Quantum Phase Diagram  
for Homogeneous Bose-Einstein Condensate

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We calculate the quantum phase transition for a homogeneous Bose gas in the plane of s-wave scattering length \(a_s\) and temperature \(T\). This is done by improving a one-loop result near the interaction-free Bose-Einstein critical temperature \(T_c(0)\) with the help of recent high-loop results on the shift of the critical temperature due to a weak atomic repulsion using variational perturbation theory. The quantum phase diagram shows a \textit{nose} above \(T_c(0)\), so that we predict the existence of a \textit{reentrant transition} \textit{above} \(T_c(0)\), where an \textit{increasing} repulsion leads to the formation of a condensate.

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I. INTRODUCTION

So far, experimental work on Bose-Einstein condensates (BECs) has dealt with magnetic traps, so that most of the recent theoretical investigations focus on such systems [1–4]. However, there are interesting theoretical problems also in homogeneous BECs with weak two-particle interactions. For instance, a very fundamental property of homogeneous BECs with a local repulsive interaction \(V_{\text{int}}(x) = g\delta^3(x)\) has been answered only recently: In which direction does this interaction push the critical temperature, and by which amount? Although this problem appears to be very simple, the answer has had an adventurous history [5–21].

The weak repulsion defines an interaction temperature \(T_{\text{int}} = gn/k_B\) where \(n\) is the particle density and \(k_B\) the Boltzmann factor. For small enough \(g\), the interaction temperature is much smaller than the interaction-free critical temperature \(T_c(0) = 2\pi\hbar^2 n^{2/3}/mk_B [\xi(3/2)]^{2/3}\), implying that calculations near \(T_c(0)\) can be done in the high-temperature limit of the theory. They can therefore be derived from the classical limit of many-body theory, where only the zero Matsubara modes of the Bose fields are included [5]. In this approximation, many groups calculated that the leading shift of the critical temperature is linear in the s-wave scattering length \(a_s = Mg/4\pi\hbar^2\):

\[
\frac{\Delta T_c}{T_c(0)} = c_1 a_s n^{1/3} + O \left( a_s^2 n^{2/3} \right).
\]

The latest and most precise Monte Carlo simulations gave a slope \(c_1 = 1.32 \pm 0.02\) [13, 14], reasonably close to the theoretical numbers 1.48 in Ref. [15], 1.15 in Ref. [16], and 0.492 in Ref. [17], which were derived by resumming a divergent perturbation series for \(c_1\) using the so-called \(\delta\)-expansion method. However, the application of this method to field theory is unjustified, as pointed out in Refs. [18, 19], since it does not take into account that field theory shows anomalous dimensions in the strong-coupling limit. This fundamental flaw was corrected in Refs. [18, 20] where the field-theoretic variational perturbation theory (VPT) developed in Refs. [22–24] was used to self-consistently determine the anomalous dimension from five- to six-loop expansions. The six-loop result is \(1.25 \pm 0.13\) [20], thus agreeing with the latest Monte Carlo value \(1.32 \pm 0.02\) [13, 14].

If we draw a phase diagram in the \(a_s-T\)-plane, the result (1) gives a curve starting linearly to the right at the critical temperature \(T_c(0)\), as illustrated in Fig. 1. A first correction to this curve has been calculated recently by Arnold and co-workers [21] by going beyond the classical limit. They find

\[
\frac{\Delta T_c}{T_c(0)} = c_1 a_s n^{1/3} + a_s^3 n^{1/3} (c_2 \ln a_s n^{1/3} + c_2) + O \left( a_s^3 n \right).
\]

Their value for the coefficient \(c_2 \approx -64\pi\zeta(1/2)/3\zeta(3/2)^{5/3} \approx 19.75\) is determined perturbatively, whereas \(c_2\) requires again resuming a divergent series which is unknown so far. With the help of Monte Carlo data they estimate \(c_2 \approx 75.7.\) If one plots (2) with \(c_1 \approx 1.3\) in the phase diagram of Fig. 1, the transition curve bends to the right. This cannot go on for higher \(a_s\) since there cannot be a condensate for high \(T\). The next correction terms must turn the transition curve in Fig. 1 to the left, so that it arrives, for \(T = 0\), at a pure quantum phase transition [25].

In this paper we follow Ref. [26] and investigate in detail the full quantum phase diagram. As it is crucial to resum asymptotic perturbation series, we present in Section II a short introduction to VPT. In Section III we derive the self-consistent Popov approximation to the effective potential of a homogeneous Bose gas using VPT. This leads to a lowest-order quantum phase diagram which already shows the interesting reentrant phenomenon. The curve is
FIG. 1: Phase diagram in the \( a_s-T \)-plane. The straight line indicates the prediction (1) of classical field theory valid locally in the vicinity of \( T_c^{(0)} \). The dashed curve illustrates the second-order result (2) of Arnold et al. [21]. The full phase diagram will be given in Fig. 3.

variationally improved in Section IV to include the five- to six-loop results near \( T_c^{(0)} \) which weakens the nose in the phase diagram but does not destroy the reentrant transition.

II. VARIATIONAL PERTURBATION THEORY

In this section we briefly outline the general procedure for resumming an asymptotic perturbation series with the help of VPT following Refs. [22–24].

A. Summary of Procedure

Perturbation expansions can only be used to calculate a physical quantity \( f(g) \) for very small values of the coupling constant \( g \). We are usually able to find a truncated power series at some finite order \( N \):

\[
f_N(g) = \sum_{n=0}^{N} a_n g^n. \tag{3}\]

If \( g \) is small enough, this can lead to an impressive agreement between theory and experiment, the most prominent example being the perturbation series for the anomalous magnetic moment of the electron \( g_e \) where \( g = \alpha \approx 1/137 \).

The smallness of \( g \) is necessary since the expansion (3) has a zero radius of convergence, as pointed out by Freeman Dyson in 1952 [27]. The point \( g = 0 \) is the endpoint of a cut (see Fig. 2) which makes the expansion divergent, with only an asymptotic validity for \( g \to 0 \). The difference between a convergent and an asymptotic series lies in the behavior of the last term \( a_N g^N \) of (3). For fixed \( g \), a convergent series has decreasing \( a_N g^N \), a typical divergent series of perturbation expansions has \( a_N \) growing factorially, so that the last term \( a_N g^N \) decreases only at small \( g \) for a few low orders, after which it increases dramatically.

These divergent series require resummation if we want to extract from them reliable results. The crudest method to approximate \( f(g) \) is via Padé approximants [28]. These are rational functions with the same power series expansions as \( f(g) \). The Padé method approximates the left-hand cut of the function \( f(g) \) in the complex \( g \)-plane by a string of poles.

A better approximation can be found by using, in addition, the knowledge of the large-order behavior of the weak-coupling coefficients \( a_n \). By means of Borel transformations the factorial growth of \( a_n \) can be eliminated [29, 30], and a Padé approximation is applied. After this, one returns back to the original function by an inverse Borel transform. This procedure can be improved further by a conformal mapping technique in which the complex \( g \)-plane is mapped into a unit circle which contains the original left-hand cut on its circumference [31].

A further simple tool for extracting physical results is provided by simple variational methods invented a long time ago by many research groups in quantum mechanics. For instance, the so-called \( \delta \)-expansion amounts to a resummation of divergent perturbation series (see, for instance, the references cited in [19]). It is based on introducing artificially a harmonic trial oscillator and optimizing the trial frequency by invoking the principle of minimal sensitivity [32]. It turns out that the \( \delta \)-expansion procedure corresponds to a systematic extension of a variational approach in quantum statistics [33–36] to arbitrary orders [22, 24, 37] and is now called VPT. It allows us to evaluate the asymptotic series...
FIG. 2: Comparing schematically analytic properties of convergent a) and asymptotic b) series.

(3) for all values of the coupling constant \( g \), even in the limit \( g \to \infty \). In particular, is it possible to derive from the initial weak-coupling expansion (3) a strong-coupling limit which has the generic form

\[
 f(g) = g^{p/q} \sum_{m=0}^{\infty} b^{(m)} g^{-2m/q} .
\]

Here \( p \) and \( q \) are real growth parameters characterizing the strong-coupling behavior. For the ground-state energy of the anharmonic oscillator with \( p = 1 \) and \( q = 3 \), the convergence was shown to be exponentially fast, even for infinite coupling strength [38–40]. It also allows us to combine a weak-coupling expansion with information on the strong-coupling expansion and interpolate between them [41].

In recent years, VPT has been extended in a simple but essential way to become applicable to quantum field theory with its anomalous dimensions. Applications to series expansions of \( \phi^4 \)-theory have led to extremely accurate critical exponents [23, 24, 42]. The field-theoretic perturbation coefficients are available up to six and partly to seven loops in \( D = 3 \) [43, 44], and up to five loops in \( D = 4 - \epsilon \) dimensions [45]. The most important feature of this new field-theoretic VPT is that it accounts for the anomalous power approach to the strong-coupling limit which the \( \delta \)-expansion cannot accommodate. As we see in Eq. (4), this approach is governed by an irrational critical exponent \( \omega = 2/q \) as was first shown by Wegner [46] in the context of critical phenomena. In contrast to the \( \delta \)-expansion, the field-theoretic variational perturbation expansions cannot be derived from adding and subtracting a harmonic term in the underlying action. The Wegner exponent \( \omega \) is determined from (3) by making the variationally resummed logarithmic derivative \( \partial \ln f(g)/\partial \ln g \) vanish at \( g \to \infty \), as we have there \( p = 0 \). The theoretical results of the field-theoretic VPT are in excellent agreement with experiment, in particular for the only challenging experimental value of the critical exponent \( \alpha \) which governs the behavior of the specific heat near the superfluid phase transition of \( ^4 \)He. The high experimental accuracy is reached in one of the few physically relevant microgravity experiments performed in a satellite orbiting around the earth [47, 48].

B. Variational Expression

Consider the truncated weak-coupling series (3) and rewrite it with the help of an auxiliary parameter \( \kappa = 1 \) as

\[
 f_N(g) = \kappa^p \sum_{n=0}^{N} a_n \left( \frac{g}{\kappa^q} \right)^n |_{\kappa=1} .
\]

Here \( p \) and \( q \) denote parameters which determine the strong-coupling behavior as we will see below. Now we introduce a variational parameter \( K \) using the substitution trick

\[
 \kappa^2 = K^2(1 + gr) ,
\]

where

\[
 r = \frac{1}{g} \left( \frac{\kappa^2}{K^2} - 1 \right) .
\]
Substituting (6) into the truncated weak-coupling series (5), and reexpanding everything in powers of \( g \) at fixed \( r \), we obtain for \( \kappa = 1 \):

\[
f_N(g, K) = \sum_{n=0}^{N} \left[ \sum_{k=0}^{N-n} \frac{(p - nq)/2}{k} \left( \frac{1}{K^2} - 1 \right)^k K^{p-nq} \right] a_n g^n.
\] (8)

According to the principle of minimal sensitivity [32], we optimize the influence of \( K \) on \( f_N(g, K) \). At first we search for local extrema, i.e., we determine \( K \) from the condition

\[
\frac{\partial f_N(g, K)}{\partial K} \bigg|_{K = K_N(g)} = 0.
\] (9)

It may happen that this condition is not solvable. In this case, we satisfy the principle of minimal sensitivity by looking for turning points, i.e., we fix the variational parameter according to

\[
\frac{\partial^2 f_N(g, K)}{\partial K^2} \bigg|_{K = K_N(g)} = 0.
\] (10)

The solutions of Eqs. (9) or (10) then yield the variational result \( f_N(g, K_N(g)) \) which turns out to be a good approximation for the function \( f(g) \) for all values of the coupling constant \( g \). The quality of this approximation can be estimated by investigating the strong-coupling limit as a special case.

C. Strong-Coupling Limit

The conditions (9) and (10) for the function (8) imply that the optimal variational parameter \( K_N(g) \) has the strong-coupling behavior

\[
K_N(g) = g^{1/q} \left( K_N^{(0)} + K_N^{(1)} g^{-2/q} + \cdots \right).
\] (11)

Thus \( f(g) \) is approximated in the limit \( g \rightarrow \infty \) by

\[
f_N(g, K_N(g)) = g^{p/q} \left[ b_N^{(0)}(K_N^{(0)}) + b_N^{(1)}(K_N^{(0)}, K_N^{(1)}) g^{-2/q} + \cdots \right].
\] (12)

The ratio \( p/q \) determines the leading \( g \)-power, and \( 2/q \) the approach to scaling. The leading strong-coupling coefficient \( b_N^{(0)}(K_N^{(0)}) \) is given by

\[
b_N^{(0)}(K_N^{(0)}) = \sum_{n=0}^{N} \sum_{k=0}^{N-n} \frac{(p - nq)/2}{k} (-1)^k (K_N^{(0)})^{p-nq} a_n,
\] (13)

where the inner sum can be further simplified, using the identity [49, see Eq. (0.151) therein]

\[
\sum_{k=0}^{m} (-1)^k \binom{x}{k} = (-1)^m \binom{x - 1}{m},
\] (14)

so that the strong-coupling coefficient (13) has the variational expression

\[
b_N^{(0)}(K_N^{(0)}) = \sum_{n=0}^{N} (-1)^{N-n} \binom{(p - nq)/2 - 1}{N - n} (K_N^{(0)})^{p-nq} a_n,
\] (15)

to be optimized in \( K_N^{(0)} \). Inserting the optimized \( K_N^{(0)} \) in (15) then leads to the variational approximation \( b_N^{(0)}(K_N^{(0)}) \) of the strong-coupling coefficient \( b^{(0)} \).

III. EFFECTIVE POTENTIAL

In order to study the Bose gas below the critical temperature, we calculate the one-loop approximation to the effective potential. In this so-called Popov approximation we determine the number of non-condensed particles. A variational resummation yields the self-consistent Popov approximation which allows us to find a lowest-order expression for the location of the quantum phase transition in the \( a_s - T \)-plane.
A. One-Loop Approximation

A grand-canonical ensemble of Bose particles with a repulsive two-particle $\delta$-function interaction is governed by the Euclidean action

$$A[\psi^*, \psi] = \int_0^{\hbar^2} d\tau \int d^D x \left\{ \psi^*(x, \tau) [\hbar \partial_\tau + \epsilon(-i\hbar \nabla) - \mu] \psi(x, \tau) + \frac{g}{2} \psi(x, \tau)^2 \psi^*(x, \tau)^2 \right\},$$

where $\epsilon(k)$ denotes the one-particle energies, $\mu$ the chemical potential, $g = 4\pi^2 \hbar^2 a_s/M$ the coupling constant, and $\beta \equiv 1/k_B T$. The one-loop approximation to the effective potential is most easily obtained with the help of the background method [22, see Subsection 3.19.4 therein]. We consider the functional integral for the partition function

$$Z = \int D\psi \int D\psi^* e^{-A[\psi, \psi^*]/\hbar}$$

performed over all Bose fields $\psi(x, \tau), \psi^*(x, \tau)$ periodic in $\tau \in (0, \hbar \beta)$, and change variables to field fluctuations $\delta\psi(x, \tau), \delta\psi^*(x, \tau)$ around a constant background $\Psi, \Psi^*$, defined by

$$\psi(x, \tau) = \Psi(x) + \delta\psi(x, \tau), \quad \psi^*(x, \tau) = \Psi^*(x) + \delta\psi^*(x, \tau).$$

The functional integral (17) is then evaluated including only the harmonic fluctuations $\delta\psi(x, \tau), \delta\psi^*(x, \tau)$. The linear terms in $\delta\psi(x, \tau), \delta\psi^*(x, \tau)$ are ignored in the background method. Thus the partition function factorizes as $Z = Z^{(0)} Z^{(1)} Z^{(rest)}$, where the zero-loop term $Z^{(0)} = e^{-A[\Psi, \Psi^*]/\hbar}$ is given by the tree-level

$$A[\Psi, \Psi^*] = \hbar \beta V \left( -\mu |\Psi|^2 + \frac{g}{2} |\Psi|^4 \right),$$

and the one-loop contribution

$$Z^{(1)} = \int D\delta\psi \int D\delta\psi^* e^{-A^{(quad)}[\delta\psi, \delta\psi^*]/\hbar}$$

involves a quadratic part whose action which can be written in matrix form:

$$A^{(quad)}[\delta\psi, \delta\psi^*] = \frac{\hbar}{2} \int_0^{\hbar^2} d\tau \int_0^{\hbar^2} d\tau' \int d^D x \int d^D x' \left( \delta\psi^*(x, \tau) \delta\psi(x, \tau) \right) G^{-1}(x, \tau; x', \tau') \left( \delta\psi(x', \tau') \delta\psi^*(x', \tau') \right).$$

The functional matrix

$$G^{-1}(x, \tau; x', \tau') = \delta(x - x') \delta(\tau - \tau') \frac{1}{\hbar} \left( \begin{array}{cc} \hbar \partial_\tau + \epsilon(-i\hbar \nabla') - \mu + 2g|\Psi|^2 & g\Psi^2 \\ -g\Psi^2 & -\hbar \partial_\tau + \epsilon(-i\hbar \nabla') - \mu + 2g|\Psi|^2 \end{array} \right)$$

is the inverse Green function. The result of the Gaussian integral in (20) reads

$$Z^{(1)} = \exp \left( -\frac{1}{2} \text{Tr} \ln G^{-1} \right).$$

Diagonalizing (22) in momentum space leads to

$$G^{-1}(k, \tau - \tau') = \delta(\tau - \tau') \frac{1}{\hbar} \left( \begin{array}{cc} \hbar \partial_\tau + \epsilon(k) - \mu + 3g|\Psi|^2 & 0 \\ 0 & -\hbar \partial_\tau + \epsilon(k) - \mu + g|\Psi|^2 \end{array} \right),$$

so that (23) reduces to

$$Z^{(1)} = \exp \left\{ -\frac{\beta}{2} \sum_k E(k) - \sum_k \ln \left[ 1 - e^{-\beta E(k)} \right] \right\}.$$  

Here we have introduced the $\Psi, \Psi^*$-dependent quasiparticle energies

$$E(k) = \sqrt{\epsilon(k) - \mu + 2g|\Psi|^2} - g^2 |\Psi|^2.$$

Combining the zero- and the one-loop contribution, we obtain for the effective potential $V(\Psi, \Psi^*) \equiv -\ln Z/\beta$ the simple expression

$$V(\Psi, \Psi^*) = V \left( -\mu |\Psi|^2 + \frac{g}{2} |\Psi|^4 \right) + \frac{\eta}{2} \sum_k E(k) + \frac{\eta}{\beta} \sum_k \ln \left[ 1 - e^{-\beta E(k)} \right] + O(\eta^2),$$

where we have introduced an expansion parameter $\eta = 1$ whose power serves to count the loop order of each term.
B. Popov Approximation

The one-loop effective potential (27) is still a function of the background fields $\Psi, \Psi^*$. If extremized in these fields, it yields the thermodynamic potential at its extremum. The extremalization condition is

$$-\mu + g|\Psi|^2 + \frac{\eta}{2V} \sum_k \frac{2g[\epsilon(k) - \mu + 2g|\Psi|^2] - g^2|\Psi|^2}{E(k)} + \frac{\eta}{V} \sum_k \frac{2g[\epsilon(k) - \mu + 2g|\Psi|^2] - g^2|\Psi|^2}{E(k) [e^{\beta E(k)} - 1]} + \mathcal{O}(\eta^2) = 0. \quad (28)$$

The extremal value of $\Psi^*\Psi$ defines the condensate density $n_0 = |\Psi|^2$, for which (28) yields the one-loop equation

$$n_0 = \frac{\mu}{g} - \frac{\eta}{V} \sum_k \frac{2\epsilon(k) + \mu}{\sqrt{\epsilon(k)^2 + 2\mu \epsilon(k)}} \left( \frac{1}{2} + \frac{1}{e^{\beta \sqrt{\epsilon(k)^2 + 2\mu \epsilon(k)}} - 1} \right) + \mathcal{O}(\eta^2). \quad (29)$$

For $\eta = 0$ we obtain the tree-level condensate density $n_0^{(0)} = \mu/g$, which leads in (26) to the quasiparticle energies found first by Bogoliubov [52]:

$$E^{(0)}(k) = \sqrt{\epsilon(k)^2 + 2\mu \epsilon(k)}. \quad (30)$$

Inserting (29) into (27) yields the grand-canonical potential:

$$\frac{\Omega(\mu, T)}{V} = -\frac{\mu^2}{2g} + \frac{\eta}{2V} \sum_k \frac{1}{\sqrt{\epsilon(k)^2 + 2\mu \epsilon(k)}} \ln \left( 1 - e^{-\beta \sqrt{\epsilon(k)^2 + 2\mu \epsilon(k)}} \right) + \mathcal{O}(\eta^2). \quad (31)$$

From this, we obtain the total particle density from the derivative

$$n(\mu, T) = -\frac{1}{V} \left. \frac{\partial \Omega(\mu, T)}{\partial \mu} \right|_T \quad (32)$$

which has the explicit form

$$n = \frac{\mu}{g} - \frac{\eta}{V} \sum_k \frac{\epsilon(k)}{\sqrt{\epsilon(k)^2 + 2\mu \epsilon(k)}} \left( \frac{1}{2} + \frac{1}{e^{\beta \sqrt{\epsilon(k)^2 + 2\mu \epsilon(k)}} - 1} \right) + \mathcal{O}(\eta^2). \quad (33)$$

Since the interesting experimental quantity is the condensate density $n_0$, we eliminate the chemical potential $\mu$ in favor of $n_0$ via (29) and find

$$n - n_0 = \frac{\eta}{V} \sum_k \frac{\epsilon(k) + gn_0}{\sqrt{\epsilon(k)^2 + 2g\mu \epsilon(k)}} \left( \frac{1}{2} + \frac{1}{e^{\beta \sqrt{\epsilon(k)^2 + 2g\mu \epsilon(k)}} - 1} \right) + \mathcal{O}(\eta^2). \quad (34)$$

The right-hand side of Eq. (34) denotes the number of non-condensed particles in the so-called Popov approximation [50, 51].

C. Self-Consistent Popov Approximation

The result (34) is valid only for $n \approx n_0$, i.e. for small $\eta$. The quantum phase transition [25] which we want to locate, however, takes place for $n \gg n_0$, i.e. at the large value $\eta = 1$ of the loop counter. This strong-coupling regime can be reached by applying VPT, following the rules reviewed in Section II. Here we introduce a variational parameter $M$ by replacing, as in (6) and (7),

$$\mu = M + r\eta, \quad (35)$$

with the abbreviation

$$r = \frac{\mu - M}{\eta}. \quad (36)$$
Inserting (35) into the grand-canonical potential (31), and reexpanding this in powers of $\eta$ at fixed $r$, we obtain

$$\frac{\Omega_{\text{trial}}(M, \mu, T)}{V} = -\frac{M^2}{2g} - \frac{M}{g} r + \frac{\eta}{2V} \sum_k \sqrt{\epsilon(k)^2 + 2M\epsilon(k)} + \frac{\eta}{\beta V} \sum_k \ln \left(1 - e^{-\beta \sqrt{\epsilon(k)^2 + 2M\epsilon(k)}}\right) + O(\eta^2).$$

(37)

Reinserting back $r$ from (36), ignoring the terms $O(\eta^2)$, and setting $\eta = 1$, we arrive at the following trial function for the grand-canonical potential:

$$\frac{\Omega_{\text{trial}}(M, \mu, T)}{V} = -\frac{M^2}{2g} - \frac{M \mu}{g} + \frac{1}{2V} \sum_k \sqrt{\epsilon(k)^2 + 2M\epsilon(k)} + \frac{1}{\beta V} \sum_k \ln \left(1 - e^{-\beta \sqrt{\epsilon(k)^2 + 2M\epsilon(k)}}\right).$$

(38)

This is optimized with respect to the variational parameter $M$, yielding

$$M_{\text{opt}} = \mu - \frac{g}{V} \sum_k \frac{\epsilon(k)}{\sqrt{\epsilon(k)^2 + 2M_{\text{opt}}\epsilon(k)}} \left(\frac{1}{2} + \frac{1}{e^{\beta \sqrt{\epsilon(k)^2 + 2M_{\text{opt}}\epsilon(k)}} - 1}\right).$$

(39)

Inserting (39) into (38) yields the optimized grand-canonical potential

$$\Omega(\mu, T) = \Omega_{\text{trial}}(M_{\text{opt}}, \mu, T).$$

(40)

However, we are more interested in a resummation of equation (34). To this end we compute the particle density (32) by using (40)

$$n = -\frac{1}{V} \frac{\partial \Omega_{\text{trial}}(M_{\text{opt}}, \mu, T)}{\partial \mu}|_{M_{\text{opt}}, T} - \frac{1}{V} \frac{\partial \Omega_{\text{trial}}(M_{\text{opt}}, \mu, T)}{\partial M_{\text{opt}}}|_{\mu, T} \frac{\partial M_{\text{opt}}}{\partial \mu}. $$

(41)

Because of Eqs. (38) and (39), this reduces to

$$n = \frac{M_{\text{opt}}}{g}. $$

(42)

Furthermore, we perform a similar variational resummation for the condensate density (29). The substitution (35) yields the variational expression

$$n_0 = \frac{M}{g} + \frac{r}{g} - \frac{\eta}{V} \sum_k \frac{2\epsilon(k) + M}{\sqrt{\epsilon(k)^2 + 2M\epsilon(k)}} \left(\frac{1}{2} + \frac{1}{e^{\beta \sqrt{\epsilon(k)^2 + 2M\epsilon(k)}} - 1}\right) + O(\eta^2).$$

(43)

Reinserting (36) and ignoring the terms $O(\eta^2)$, this becomes at $\eta = 1$

$$n_0 = \frac{\mu}{g} - \frac{1}{V} \sum_k \frac{2\epsilon(k) + M}{\sqrt{\epsilon(k)^2 + 2M\epsilon(k)}} \left(\frac{1}{2} + \frac{1}{e^{\beta \sqrt{\epsilon(k)^2 + 2M\epsilon(k)}} - 1}\right).$$

(44)

Evaluating this expression at $M = M_{\text{opt}}$ with (39), we find by taking into account (42)

$$n - n_0 = \frac{1}{V} \sum_k \frac{\epsilon(k) + gn}{\sqrt{\epsilon(k)^2 + 2gne\epsilon(k)}} \left(\frac{1}{2} + \frac{1}{e^{\beta \sqrt{\epsilon(k)^2 + 2gne\epsilon(k)}} - 1}\right).$$

(45)

Thus we have arrived at the self-consistent Popov approximation, which differs from the usual Popov approximation (34) by having the total particle density $n$ on the right-hand side rather than the condensate density $n_0$. Note that Eq. (45) could also be obtained by just replacing $n_0$ in the right-hand side of Eq. (34) by $n$, the error involved in this substitution being of order $O(\eta^2)$. The above VPT analysis puts such a “dressing” procedure on a rigorous footing. Furthermore, we remark that the location of the quantum phase transition [25] for all $T$ is obtained from (45) by solving this equation for $n_0 = 0$ [52, 53].

**IV. LOWEST-ORDER TRANSITION CURVE**

In this section we determine the quantum phase transitions for a homogeneous BEC in the $a_s-T$-plane from (45).
A. Zero-Temperature Limit

Inserting into (45) the free-particle energies
\[ \epsilon(k) = \frac{\hbar^2 k^2}{2m}, \quad (46) \]
and going to the thermodynamic limit, in which we can replace the momentum sum by an integral
\[ \sum_k \rightarrow V \int \frac{d^Dk}{(2\pi)^D}, \quad (47) \]
we find the zero-temperature equation
\[ n = n_0 + \frac{1}{2} \int \frac{d^Dk}{(2\pi)^D} E(k) \left( \frac{\hbar^2 k^2}{2m} + gn \right), \quad (48) \]
with the Bogoliubov quasi-particle energies
\[ E(k) = \sqrt{\left( \frac{\hbar^2 k^2}{2m} \right)^2 + 2gn} \frac{\hbar^2 k^2}{2m}. \quad (49) \]
For large values of \( k \), the Bogoliubov energies coincide with (46). For small values of \( k \), however, the Bogoliubov spectrum (49) has a linear \( k \)-dependence
\[ E(k) \approx c \hbar |k|, \quad c = \sqrt{\frac{4\pi \hbar^2 n a_s}{m^2}}. \quad (50) \]
Since \( E(k)/|k| \) is bounded from below, the interacting Bose gas is superfluid. Recently, the Bogoliubov sound velocity (50) was measured in a trapped BEC at MIT [54].

As the integrand in (48) depends only on the absolute value of the wave vector \( k \), the integrals are effectively one-dimensional, and we may rewrite (48) as
\[ n - n_0 = \frac{1}{2} \left[ J_D \left( 1, \frac{1}{2}, 2gn \right) + gn J_D \left( 0, \frac{1}{2}, 2gn \right) \right]. \quad (51) \]
Here we have introduced the master integral
\[ J_D(\alpha, \beta, a) = \frac{1}{\Gamma(D/2)} \left( \frac{m}{2\pi \hbar^2} \right)^{D/2} \int_0^\infty \frac{dx}{x^\alpha (x+a)^\beta} \frac{x^{D/2-\beta-1}}{\Gamma(D/2)} \int_0^\infty dx \frac{x^{\alpha+D/2-\beta-1}}{(x+a)^\beta}, \quad (52) \]
which is related to the integral representation of the Beta function
\[ B(x, y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)} = \int_0^\infty dt \frac{t^{x+y}}{(t+1)^{x+y}} \quad (53) \]
according to
\[ J_D(\alpha, \beta, a) = \frac{a^{D/2+\alpha-2\beta}}{\Gamma(D/2)} \left( \frac{m}{2\pi \hbar^2} \right)^{D/2} B \left( \frac{D}{2} + \alpha - \beta, \frac{D}{2} - \alpha + 2\beta \right). \quad (54) \]
Thus we find for the particle density (51) in \( D = 3 \) dimensions the equation:
\[ \frac{n - n_0}{n} = \frac{\sqrt{m^3 n^3 a_s}}{3\pi^2 \hbar^3}, \quad (55) \]
which gives the so-called deformation of the condensate. Expressing \( g \) in terms of the \( s \)-wave scattering length \( a_s \) leads to the well-known Bogoliubov depletion [52]:
\[ \frac{n - n_0}{n} = \frac{8}{3} \sqrt{\frac{a_s^2 n}{\pi}}. \quad (56) \]
Since this self-consistent equation was derived by variational perturbation theory which we know to be very good up to strong couplings [22], we may use it to find the strong-coupling value of \( a_s \) where the depletion is complete. This is the point of a quantum phase transition [25] at zero temperature, taking place at
\[ a_s^c(T = 0)n^{1/3} = \left( \frac{9\pi}{64} \right)^{1/3}. \quad (57) \]
9

FIG. 3: Quantum phase diagram of Bose-Einstein condensation in variationally improved one-loop approximation without (dotted) and with properly imposed higher-loop slope properties at $T_c^{(0)}$ (dashed length increasing with VPT order). Short solid curve starting at $T_c^{(0)}$ is due to Arnold et al. [21]. Dashed straight line indicates the slope of our curve extracted either from Monte-Carlo data [13, 14] or recent analytic results [18, 20]. Diamonds correspond to the Monte-Carlo data of Ref. [6] and dots stem from Ref. [58], both scaled to their critical value $a_s(T = 0) \approx 0.63$.

B. Full Quantum Phase Diagram

We now calculate the temperature dependence of the quantum phase transition. Using (45)–(47), we obtain instead of the zero-temperature equation (55)

$$a_s n^{1/3} \left[ 1 + \frac{3\alpha}{16} I(\alpha) \right]^{2/3} = \left( \frac{n-n_0}{n} \right)^{2/3} \left( \frac{9\pi}{64} \right)^{1/3},$$

where $I(\alpha)$ abbreviates the integral

$$I(\alpha) = \int_0^\infty dx \frac{x\alpha + 8}{2\sqrt{x\alpha} + 16(e^{\sqrt{x}2\alpha/16} + 1)}.$$

The dimensionless parameter $\alpha$ is given by

$$\alpha = \left[ \frac{t}{a_s n^{1/3} \zeta(3/2)^{2/3}} \right]^2,$$

where $t = T/T_c^{(0)}$ denotes the reduced temperature. The quantum phase transition at $n_0 = 0$ obeys now the equation

$$a_c n^{1/3} \left[ 1 + \frac{3\alpha_c}{16} I(\alpha_c) \right]^{2/3} = \left( \frac{9\pi}{64} \right)^{1/3}.$$ (61)

Near $T = 0$ we perform a Taylor expansion in the parameter $\alpha_c$, i.e.

$$a_c n^{1/3} = \sum_{k=0}^N a_k \alpha_c^k + O(\alpha_c^{N+1}),$$ (62)

and obtain for the coefficients:

$$a_0 = \left( \frac{9\pi}{64} \right)^{1/3} \approx 0.762, \quad a_1 \approx -0.313, \quad a_2 \approx 0.200, \quad a_3 \approx -0.207.$$ (63)

The series has Borel character — the sign of the coefficients is alternating. This expansion is inapplicable for small $a_s$ since $\alpha$ diverges in this limit. There we solve (61) by rescaling and expanding the integrand in (59), yielding

$$I(\alpha) = \frac{\sqrt{\alpha}}{2} \int_0^\infty dz \sqrt{z} \exp \left( \frac{1}{\sqrt{\alpha z/4 + 2/\sqrt{\alpha}}} \right) - 1 + O \left( \frac{1}{\alpha} \right).$$ (64)
Using the series representation of the Bose distribution function, we obtain
\[ I(\alpha) = \frac{4\Gamma(3/2)}{\alpha^{1/4}} \zeta_{3/2}(e^{-2/\sqrt{\alpha}}) + \mathcal{O}\left(\frac{1}{\alpha}\right), \tag{65} \]
where we have introduced the polylogarithmic function
\[ \zeta_\nu(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^\nu}. \tag{66} \]
It has the Robinson expansion [55]
\[ \zeta_\nu(e^{\beta \mu}) = \Gamma(1 - \nu)(-\beta \mu)^{\nu-1} + \sum_{k=0}^{\infty} \frac{(\beta \mu)^k}{k!} \zeta(\nu - k), \quad \mu < 0, \tag{67} \]
which can easily be proved with the help of Poisson’s summation formula [22, Chap. 2]. Thus we obtain for large \( \alpha \):
\[ I(\alpha) \approx \frac{2\sqrt{2\pi}\zeta(3/2)}{\alpha^{1/4}} - \frac{4\sqrt{2}\pi}{\sqrt{\alpha}} + \mathcal{O}\left(\frac{1}{\alpha^{3/4}}\right), \tag{68} \]
Inserting this into (61) yields:
\[ 1 = t_c^{3/2} - \frac{2\sqrt{2\pi}a_c n^{1/3}t_c}{\zeta(3/2)^{2/3}}. \tag{69} \]
From this equation we can derive a shift in the critical temperature due to the interaction. We expand
\[ t_c = 1 + \frac{\Delta T_c}{T_c^{(0)}}, \tag{70} \]
and obtain from (69)
\[ \frac{\Delta T_c}{T_c^{(0)}} = \frac{4\sqrt{2}\pi}{3\zeta(3/2)^{2/3}} \sqrt{a_c n^{1/3}} + \mathcal{O}(a_c n^{1/3}). \tag{71} \]
This has the square-root behavior found before in Refs. [56, 57], with the positive sign agreeing with Ref. [57]. The full phase diagram is displayed in Fig. 3. It shows the interesting phenomenon of a reentrant transition above the critical temperature \( T_c^{(0)} \) of the free system, which shows up as a nose in the transition curve. This implies that a condensate can be produced above \( T_c^{(0)} \) by increasing \( a_s \), which disappears upon a further increase of \( a_s \). The transition curve differs so far considerably from early Monte-Carlo simulations [6], also shown in Fig. 3.

From recent work we know, however, that the square-root behavior (71) is incorrect, since its derivation ignores the pile-up of infrared singularities to high orders at the critical point. As explained in the beginning, Monte-Carlo simulations [13, 14] and precise high-temperature calculations [18, 20] have derived a temperature shift (1) which is linear in the scattering length \( a_s \), with a slope \( c_1 \approx 1.3 \). Thus it becomes necessary to improve our resummed one-loop approximation (61) for the transition line via VPT in such a way that the \( a_c \to \infty \) behavior of the expansion (62) is given by (1) and not by (71). In doing so we can follow the interpolation program between weak and strong-coupling expansions which was developed in Ref. [41].

### C. Variationally Improved Quantum Phase Diagram

We now calculate a more reliable transition curve for the quantum phase diagram interpolating the weak-coupling expansions (62) to a strong-coupling expansion which is compatible with the linear increase (1). The generic strong-coupling expansion is
\[ a_c^{\nu_1/3} = \alpha^{p/q}_c \sum_{k=0}^{N} b_k \alpha^{2k/q}_c. \tag{72} \]
We shall use only the accurate knowledge of the small-\(a_s\) behavior (1) so that we possess only the two leading terms in (72):

\[
a_s^c n^{1/3} = \alpha_c^{b/q} \left( b_0 + b_1 \alpha_c^{-2/q} \right). \tag{73}
\]

Expressed in terms of the parameter \(\alpha\) of Eq. (60) and replacing \(t_c\) via (70), this reads:

\[
b_0 - \left( a_s^c n^{1/3} \right)^{1+2p/q} \zeta(3/2)^{4p/3q} + b_0 \frac{2p}{q} \frac{T_c}{T_c^{(0)}} + b_1 \zeta(3/2)^{8/3q} \left( a_s^c n^{1/3} \right)^{4/q} = 0. \tag{74}
\]

This equation is satisfied if

\[
1 + \frac{2p}{q} = 0, \quad \frac{4}{q} = 1,
\]

which fixes the values of \(p, q\) to \(p = -2, q = 4\). Comparison between (1) and (74) yields

\[
b_0 = \frac{1}{\zeta(3/2)^{2/3}}, \quad b_1 = \frac{c_1}{\zeta(3/2)^{4/3}}. \tag{76}
\]

This result will now be combined with our self-consistent one-loop approximation (61) for small \(\alpha\). The philosophy will be to use only the first \(W+1\) weak-coupling coefficients \(a_0, \ldots, a_W\) in (62). We allow for two extra weak-coupling coefficients \(\tilde{a}_{W+1}\) and \(\tilde{a}_{W+2}\) chosen such that the strong-coupling limit calculated with VPT matches the coefficients \(b_0\) and \(b_1\) in (76). Afterwards we determine the whole quantum phase diagram from the variationally resummed series

\[
a_s^c n^{1/3} = \sum_{k=0}^{W} a_k \alpha_c^k + \tilde{a}_{W+1} \alpha_c^{W+1} + \tilde{a}_{W+2} \alpha_c^{W+2}. \tag{77}
\]

Let us illustrate this procedure for \(W = 0\) and determine the subsequent weak-coupling coefficients \(\tilde{a}_1, \tilde{a}_2\) from the strong-coupling coefficients \(b_0, b_1\). To this end we follow the VPT procedure of Section II by identifying \(\alpha_c \equiv g\) and by specifying (8) for \(N = 2, p = -2,\) and \(q = 4:\)

\[
f_2(g, K) = \frac{3a_0}{K^2} - \frac{3a_0}{K^4} + \frac{a_0 + 4g\tilde{a}_1}{K^6} - \frac{3g\tilde{a}_1}{K^8} + \tilde{a}_2 g^2 \alpha_c K^4 \tag{78}
\]

where the last two coefficients in (8) were replaced by \(\tilde{a}_1, \tilde{a}_2\). According to the principle of minimal sensitivity [32] we have to optimize (78) with respect to \(K\) and solve Eq. (9) which leads to

\[
-6a_0 \alpha_c + \frac{12a_0}{K^3} - 6a_0 + 4g\tilde{a}_1 \alpha_c K^7 - 24g\tilde{a}_1 \alpha_c K^9 - 10\tilde{a}_2 g^2 \alpha_c \alpha_c K^{11} = 0. \tag{79}
\]

Inserting the ansatz (11) with the two leading coefficients \(K_2^{(0)}\) and \(K_2^{(1)}\), i.e.

\[
K_2(g) = K_2^{(0)} g^{-1/4} + K_2^{(1)} g^{-1/4} + \mathcal{O}(g^{-3/4}),
\]

into (79) and comparing the coefficients of the two leading powers \(g^{-1/2}\), \(g^{-1/4}\) in the coupling constant \(g\), yields the following two equations:

\[
0 &= 3K_2^{(0)} a_0 - 12K_2^{(1)} \tilde{a}_1 + 5\tilde{a}_2, \tag{80}
\]

\[
0 &= 6K_2^{(0)} a_0 + 9K_2^{(0)} K_2^{(0)} a_0 + 12K_2^{(0)} \tilde{a}_1 + 84K_2^{(0)} K_2^{(1)} \tilde{a}_1 + 55K_2^{(1)} \tilde{a}_2.
\]

As we have four unknown variables \(\tilde{a}_1, \tilde{a}_2, K_2^{(0)}\) and \(K_2^{(1)}\), we need two more equations for their unique determination. It turns out that they can be obtained from the known strong-coupling coefficients \(b_0\) and \(b_1\) in (76) as follows. Inserting (80) into (78) and comparing with (12) yields:

\[
b_0 = \frac{1}{K_2^{(0)}} \left( 3K_2^{(0)} a_0 + 4K_2^{(0)} \tilde{a}_1 + \tilde{a}_2 \right), \tag{83}
\]

\[
b_1 = \frac{1}{K_2^{(0)}} \left( -3K_2^{(0)} a_0 + 6K_2^{(0)} K_2^{(1)} a_0 + 3K_2^{(0)} \tilde{a}_1 + 24K_2^{(0)} K_2^{(1)} \tilde{a}_1 + 10K_2^{(1)} \tilde{a}_2 \right).
\]
From (81) and (83), we determine $\tilde{a}_1$ and $\tilde{a}_2$ as functions of $K_2^{(0)}$:

$$\tilde{a}_1 = -\frac{3}{2} K_2^{(0)^4} \left( a_0 - \frac{5}{12} b_0 K_2^{(0)^2} \right), \quad \tilde{a}_2 = 3K_2^{(0)^8} \left( a_0 - \frac{1}{2} b_0 K_2^{(0)^2} \right).$$

Furthermore, Eq. (82) can be solved for $K_2^{(1)}$:

$$K_2^{(1)} = -K_2^{(0)^3} \frac{b_1 K_2^{(0)^8} + 3a_0 K_2^{(0)^4} + 3\tilde{a}_1}{6K_2^{(0)^8} a_0 + 24K_2^{(0)^4} \tilde{a}_1 + 10\tilde{a}_2}.$$

This expression has the interesting property, that the denominator is zero, if we insert (85). As $K_2^{(1)}$ should be a finite quantity, we have to demand that the numerator also vanishes. This leads to an explicit algebraic expression for $K_2^{(0)}$, which is solved by

$$K_2^{(0)} = \pm \left( -\frac{3a_0}{2b_1} + \sqrt{\frac{9a_0^2}{4b_1^2} - \frac{3\tilde{a}_1}{b_1}} \right)^{1/4}.$$

Note that with that the choice (84) is satisfied although it was not needed for deriving (87). We now insert the weak-coupling coefficient $a_0 \approx 0.762$ from (63) and the correct strong-coupling coefficients (76) with $c_1 \approx 1.3$ to yield $K_2^{(0)} \approx \pm 0.93461$. This result leads via (85) to the new coefficients:

$$W = 0 : \quad \tilde{a}_1 \approx -0.654, \quad \tilde{a}_2 \approx 0.935.$$

Finally, the trial function (78) follows to be

$$f_2(g,K) \approx 2.284 \frac{1}{K^2} - 2.284 \frac{1}{K^4} + (0.761 - 2.616g) \frac{1}{K^6} + 1.962g \frac{1}{K^8} + 0.935g^2 \frac{1}{K^{10}}.$$

and leads together with the optimization (9) to our first resummation improved transition line which is valid for arbitrary values of the coupling constant. The result, shown in Fig. 3 as VPT order 1, has now the correct asymptotic behavior near $T_c^{(0)}$ as well as near $T = 0$. In a similar way we also determined the new computed weak-coupling coefficients of the improved resummed one-loop approximation for the two subsequent orders $W = 1, 2$:

$$W = 1 : \quad \tilde{a}_2 = -1.864, \quad \tilde{a}_3 = 16.66,$$

$$W = 2 : \quad \tilde{a}_3 = -29.53, \quad \tilde{a}_4 = 622.0.$$

A resummation of the corresponding weak-coupling series (77) shows the fast converging phase curves with VPT order 2 and 3 in Fig. 3. It is interesting that the new computed coefficients in (90) and (91) deviate significantly from the original ones in (63). The reason is that the influence of higher orders becomes smaller in a weak-coupling expansion and it needs higher deviations to obtain the correct strong-coupling behavior.

The agreement with the Monte Carlo points in Fig. 3 is now much better than with the initial one-loop transition curve. However, it is not perfect since the simulations are quite inaccurate in the nose region. In fact, the slope parameter of the Monte Carlo data is $c_1 \approx 0.3$ [6], which is a factor 4 smaller than the true value. The disagreement is therefore no cause of worry.

Let us end by remarking that a nose in the phase diagram was also found in Ref. [59]. The authors did not, however, take this phenomenon seriously but considered it as an artefact of their slave boson approach.

V. SUMMARY AND OUTLOOK

In this article we have investigated the condensation of a homogeneous Bose gas in the $a_s-T$-plane. The result was obtained by applying VPT at two stages. First, we variationally resummed the Popov approximation to the effective potential in order to reach the quantum phase transition. Second, the lowest-order quantum phase diagram was variationally improved by taking into account recent results on the leading temperature shift for small scattering length $a_s$.

Finally, we mention that the self-consistent Popov approximation is also applicable to BECs trapped in optical lattices [26]. There the periodicity of the lattice leads to a quasi-free behavior due to Bloch’s theory which enables
us to treat this system as effectively homogeneous [60–65]. At \( T = 0 \), this yields a quantum phase transition from a superfluid phase to a Mott insulator, in good agreement with recent experimental data [66]. The theory in Ref. [26] predicts again a reentrant phenomenon in the quantum phase diagram which might be observed experimentally. The only problem is the need of a soft magnetic trap with frequency of the order of 10 Hz which holds the atoms in the optical lattice. This could in principle destroy the reentrant transition, since the temperature shift in a trap is negative. It is not yet clear whether for very small trap frequency, there exists a crossover from negative to positive slope \( c_1 \).

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