion of finite temperature effects is also straightforward in the formulation we use, so that thermodynamic properties can be studied rather easily. We show that several of the old results can be retrieved from truncated versions of the full gaussian approximation, including ground state energy and phonon spectrum. This last feature is lost when one adheres to the full gaussian approximation, notwithstanding the fact that it is supported theoretically by the Hugenholtz-Pines theorem [13, 14] to all perturbative orders, a feature which has been noted long ago by Girardeau and Arnowitz [15]. The phonon spectrum can be recovered in a generalized RPA treatment [16] or by using the functional derivative method developed by Hohenberg and Martin [17] and recently re-discussed by Griffin [18]. Problems of thermodynamic instability develop for contact forces when one uses a renormalization procedure in which the coupling constant is made to approach zero from it negative values, which has been considered in a relativistic context e.g. by Bardeen and Moshe [19] and which has also been extensively discussed by Stevenson as the “precarious” renormalized $\lambda \phi^4$ theory [20] and more recently by Türköz [10] and by Kerman and Lin [11].

The formulation which we adopt is reviewed in Section 2, where the formal, finite temperature equilibrium solutions for a contact repulsive interaction are obtained. A truncated version of the gaussian variational equations is analyzed in Section 3. In Section 4, we deal with the full gaussian approximation. Two different prescriptions for dealing with the divergences are considered. The first one involves a renormalization scheme related to that proposed by Stevenson. As a second, alternative scheme we treat the Hamiltonian with contact interactions as an effective theory to be implemented with a fixed cut-off in momentum
space. Numerical results are given in this case for properties of the different phases and phase equilibria. Section 5 contains our conclusions.

2 Thermal gaussian approximation

We consider an extended, uniform and isotropic system of non-relativistic, interacting, spinless bosons described by the Hamiltonian (in momentum representation with periodic boundary conditions in volume $V$)

$$H = \sum_{k} e(k) a_{k}^\dagger a_{k}^\dagger + \frac{\lambda}{2V} \sum_{k_1 k_2 q} a_{k_1 + q}^\dagger a_{k_2 - q}^\dagger a_{k_2} a_{k_1}$$

where $e(k) = \frac{\hbar^2 k^2}{2m}$ is the free particle kinetic energy, and the contact repulsive ($\lambda > 0$) interaction between a pair of particles is $\lambda \delta(\vec{r} - \vec{r}')$. The field operators satisfy standard boson commutation relations. Within a grand canonical description the state of the system is described by the density operator

$$\mathcal{F} = \frac{1}{Z} e^{-\beta \mathcal{H}}$$

where $\mathcal{H} = H - \mu N$, $N$ being the boson number operator, and $Z$ the grand canonical partition function

$$Z = \text{Tr} e^{-\beta \mathcal{H}}.$$

Following the variational approach of Balian and Vénéroni [21], we look for extrema of the object

$$f(M) = \text{Tr} e^{-M}$$

under the constraint $M - \beta \mathcal{H} = 0$, which is taken into account through the introduction of a Lagrange multiplier matrix $B$. This leads to the variational problem
\[ \delta \Phi(M, B) = \delta Tr \left[ e^{-M} + B(M - \beta \mathcal{H}) \right] = 0. \] (2)

Variation of \( M \) gives \( B = e^{-M} \), and elimination of \( B \) from Eq. 2 leads to the \( M \)-dependent object

\[ \Phi(M, B) \rightarrow \Psi(M) = Tr \left[ e^{-M} (1 + M - \beta \mathcal{H}) \right]. \] (3)

Balian and Vénéroni show that \( Z \geq \Psi(M) \) for any \( M \). Defining \( z = Tr e^{-M} \) we can write

\[ e^{-M} = z \mathcal{F}_0 \]

where now \( Tr \mathcal{F}_0 = 1 \). Substituting this in Eq. 3 and varying \( z \) we find the variational expression for the grand potential \( \Omega \)

\[ \Omega = -\frac{1}{\beta} \ln Z \leq Tr [ (\mathcal{H} + KT \ln \mathcal{F}_0) \mathcal{F}_0 ] \] (4)

where \( \mathcal{F}_0 \) is an arbitrary density with unit trace, and we used the notation \( 1/\beta = KT \). In Eq. 4 we can in particular identify an entropy factor as \( S_0 = -K \ TR[\mathcal{F}_0 \ln \mathcal{F}_0] \).

The most general gaussian approximation consists in adopting for \( M \) an ansatz of the form [22]

\[ M \rightarrow \sum_{\vec{k}\vec{k}'}[A_{\vec{k}\vec{k}'} a_{\vec{k}}^{\dagger} a_{\vec{k'}} + (B_{\vec{k}\vec{k}'} a_{\vec{k}}^{\dagger} a_{\vec{k}'}^{\dagger} + h.c.) + (C_{\vec{k}} a_{\vec{k}}^{\dagger} + h.c.)] \]

where the matrix \( A_{\vec{k}\vec{k}'} \) is hermitean. The quadratic form appearing in \( M \) can be diagonalized by a general canonical transformation of the Bogolyubov type, which amounts to changing to the natural orbital representation of the extended one boson density corresponding to the gaussian density \( \mathcal{F}_0 \) [8, 9]. The uniformity and isotropy assumptions we make allow us to restrict this general ansatz so that \( A_{\vec{k}\vec{k}'} \) is diagonal, \( B_{\vec{k}\vec{k}'} \) vanishes unless \( \vec{k} = -\vec{k}' \) and both
of these matrices and the $C_{\vec{n}}$ depend only on the magnitudes of the momentum vectors. The diagonalization of the quadratic form is achieved in this case by defining transformed boson operators as

$$
\eta_{\vec{k}} = x_{\vec{k}} b_{\vec{k}} + y_{\vec{k}} b_{-\vec{k}}
$$

$$
\eta_{\vec{k}}^\dagger = x_{\vec{k}} b_{\vec{k}}^\dagger + y_{\vec{k}} b_{-\vec{k}}
$$

where

$$
b_{\vec{k}} = a_{\vec{k}} - \Gamma_{\vec{k}}
$$

and we have used the isotropy of the uniform system to make the c-number transformation parameters $x_{\vec{k}}$, $y_{\vec{k}}$ and $\Gamma_{\vec{k}}$ dependent only on the magnitude of $\vec{k}$. In order for this transformation to be canonical we have still to impose on the $x_{\vec{k}}$ and $y_{\vec{k}}$ the usual normalization condition

$$
|x_{\vec{k}}|^2 - |y_{\vec{k}}|^2 = 1.
$$

The trace-normalized gaussian density operator is now written explicitly as

$$
\mathcal{F}_0 = \prod_{\vec{k}} \frac{1}{1 + \nu_{\vec{k}}} \left( \frac{\nu_{\vec{k}}}{1 + \nu_{\vec{k}}} \right)^{\eta_{\vec{k}}^\dagger \eta_{\vec{k}}}
$$

Straightforward calculation shows that

$$
Tr(\eta_{\vec{k}}^\dagger \eta_{\vec{\kappa}} \mathcal{F}_0) = \nu_{\vec{k}} \delta_{\vec{k} \vec{\kappa}}
$$

so that the $\nu_{\vec{k}}$ are positive quantities corresponding to mean occupation numbers of the $\eta$-bosons. One also finds that

$$
Tr[(x_{\vec{k}}^* a_{\vec{k}} + y_{\vec{k}}^* a_{-\vec{k}}^\dagger)^n \mathcal{F}_0] = Tr[(\eta_{\vec{k}} + A_{\vec{k}})^n \mathcal{F}_0] = A_{\vec{k}}^n
$$
with \( A_k = x_k \Gamma_k + y_k \Gamma_k^* \) so that non vanishing values of the \( \Gamma_k \) correspond to coherent condensates of unshifted, Bogolyubov transformed bosons. We again invoke the system uniformity to impose

\[
\Gamma_k = \delta_{k,0} \Gamma_0
\]

in the calculations to follow.

It is important to note that the truncated density \( \mathcal{F}_0 \) in general breaks the global gauge symmetry of \( H \) which is responsible for the conservation of the number of \( a \)-bosons. The quadratic dispersion of the number operator \( N = \sum_k \hat{a}_k^\dagger \hat{a}_k \) in this state can in fact be obtained explicitly as

\[
\langle N^2 \rangle - \langle N \rangle^2 = 2|\Gamma_0|^2[|x_0|^2 \nu_0 + |y_0|^2(1 + \nu_0)] - 2\Gamma_0^2 x_0 y_0^* (1 + 2\nu_0) - \\
-2\Gamma_0^2 y_0 x_0^* (1 + 2\nu_0) + |\Gamma_0|^2 + \sum_k [|x_k|^2 \nu_k + (1 + \nu_k)|y_k|^2] + \\
+ \sum_k \{[|x_k|^2 \nu_k + (1 + \nu_k)|y_k|^2]^2 + |x_k|^2 |y_k|^2 (1 + 2\nu_k)^2 \}.
\]

Furthermore, mean values of many-boson operators taken with respect to \( \mathcal{F}_0 \) will contain no irreducible many-body parts, so that the replacement of \( \mathcal{F} \) by \( \mathcal{F}_0 \) amounts to a mean field approximation. The states described by \( \mathcal{F}_0 \) have therefore to be interpreted as “intrinsic” mean field states.

An important simplification which occurs in the case of stationary states such as we consider here is that the transformation parameters \( x_k, y_k \) and \( \Gamma_0 \) can be taken to be real and we can use a simple parametric representation that automatically satisfies the canonicity condition. It reads
\[ x_k = \cosh \sigma_k, \quad y_k = \sinh \sigma_k. \]  

(7)

It is then straightforward to evaluate the traces involved in Eq. 4 to obtain

\[ \Omega \leq \sum \left( e(k) - \mu + \frac{2\lambda \Gamma_0^2}{V} \right) \left[ \frac{(1 + 2\nu_k) \cosh 2\sigma_k - 1}{2} \right] - \mu \Gamma_0^2 + \frac{\lambda \Gamma_0^4}{2V} \]

\[ - \frac{\lambda \Gamma_0^2}{2V} \sum (1 + 2\nu_k) \sinh 2\sigma_k + \frac{\lambda}{V} \left\{ \sum \left[ \frac{(1 + 2\nu_k) \cosh 2\sigma_k - 1}{2} \right] \right\}^2 \]

\[ + \frac{\lambda}{8V} \left\{ \sum (1 + 2\nu_k) \sinh 2\sigma_k \right\}^2 \]

\[ - K T \sum [(1 + \nu_k) \ln(1 + \nu_k) - \nu_k \ln \nu_k]. \]

In a similar way the number fixing condition \( \text{Tr}[\mathcal{F}_0 N] = \langle N \rangle \) evaluates to

\[ \langle N \rangle = \Gamma_0^2 + \sum_{\vec{k}} \left[ \frac{(1 + 2\nu_k) \cosh 2\sigma_k - 1}{2} \right]. \]  

(9)

2.1 Formal equilibrium solutions

Equations determining the form of the truncated density \( \mathcal{F}_0 \) appropriate for thermal equilibrium are in general derived by requiring that \( \Omega \), eq. 8, is stationary under arbitrary variations of \( \Gamma_0, \sigma_k \) and \( \nu_k \). Variation with respect to \( \Gamma_0 \) gives the gap equation

\[ \Gamma_0 \left\{ \frac{2\lambda}{V} \Gamma_0^2 - 2\mu - \frac{\lambda}{V} \sum_{\vec{k}} [(1 + 2\nu_k)(\sinh 2\sigma_k - 2 \cosh 2\sigma_k) + 2] \right\} = 0 \]  

(10)

which, besides the trivial solution \( \Gamma_0 = 0 \), may also admit a solution with a non vanishing value of \( \Gamma_0 \) obtained by requiring that the expression in curly brackets vanishes. This solution involves the number constraint, Eq. 9, in addition to the values of \( \nu_k \) and \( \sigma_k \), which are determined by the remaining variational conditions on \( \Omega \). In order to simplify the algebraic
work involved in the study of this class of solutions it is convenient to use the number
constraint Eq.9 to eliminate Γ₀ from the right hand side of Eq.8 which then assumes the
form

Ω ≤ F − µ⟨N⟩

with ⟨N⟩ given by Eq.4. This identifies a free energy F as

\[
F = \sum_{\vec{k}} (e(k) + \lambda \rho) \left[ \frac{(1 + 2\nu_k) \cosh 2\sigma_k - 1}{2} \right] - \frac{\lambda \rho}{2} \sum_k (1 + 2\nu_k) \sinh 2\sigma_k \\
- \frac{\lambda}{2V} \left\{ \sum_{\vec{k}} \left[ \frac{(1 + 2\nu_k) \cosh 2\sigma_k - 1}{2} \right] \right\}^2 + \frac{\lambda}{8V} \{ \sum_k (1 + 2\nu_k) \sinh 2\sigma_k \}^2 \\
+ \frac{\lambda}{2V} \sum_{\vec{k}, \vec{k}'} (1 + 2\nu_{k'}) \sinh 2\sigma_{k'} \left[ \frac{(1 + 2\nu_k) \cosh 2\sigma_k - 1}{2} \right] + \frac{\lambda \rho^2 V}{2} \\
- KT \sum_{\vec{k}} [(1 + \nu_k) \ln(1 + \nu_k) - \nu_k \ln \nu_k]
\]

Extremizing F by setting derivatives with respect to σ_k and ν_k equal to zero one gets

\[
\tanh 2\sigma_k = \frac{\lambda \rho - \frac{\lambda}{2V} \sum_k [(1 + 2\nu_k) \cosh 2\sigma_k - 1] - \frac{\lambda}{2V} \sum_k (1 + 2\nu_k) \sinh 2\sigma_k}{e(k) + \lambda \rho - \frac{\lambda}{2V} \sum_k [(1 + 2\nu_k) \cosh 2\sigma_k - 1] + \frac{\lambda}{2V} \sum_k (1 + 2\nu_k) \sinh 2\sigma_k}
\]

and

\[
\nu_k = \frac{1}{\{e \exp[\sqrt{\Delta}/KT] - 1\}}
\]

where

\[
\Delta = e(k)^2 + 2\lambda e(k) \times
\]
\[
\times \{ \rho - \lambda \frac{1}{2V} \sum_k [(1 + 2\nu_k) \cosh 2\sigma_k - 1] + \lambda \frac{1}{2V} \sum_k (1 + 2\nu_k) \sinh 2\sigma_k \} \\
+ 4\lambda^2 \{ \rho - \lambda \frac{1}{2V} \sum_k [(1 + 2\nu_k) \cosh 2\sigma_k - 1] \} \times \\
\times \lambda \frac{1}{2V} \sum_k (1 + 2\nu_k) \sinh 2\sigma_k \tag{14}
\]

As for the trivial solution \( \Gamma_0 = 0 \), we differentiate \( \Omega \) as written in Eq.8 and get

\[
\tanh 2\sigma_k = \frac{-\lambda \sum_k (1 + 2\nu_k) \sinh 2\sigma_k}{e(k) - \mu + \frac{1}{\beta} \sum_k [(1 + 2\nu_k) \cosh 2\sigma_k - 1]}. \tag{15}
\]

Finally, we stress that the results obtained in the present section are largely formal, as they involve divergent sums. In order to allow for the derivation of thermodynamic properties of the different phases they must therefore be supplemented by suitable regularization and renormalization procedures. These will be discussed in sections 3 and 4 below.

### 3 Independent \( \eta \)-bosons and dilute system limit

In this section we consider two different truncation schemes of the gaussian variational equations which lead to well known results for the low temperature properties of the interacting boson system. The first and most drastic truncation of the gaussian approximation consists in neglecting all terms representing interactions between \( \eta \)-bosons. The result is entirely trivial in the case \( \Gamma_0 = 0 \) since this implies \( \sigma_k = 0 \). All effects of the interaction are thus discarded, giving us just the ideal gas results

\[
\nu_k = \frac{1}{\exp\left[\frac{e(k) - \mu}{kT}\right] - 1} \tag{16}
\]

where \( \mu \) is determined by the number constraint.
\[
\rho = \frac{1}{4\pi^2} \int_0^\infty \frac{k^2 dk}{\exp\left[\frac{e(k)-\mu}{kT}\right] - 1}.
\]  

(17)

As for the solution corresponding to \( \Gamma_0 \neq 0 \), discarding interaction between \( \eta \)-bosons amounts to dropping all double sums in Eq. (9). The variational conditions on \( \sigma_k \) and \( \nu_k \) appear then as

\[
\tanh 2\sigma_k = \frac{\lambda \rho}{e(k) + \lambda \rho}
\]

(18)

and

\[
\nu_k = \frac{1}{e^{\frac{1}{\pi T} \sqrt{e(k)^2 + 2\lambda \rho e(k)}} - 1}.
\]

(19)

When using these results for calculating \( F \) we replace sums by integrals and introduce a cut-off \( \Lambda \) in the range of integration over momenta. Ignoring terms that vanish in the limit \( \Lambda \to \infty \) we get

\[
\frac{F}{\mathcal{V}} = \frac{\lambda \rho^2}{2} - \frac{\lambda^2 m \Lambda \rho^2}{4\pi^2 \hbar^2} + \frac{8m^{3/2} \lambda^{5/2} \rho^{5/2}}{15\pi^2 \hbar^3} \\
+ \frac{KT}{2\pi^2} \int_0^\Lambda k^2 \ln \left\{ 1 - \exp \left[ -\frac{\sqrt{e(k)^2 + 2e(k)\lambda \rho}}{KT} \right] \right\} dk
\]

(20)

which shows that we get a linearly divergent term proportional to \( \lambda^2 \). This term is a leftover of the non-normal ordered terms of \( H \) which involve two \( \eta \)-operators. It is therefore a direct consequence of the non-trivial nature of the Bogolyubov transformation, and can be compensated by introducing the Fermi pseudo-potential, where the contact interaction is replaced by
\[ V_p(\vec{r} - \vec{r}') = \lambda \frac{\partial}{\partial(|\vec{r} - \vec{r}'|)} [(|\vec{r} - \vec{r}'|)\delta(\vec{r} - \vec{r}')] \]

\[ = \lambda \delta(\vec{r} - \vec{r}') + (|\vec{r} - \vec{r}'|)\lambda'\delta'(\vec{r} - \vec{r}') \]

which can be related, in the case of dilute, cold systems to the two boson scattering length \(a\) through

\[ \lambda = \frac{4\pi \hbar^2 a}{m} \]

The regularized ground state energy becomes

\[ \frac{E_0}{V} = \frac{\lambda \rho^2}{2} \left( 1 + \frac{128 (a^3 \rho)^{1/2}}{15 \pi^{1/2}} \right) \]

and the chemical potential appears as

\[ \mu = \lambda \rho + \frac{4\rho^{3/2}m^{3/2}\lambda^{5/2}}{3\pi^2\hbar^3} \]

\[ + \frac{1}{2\pi^2} \int_0^\infty \frac{\lambda e(k)k^2dk}{\exp\left[\frac{\sqrt{e(k)^2 + 2e(k)\lambda\rho}}{K_F}\right] - 1} \sqrt{e(k)^2 + 2e(k)\lambda\rho} \]

(21)

These are just the results obtained by Lee, Huang and Yang [23], by Beliaev [25] and by Hugenholtz and Pines [13] under the assumption of a macroscopic (c-number) occupation of the zero momentum mode. Note however that in the present formulation this is replaced by the coherent condensate associated with \(\Gamma_0\). In addition to this we still have non-coherent occupation of the zero momentum mode as given by the limit of \(\nu_k\), Eq. (17), for \(k \to 0\). For small, non-zero temperatures this diverges as \(1/k\) and therefore does not contribute to the density of the system. Finally, the values obtained for the chemical potential in the condensate (\(\Gamma_0 \neq 0\)) and non-condensate (\(\Gamma_0 = 0\)) phases indicate the instability of the
former. This may be seen very easily from the fact that $\mu$ is always positive in Eq. (19) and always negative or zero in Eq. (15).

A possible way to circumvent this drawback in the framework of the gaussian approximation is to perform a somewhat less drastic if more delicate truncation of the complete variational expressions, which relies on the fact that we are working with dilute systems. There is little change in the case of the $\Gamma_0 \neq 0$ phase. Eqs. (7) and (16) give the depletion

$$\rho = \rho_0 + \frac{8 (a^3 \rho)^{1/2}}{3 \pi^{1/2}}.$$  

In the limit of a dilute system one has $(a^3 \rho_0)^{1/2} \approx (a^3 \rho)^{1/2} \ll 1$ so that one may replace $\rho$ by $\rho_0$ in Eq. (16). With this replacement the excitation spectrum of the truncated Hamiltonian is related to the density of the condensate as

$$w(k) = \sqrt{e(k)^2 + 2\lambda \rho_0 e(k)}$$  

As for the phase with $\Gamma_0 = 0$, the occupation numbers $\nu_k$ are obtained by keeping $\sigma_k = 0$ but with no truncation. The chemical potential $\mu$ is determined using the constraint condition (7) that in this case reads

$$\rho = \frac{1}{4\pi^2} \int_0^\infty \frac{k^2 dk}{\exp \left( \frac{e(k) - \mu + 2\lambda \rho}{kT} \right) - 1}.$$  

Since the truncation has been avoided in the case when $\Gamma_0 = 0$, this phase is no longer treated as a free bose gas, and calculation shows that at $T = 0$ the condensate phase now appears as the stable one, since its chemical potential $\mu = \lambda \rho$ is lower than that of the non condensed phase, for which $\mu = 2\lambda \rho$. It is apparent that in this derivation the two phases are not treated on the same footing as far as the truncation is concerned. However the truncation of the two body terms has a quite different significance in each of the two cases. The rationale for this procedure rests in fact on the expectation that the most relevant effects of the two
body interaction are incorporated to the result via the symmetry breaking processes which take place in the treatment of the $\Gamma_0 \neq 0$ phase but not in that of the $\Gamma_0 = 0$ phase.

4 Handling the full gaussian approximation

In this section we examine two different prescriptions for dealing with the divergences of the complete gaussian approximation developed in section 2. The first prescription involves a renormalization scheme similar to the one proposed by Stevenson [20] in the context of the relativistic $\phi^4$ theory under the name of “precarious theory”, in which the bare coupling constant is made to approach zero by negative values. It represents an attempt at sticking as much as possible to the dynamics of contact interactions as such in the present context. Although successful in removing the divergences in a consistent way, this scheme will be shown to lead to a thermodynamically unstable system. We therefore consider also, as a second prescription, the simple alternate “effective theory” scheme in which a fixed cut-off is introduced in momentum space in the spirit of the work of Amelino-Camelia and Pi [26].

4.1 Contact forces: precarious theory

In order to reduce unessential complications to a minimum we restrict ourselves in the following development to the properties of the system at $T = 0$ in the phase corresponding to $\Gamma_0 \neq 0$, since the extension to $T \neq 0$ involves no additional divergences. The gap equation, Eq. (8), combined with the number constraint, Eq. (7), gives

\[
\mu = \lambda \rho + \frac{\lambda}{2V} \sum_k [\cosh 2\sigma_k - 1] - \frac{\lambda}{2V} \sum_k \sinh 2\sigma_k.
\]

and from Eqs. (10) to (12) we get
tanh 2\sigma_k = \frac{\lambda \rho - \frac{\lambda}{2} \sum \kappa \left[ \cosh 2\sigma_k - 1 \right] - \frac{\lambda}{4} \sum \kappa \sinh 2\sigma_k}{e(k) + \frac{\lambda}{2} \rho - \frac{\lambda}{2} \sum \kappa \left[ \cosh 2\sigma_k - 1 \right] + \frac{\lambda}{2} \sum \kappa \sinh 2\sigma_k}. \tag{23}

This is an implicit equation for the transformation parameters \sigma_k which appear in the sums of Eqs. (20) and cut-off Λ and, again neglecting contributions that vanish in the limit Λ → ∞, make the ansatze

\frac{1}{2V} \sum_k \sinh 2\sigma_k = \alpha + \beta \Lambda \tag{24}

and

\frac{1}{2V} \sum_k \left( \cosh 2\sigma_k - 1 \right) = \gamma \tag{25}

where \alpha, \beta, and \gamma are assumed to approach finite values in the limit Λ → ∞. We next introduce a renormalized coupling constant \lambda_r as

\lambda = \frac{\lambda_r}{1 - \frac{\lambda_r m \Lambda}{2\pi^2 \hbar^2}} \tag{26}

so that when Λ → ∞ the bare coupling constant \lambda approaches zero from negative values \[11, 10, 20\]. Eq. (21) becomes

\tanh 2\sigma_k = \frac{\lambda_r \rho - \lambda_r \gamma - \frac{\lambda_r}{2} \rho - \lambda_r \beta \Lambda}{e(k) + \frac{\lambda_r}{2} \rho - \lambda_r \gamma + \frac{\lambda_r}{2} \alpha + \lambda_r \beta \Lambda} \equiv - \frac{M + \frac{Q}{\Lambda} + O(\Lambda^{-2})}{e(k) + M + \frac{R}{\Lambda} + O(\Lambda^{-2})}

with

\begin{align*}
M &= - \frac{2\pi^2 \hbar^2 \beta}{m}, \\
Q &= \frac{2\pi^2 \hbar^2}{m} \left( \rho - \gamma - \alpha - \frac{2\pi^2 \hbar^2 \beta}{\lambda_r m} \right), \\
R &= \frac{2\pi^2 \hbar^2}{m} \left( \rho - \gamma + \alpha + \frac{2\pi^2 \hbar^2 \beta}{\lambda_r m} \right). \tag{27}
\end{align*}
This makes good sense for all $\vec{k}$ and for any $\Lambda$ provided $M$ is positive. We can also obtain sinh $2\sigma_k$ and cosh $2\sigma_k$ in terms of $M$, $Q$ and $R$ to evaluate the sums of Eqs. (22) and (23) up to terms $O(\Lambda^{-1})$ with the results

$$\alpha + \beta \Lambda = -\frac{1}{4\pi^2} \int_0^\Lambda k^2 \frac{(M + \frac{Q}{\Lambda})}{\sqrt{c(k)^2 + 2(M + \frac{Q}{\Lambda})c(k) + G}} dk$$

$$= \frac{m^{3/2}M^{3/2}}{\pi^2\hbar^4} - \frac{mQ}{2\pi^2\hbar^2} - \frac{mM\Lambda}{2\pi^2\hbar^2},$$

which is consistent with the expression for $M$ in Eq. (25), and

$$\gamma = \frac{1}{4\pi^2} \int_0^\Lambda k^2 \left\{ \frac{[e(k) + M + \frac{R}{\Lambda}]}{\sqrt{e(k)^2 + 2(M + \frac{Q}{\Lambda})e(k) + G}} - 1 \right\} dk = \frac{m^{3/2}M^{3/2}}{3\pi^2\hbar^3}$$

where we defined

$$G = \frac{2M(R - Q)}{\Lambda} + \frac{R^2 - Q^2}{\Lambda^2}.$$  

It is easy to see that for $M = 0$ we obtain the ideal Bose gas results (free theory). For $M > 0$, in order to evaluate $F$ (which for $T = 0$ reduces to the ground state energy $E_0$), we also need

$$\frac{1}{2V} \sum_{\vec{k}} e(k)(\cosh 2\sigma_k - 1) = \frac{mM^2\Lambda}{4\pi^2\hbar^2} + \frac{mMQ}{2\pi^2\hbar^2} - \frac{4m^{3/2}M^{5/2}}{5\pi^2\hbar^3}.$$  

Taking these results to Eq. (9) (with $\nu_k = 0$ for $T = 0$) we see that the remaining linearly divergent terms cancel and we are left with

$$\frac{F(T = 0)}{V} = \frac{E_0}{V} - \frac{8m^{3/2}M^{5/2}}{15\pi^2\hbar^3} - M\rho - \frac{M^2}{2\lambda_r}$$  

which identifies the chemical potential as $\mu = -M$. Note that $M > 0$ now implies $\mu < 0$.

Finally, in order to relate $\mu$ (or $M$) to the density of the system we evaluate the grand potential, Eq. (6), with the result
\[ \Omega(T = 0) = \frac{8m^{3/2}(-\mu)^{5/2}V}{15\pi^2\hbar^3} - \frac{\mu^2V}{2\lambda_r} \quad (29) \]

and use the relation \( N = -(\frac{\partial\Omega}{\partial\mu})_{T,V} \) to obtain

\[ \rho = \frac{\mu}{\lambda_r} + \frac{4m^{3/2}(-\mu)^{3/2}}{3\pi^2\hbar^3}. \quad (30) \]

With the condition \( \mu < 0 \) when \( \Lambda \to \infty \), we get a phonon-like spectrum as in Sec. 3,

\[ E(k) = \sqrt{e(k)^2 - 2\mu e(k)}. \]

We can also take the appropriate derivative of \( F \) (or, equivalently, evaluate \(-\Omega/V\) using Eq. (27)) to get the pressure at \( T = 0 \) as

\[ P = -\left( \frac{\partial F}{\partial V} \right)_{T,N} = -\frac{\Omega}{V} = -\frac{8m^{3/2}(-\mu^{5/2})}{15\pi^2\hbar^3} + \frac{\mu^2}{2\lambda_r} \quad (31) \]

and it is easy to show, using Eqs. (26), (28), (29) and \( \rho > 0 \), that \( \frac{dP}{d\rho} \) and \( E_0/V \) are always negative. This shows that the renormalized theory is thermodynamically unstable. As a matter of fact, this instability should be seen as the non-relativistic counterpart of the “intrinsic instability” pointed quite some time ago by Bardeen and Moshe \[15\] in their analysis of the phase-structure of the relativistic \( \lambda\phi^4 \) theory in four dimensions, which has also been raised recently in the context of multi-field theories \[27\]. It underlies also the “precariousness” of this theory in Stevenson’s treatment \[20\].

Another possible phase to be studied corresponds to a solution where \( \Gamma_0 = 0 \). In order to account for the fact that in this case a macroscopic occupation \( \nu_0 \) may develop, we separate the \( \vec{k} = 0 \) contribution in the sums

\[ \frac{1}{2V} \sum_{\vec{k}} (\cosh 2\sigma_{\vec{k}} - 1) \to c + \frac{1}{2V} \sum_{\vec{k} \neq 0} (\cosh 2\sigma_{\vec{k}} - 1) \quad (32) \]
\[
\frac{1}{2V} \sum_{\mathbf{k}} \sinh 2\sigma_{\mathbf{k}} \rightarrow d + \frac{1}{2V} \sum_{\mathbf{k} \neq 0} \sinh 2\sigma_{\mathbf{k}}
\]

so that Eq. (13) becomes

\[
\tan 2\sigma_{\mathbf{k}} = \frac{-\lambda d - \frac{1}{2V} \sum_{\mathbf{k} \neq 0} \sinh 2\sigma_{\mathbf{k}}}{e(k) - \mu + 2\lambda \rho}.
\]

Using the ansatze (22) and (23) we obtain

\[
\tanh 2\sigma_{\mathbf{k}} = \frac{-\lambda d - \frac{1}{2V} \sum_{\mathbf{k} \neq 0} \sinh 2\sigma_{\mathbf{k}}}{e(k) - \mu + \frac{2\lambda \rho}{1 - \frac{\beta m}{2\pi \hbar^2}}} \equiv - \frac{M + \frac{Q}{\Lambda} + \mathcal{O}(\Lambda^{-2})}{e(k) - \mu + \frac{R}{\Lambda} + \mathcal{O}(\Lambda^{-2})}
\]

with

\[
M = - \frac{2\pi^2 \hbar^2 \beta}{m},
\]

\[
Q = + \frac{2\pi^2 \hbar^2}{m} d,
\]

\[
R = - \frac{4\pi^2 \hbar^2}{m} \rho.
\]

If we examine

\[
\gamma = \frac{1}{4\pi^2} \int_{0}^{\Lambda} k^2 \left[ \frac{e(k) - \mu}{\sqrt{[e(k) - \mu]^2 - M^2}} - 1 \right] dk
\]

we see that the only acceptable solution is \(M = \mu\). If \(M = 0\) it follows that \(\sigma_{\mathbf{k}} = 0\), leading to a possible solution \(c = d = v_0/V\) which corresponds essentially a free Bose gas. If, on the other hand, \(M \neq 0\) we are again led to a thermodynamically unstable situation.
4.2 Effective theory

The renormalization prescription of the preceding subsection tells us that if \( \lambda_r \) is positive and held fixed when \( \Lambda \to \infty \) we must have \( \lambda \to 0^- \) which results in a thermodynamically unstable theory that we want to avoid. Since a positive value of \( \lambda \) leads to a trivial theory with \( \lambda_r = 0 \) when the limit \( \Lambda \to \infty \) is taken, we next consider the results that one obtains for the non-trivial effective theory in which \( \Lambda \) is kept fixed at a finite value allowing for both \( \lambda_r > 0 \) and \( \lambda > 0 \). This requires that one must have

\[
\frac{\lambda_r m \Lambda}{2\pi^2 h^2} < 1
\]

and implies a finite resolution \( \mathcal{O}(\Lambda^{-1}) \) in configuration space. The restricted momentum space also implies that the validity of the results will be restricted to temperatures which are low in the scale

\[
\frac{\hbar^2 \Lambda^2}{2Km}.
\]

Because in the derivations given in the preceding subsection all terms that vanish in the limit \( \Lambda \to \infty \) were neglected, we use here the general expressions given in Section 2. Eq. (24) will be used with a fixed value of \( \Lambda \) to relate the bare and effective coupling constants \( \lambda \) and \( \lambda_r \) respectively.

Consider first the condensed phase, \( \Gamma_0 \neq 0 \). The sums appearing in Eqs. (9), (10) and (11) are now finite, and we therefore define

\[
A = \frac{1}{2V} \sum_k' (1 + 2\nu_k) \sinh 2\sigma_k
\]

\[
B = \frac{1}{2V} \sum_k' [(1 + 2\nu_k) \cosh 2\sigma_k - 1]
\]
\[ C = \frac{1}{2V} \sum_k' e(k) \left[ (1 + 2\nu_k) \cosh 2\sigma_k - 1 \right]. \]

where the primed sums are restricted to \(|\vec{k}| \leq \Lambda\). Eqs. (8), (10) and (12) appear then as

\[ \mu = \lambda \rho - \lambda A + \lambda B \quad (38) \]

\[ \tanh 2\sigma_{\vec{k}} = \frac{\lambda[\rho - B - A]}{e(k) + \lambda[\rho - B + A]} \]

and

\[ \Delta = e(k)^2 + 2\lambda e(k)[\rho - B + A] + 4\lambda^2[\rho - B]A. \]

This last quantity determines \(\nu_k\) through Eq. (11) and shows explicitly the presence of an energy gap in the quasiparticle spectrum which is related to the quasiparticle interaction term \(2\lambda\rho_0 A\) (we use \(\rho - B = \rho_0\), the density of the coherent condensate). The free energy \(F\) and the pressure \(P\) are given by

\[ F = CV - \lambda \rho(A - B)V + \frac{\lambda}{2}(\rho^2 + A^2 - B^2)V + \lambda ABV \]

\[ -KT\sum_{\vec{k}}'[(1 + \nu_k) \ln(1 + \nu_k) - \nu_k \ln \nu_k] \quad (39) \]

and

\[ P = \frac{\lambda B^2}{2} + \frac{\lambda \rho^2}{2} - C - \lambda AB - \frac{\lambda A^2}{2} + \frac{1}{V} \sum_{\vec{k}}' \nu_{\vec{k}} \sqrt{\Delta} \]

\[ -KT \sum_{\vec{k}}' \ln\left\{ 1 - \exp\left[ -\sqrt{\Delta}/KT \right] \right\} \quad (40) \]

After going to the continuum limit, we can calculate \(A\) and \(B\) for given values of \(\rho\) and \(T\) by solving numerically the system of equations.
A = \frac{1}{4\pi^2} \int_0^\Lambda k^2 \left\{ \frac{\lambda (\rho - B - A)}{\sqrt{\Delta}} \left[ 1 + \frac{2}{\exp \left( \frac{\sqrt{\Delta}}{KT} \right) - 1} \right] \right\} dk

B = \frac{1}{4\pi^2} \int_0^\Lambda k^2 \left\{ e(k) + \frac{\lambda (\rho - B + A)}{\sqrt{\Delta}} \left[ 1 + \frac{2}{\exp \left( \frac{\sqrt{\Delta}}{KT} \right) - 1} \right] - 1 \right\} dk.

Finally, in terms of the values of $A$ and $B$ we can calculate $C$ and the thermodynamic functions also numerically.

As for the case $\Gamma_0 = 0$ with the sums restricted to the cut-off, it’s easy to see that the only solution is $\sigma_k = 0$. In the continuum limit,

$$\rho = \frac{1}{2\pi^2} \int_0^\Lambda \frac{k^2 dk}{\exp[(e(k) - \mu + 2\lambda \rho)/KT] - 1} \quad (41)$$

which serves to determine $\mu$. The pressure is in this case given by

$$P = \lambda \rho^2 - \frac{KT}{2\pi^2} \int_0^\Lambda k^2 \ln \left\{ 1 - \exp\left\{ -(e(k) - \mu + 2\lambda \rho)/KT \right\} \right\}. \quad (42)$$

### 4.3 Numerical results

#### 4.3.1 Cut-off dependence

In order to perform numerical calculations we used a system of units such that the Boltzmann constant $K = 1$ and $c = 1$, so that energies are expressed in degrees Kelvin. We use $m = 4 \times 10^{13}$ oK and $\lambda_r = 50$ oKÅ$^3$. In Fig. (1), we show the dependence of the ground state energy, for a density $\rho = 0.01$ Å$^{-3}$ as the cut-off is varied in the interval $1.0$ Å$^{-1} < \Lambda < 5.0$ Å$^{-1}$. For the calculations described below we take $\Lambda = 3.0$ Å$^{-1}$. According to Eq. (24), this corresponds to a bare coupling constant $\lambda = 119.124$ oKÅ$^3$. For densities larger than the quoted value one starts having stronger cut-off dependence, so that the present scheme is, in this sense, also limited to rather dilute systems.
4.3.2 Phase transition

Results of some sample calculations using the various expressions of the preceding section are shown in Figs. (2) to (5). For the range of temperatures and densities considered here, the adopted value of the cut-off momentum $\Lambda$ essentially saturates the values of the finite momentum integrals involved. The density $\rho$ is plotted in the figures as the number density in units of Å$^{-3}$.

In order to study the properties of the condensed ($\rho_0 > 0$) and of the non-condensed ($\rho_0 = 0$) phases, as well as their coexistence, we show in Fig. 2 the chemical potential $\mu$ calculated as a function of the density $\rho$ in each of these two cases, for a constant temperature fixed as $T = 2^oK$, using Eqs. (38) and (41) respectively. The condensed phase has two different branches with different chemical potentials in the range $\rho > \sim 7 \times 10^{-2} \text{Å}^{-3}$ and ceases to exist for lower values of the density. The chemical potential of the non-condensed phase increases monotonically approaching the upper branch of the condensed phase asymptotically from above. It is interesting to note that these two solutions essentially merge at a density where the non-condensed solution develops a macroscopic occupation $\nu_0$ of the zero momentum state, and that the solution involving instead a coherent condensate ($\rho_0 > 0$) leads to a lower value of $\mu$. In order to decide about the thermodynamic stability of the various solutions we give in Fig. 3 the corresponding plot of $\mu$ against the pressure $P$, which displays the pattern of a first order transition. The densities of the two stable phases are indicated by the light dashed lines in Fig. 2. Fig. 4 shows the $T = 2^oK$ and the $T = 0^oK$ isotherms in a standard $P \times \rho^{-1}$ diagram together with the appropriate Maxwell construction for $T = 2^oK$. The condensed solution is the only one stable at $T = 0^oK$. The pattern found for $T = 2^oK$ repeats itself for higher temperatures with no evidence of a critical temperature within the range allowed by the limitations of the effective theory. The stable isotherms for
temperatures of 0, 2, 3 and 4 °K are shown in Fig. 5.

5 Concluding remarks

In the gaussian approximation it is possible to renormalize a repulsive contact interaction using a procedure akin to the so called precarious renormalization scheme of Stevenson[20]. Despite being finite and exhibiting some desirable properties, such as an excitation spectrum of the phonon type, the condensate phase is thermodynamically unstable for all system densities. This is a manifestation of a corresponding instability pointed out in a relativistic context by Bardeen and Moshe [19]. Solutions with no pairing ($\sigma_k = 0$), on the other hand, can be verified to correspond just to a free bose gas. We stress that the thermodynamic instability of the paired, condensed phase cannot be recognized just from the expression for the ground state energy, Eq. (27), but requires the use of the equation of state.

As an alternative to such an unstable, renormalized theory we considered a cut-off dependent effective theory for a dilute system. Among the results of this theory we have a gap in the excitation spectrum in disagreement with the Hugenholz-Pines theorem[13], and a first order transition between a condensed phase and a non-condensed phase. The occurrence of the gap can be associated to the drastic reordering and infinite partial ressumation of the perturbative series implied in the Gaussian variational approximation. It should be noted in this connection that the variational calculation involving the truncated density $F_0$ is designed to optimize the determination of the grand-potential, and that this does not imply the variational optimization of the thermal occupation probabilities from which the excitation spectrum is derived [21]. On the other hand, the sensitivity of the excitation spectrum to the dynamical ingredients included in the calculation can be illustrated by the fact that, using the free quasi-boson truncation described in section 3 (which breaks the variational
self consistency of the calculation), the results obtained agree with the Hugenholtz-Pines theorem.

We also remark that it is a well known tendency of mean field approximations to over-represent discontinuities in situations involving phase transitions, e.g. by predicting discontinuous behaviors in the case of finite systems. This recommends, as already observed in ref. [26] on the basis of a reliability analysis of power-counting type, that caution should be exerted in the interpretation of the first order character obtained for the phase transition in this calculation.

In conclusion, the introduction of quantum effects at the level of a paired mean field calculation for a non-ideal bose system gives results which differ even qualitatively from usual perturbative results. Comparison with experiment is still hampered by the fact that a very dilute though sufficiently non-ideal system has not yet been realized in practice.

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Figure Captions

FIG. 1. Cut-off dependence of the ground state energy per particle. See text for details.

FIG. 2. Chemical potential as a funcion of number density for T=2°K and Λ = 3Å⁻¹. See text for other parameter values. The highlighted values of μ and ρ correspond to the Maxwell
construction shown in Figs. 3 and 4.

FIG. 3. Chemical potential as a function of pressure for the isotherm depicted in Fig. 2. The highlighted point indicates the first order phase transition.

FIG. 4. Equation of state isotherms for T=0 and 2 °K showing the Maxwell construction identifying the phase coexistence region in the T=2 °K isotherm.

FIG. 5. Equation of state stable isotherms for T=0, 2, 3 and 4 °K.