Quantum-unbinding near a zero temperature liquid–gas transition

Wilhelm Zwerger
Technische Universität München, Physik Department, James-Franck-Strasse, 85748 Garching, Germany
E-mail: zwerger@ph.tum.de

Received 28 June 2019
Accepted for publication 8 August 2019
Published 22 October 2019

Abstract. We discuss the quantum phase transition from a liquid to a gaseous ground state in a Bose fluid with increasing strength of the zero point motion. It is shown that in the zero pressure limit, the two different ground states are separated by a quantum tricritical point whose position is determined by a vanishing two-body scattering length. In the presence of a finite three-body scattering amplitude, the superfluid gas at this point exhibits sound modes whose velocity scales linearly with density while the compressibility diverges $\sim p^{-1/3}$ in the limit of vanishing pressure $p$. In the liquid regime of negative scattering lengths, it is shown that $N$-body bound states exist up to arbitrary $N$, consistent with a theorem by Seiringer. The asymptotic scaling $a_-(N) \sim N^{-1/2}$ of the scattering lengths where they appear from the continuum is determined from a finite size scaling analysis in the vicinity of the quantum tricritical point. This also provides a qualitative understanding of numerical results for the quantum unbinding of small clusters.

Keywords: quantum phase transitions, Bose–Einstein condensation, cold atoms, quantum fluids
Quantum-unbinding near a zero temperature liquid–gas transition

Contents

1. Introduction .......................................................... 2
2. Microscopic model and few-body physics ..................... 5
3. Zero temperature phase diagram and quantum tricritical point 10
4. Quantum unbinding for finite particle numbers ............... 15
5. Conclusion ................................................................ 16
   Acknowledgments .......................................................... 18
   References .................................................................. 18

1. Introduction

It is an empirical fact that the generic equilibrium state of matter at low temperatures is a solid. The only exceptions are the two isotopes of Helium which remain in a liquid phase down to zero temperature. On a microscopic level, this is a consequence of zero point motion, which plays an only minor role in most solids. In Helium, however, it is large enough to destroy crystalline order of the ground state below a critical external pressure $p_c$. For particles obeying Bose statistics, which will be considered here, the phase diagram can be determined in quantitative terms within a fully microscopic approach even for a strongly interacting system like $^4$He [1]. The approach also reveals the importance of Bose statistics in the stability of a liquid state at low temperatures and pressure. Indeed, as shown by Boninsegni et al [2], distinguishable particles with the same amount of zero point energy would actually form a crystal even at $p < p_c$ unless the temperature is close to zero. The aim of the present work is to investigate a scenario in which the zero point energy is even larger than the one in $^4$He. The ground state is then eventually a superfluid gas and the resulting finite temperature phase diagram, shown schematically in figure 1, exhibits neither a triple- nor a critical point. In practice, such a scenario is realized only in the case of spin-polarized hydrogen. As a long lived metastable configuration, however, a gaseous state is also present in dilute, ultracold Bose gases. Some of the results found here are thus expected to be of relevance also in this context. Note that for Bose systems which are liquid or gaseous with a uniform density, the ground state is a superfluid by a rather general argument due to Leggett [3].

In order to understand the quantum phase transition between a liquid and a gaseous ground state with increasing strength of the zero point motion, we follow an approach due to Sachdev [4] and consider the transition out of the vacuum state into one with a finite particle density $n$ as a function of the chemical potential $\mu$. In the case where the ground state is a gas, the associated effective field theory is the well known $\psi^4$-theory for a complex scalar field. Specifically, the finite density gas with $n(\mu) = \mu/g + \ldots$ is separated from the vacuum at $\mu < 0$ by a line of fixed points with infinite correlation.
length. For a liquid ground state, in turn, the transition out of the vacuum appears at a negative chemical potential \( \mu_c < 0 \). It is of first order, i.e. the density jumps from zero to a finite value \( \bar{n} \) at \( \mu = \mu_c^* \). The associated line of critical points thus has a finite correlation length which approaches infinity, however, close to the point where \( \mu_c \) reaches zero. Microscopically, the location of the quantum tricritical point which separates the liquid and gaseous ground states is determined by the condition \( g = 4\pi\hbar^2a/m \equiv 0 \) of a vanishing two-body scattering length. At this point and also in the liquid regime at small negative scattering lengths, the Bose system is stabilized by three-body interactions. The effective field theory thus features a \( \psi^4 \)-term as in the standard description of tricritical points. Expressed in terms of the de Boer parameter \( \Lambda_{dB} \), which measures the strength of the zero point motion \([5]\), the ground state at vanishing pressure changes from a liquid to a gas at a critical value \( \Lambda_{dB,c} \approx 0.7 \). For a finite particle number \( N \), the quantum unbinding transition is shifted to lower values \( \Lambda_{dB}^*(N) < \Lambda_{dB,c}^* \) of the de Boer parameter. This shift can be understood within a finite size scaling analysis in the vicinity of the quantum tricritical point, where both the bulk and the surface energy vanish, providing a qualitative understanding of numerical results for the unbinding of small clusters \([6, 7]\).

In standard ultracold Bose gases, the de Boer parameter is much less than one and thus the interaction supports a large number of two-body bound states. At very low densities, however, they are of no relevance since they are inaccessible kinematically with just two-body collisions. In particular, Bose gases with a positive scattering length form an essentially stable system down to zero temperature. For negative scattering lengths, in turn, stability of the ground state may be preserved only for small enough particle numbers \( N < N_c \approx 0.6 \ell_0/|a| \) and in the presence of a harmonic trap with an associated oscillator length \( \ell_0 \). At finite temperatures, however, an essentially
homogeneous Bose gas with attractive interactions can be studied in a moderately
degenerate, non-condensed regime \( n \lambda_T^3 \lesssim 1 \), even if the magnitude \(|a|\) of the scattering
length is increased to values of the order of the average interparticle spacing \( n^{-1/3} \)
or the thermal wavelength \( \lambda_T \) by the use of Feshbach resonances [8]. This allows to
explore basic few-body phenomena like the existence of three-body bound states for
identical bosons, which were predicted by Efimov [9] in a nuclear physics context. Efimov
states were first observed in an ultracold gas of Cesium atoms, where the for-
formation of a trimer bound state near zero energy shows up as a pronounced maximum
in the three-body loss coefficient [10]. Theoretically, one expects an infinite sequence
of trimers which may be thought of as excited states of the lowest lying 3-body bound
state. They emerge from the two-particle continuum at a sequence of increasingly
more negative scattering lengths \( a_{(n)}(3) \) which approach \( a = \pm \infty \) in a geometric manner.
Near this accumulation point, the effective range of the interactions is irrelevant.
For \( n \gg 1 \), therefore, the series displays universal behavior \( a_{(n+1)}(3)/a_{(n)}(3) \rightarrow 22.69 \ldots
\) which is associated with an underlying renormalization group limit cycle [11]. In prac-
tice, only the lowest or possibly the second lowest [12] of these trimers are accessible,
where universality is violated due to the finite range of the interactions. As shown by
Schmidt et al [13], this leads e.g. to a ratio \( a_{(1)}(3)/a_{(0)}(3) \simeq 17 \), much smaller than
in the universal limit. Many-body bound states exist also for larger particle numbers
\( N > 3 \). This has been studied in detail for \( N = 4 \), where theory predicts an infinite
sequence of two tetramer states per Efimov trimer [14–17]. Experimentally, the lowest
tetramer state has been observed by Ferlaino et al [18] at \( a_-(4) \simeq 0.47 a_-(3) \) and even
signatures of a five-body bound state have been inferred from a characteristic feature
in the recombination rate of Cesium near a scattering length \( a_-(5) \simeq 0.64 a_-(4) \) [19]. In
the present work, we will restrict ourselves to the energetically lowest \( N \)-body bound
states. The magnitude of the scattering lengths \( a_-(N) < 0 \) where they detach from the
continuum form a sequence which apparently approaches zero in a monotonic manner.
This has been investigated by von Stecher via numerical solutions of the Schrödinger
equation up to \( N = 13 \) [20]. In particular, it turns out that the consecutive ratios
\( a_-(4)/a_-(3) \simeq 0.44 \), \( a_-(5)/a_-(4) \simeq 0.64 \) and \( a_-(6)/a_-(5) \simeq 0.73 \) are not very sensitive
to the detailed form of the two-body interactions [21].

A natural question which arises in this context is whether the sequence of \( N \)-body
bound states continues up to \( N = \infty \). As will be discussed below, this is indeed the
case, at least near the quantum tricritical point, where the interaction changes from
an overall attractive to a repulsive behavior and there is no longer any two-body
bound state. The existence of an infinite sequence of \( N \)-body bound states with an
accumulation point at \( a = 0 \) is consistent with a theorem due to Seiringer [22], which
states that some \( N \)-body bound state must exist for arbitrary small negative scattering
lengths. Specifically, it turns out that the asymptotic dependence \(|a_-(N)| \sim N^{-1/2}\)
of the magnitude of the scattering lengths below which no \( N \)-body bound states exist,
is determined by a finite size scaling analysis in the vicinity of the quantum tricriti-
cal point. It is important to note that these results rely crucially on the assumption
of two-body interactions which have a strong repulsive part at short distances and a
finite range, guaranteeing thermodynamic stability and a stable liquid ground state as
in \( ^4 \)He. By contrast, within zero range or purely attractive interactions, the issue of
$N$-body bound states is ill-defined for large $N$. An example is provided by a Bose gas with zero range attractive interactions in two dimensions. As shown by Hammer and Son [23], it exhibits an infinite sequence of $N$-body bound states. Due to the logarithmic increase of the effective interaction strength at large distances, their binding energies $B_N$ increase exponentially according to $B_{N+1}/B_N \to 8.567 \ldots$ while their size $R_N$ goes to zero as $R_{N+1}/R_N = 0.3417 \ldots$ (see also the recent work by Bazak and Petrov [24]). For large $N$, therefore, the behavior of the interaction at short distance becomes relevant. An exceptional situation appears in one dimension, where the quantum dissociation of a Luttinger liquid into a gaseous phase has been discussed by Kolomeisky et al [25]. In this case, an attractive Bose gas with zero range interactions exhibits a finite temperature liquid–gas transition as shown by Herzog et al [26].

The paper is structured as follows: in section 2, we introduce the microscopic model and discuss the resulting two- and three-body problem. For vanishing scattering length and in a regime, where no two-body bound state exists, a repulsive three-body interaction arises from a positive value of the associated scattering hypervolume introduced by Tan [27]. An effective field theory description of the zero temperature liquid–gas transition in the many-body system near vanishing scattering length is developed in section 3, extending the early numerical approach to this problem by Miller et al [28]. Depending on the sign of $a$, the finite density superfluid is separated from the vacuum state by an either first or a second order line of fixed points which meet at a quantum tricritical point. Its position is determined by the condition of vanishing scattering length, i.e. by two-body physics. Moreover, in section 4, we address the problem for finite particle numbers. It is shown that the threshold scattering lengths $a_\pm(N)$ for the existence of $N$-body bound states in the limit $N \gg 1$ are determined by a finite size scaling analysis in the vicinity of the quantum tricritical point, which separates the liquid and gaseous ground states of the bulk system. A conclusion and a discussion of open problems is presented in section 5.

2. Microscopic model and few-body physics

We consider a generic Hamiltonian for a system of bosons with pure two-body interactions. The associated first quantized Hamiltonian

$$\hat{H}_N = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \nabla_i^2 + \sum_{1 \leq i < j \leq N} V(x_i - x_j)$$

(1)

gives rise to a proper thermodynamics provided the interaction fulfills certain conditions. Specifically, as shown by Fisher [29], a sufficient condition for the existence of a well defined thermodynamic limit is that the two-body potential $V(r) \geq -\epsilon$ has a finite lower bound, decays faster than $1/r^3$ at large distances and increases more rapidly than $1/r^3$ for separations smaller than a short range scale $\sigma$. Interactions of this type guarantee stability of the many-body problem since they obey

$$\sum_{1 \leq i < j \leq N} V(x_i - x_j) > -B \cdot N$$

(2)

https://doi.org/10.1088/1742-5468/ab3ccc
for all possible configurations with a positive constant $B$, which depends on $\epsilon$ but not on other variables like density, which are specific for different ground states. The characteristic energy and length scales $\epsilon$ and $\sigma$ determine the de Boer parameter

$$\Lambda_{\text{dB}} = \frac{\hbar}{\sigma \sqrt{m \epsilon}}$$

(3)
as the square root of the ratio between the zero point energy on the scale $\sigma$ and the depth $\epsilon$ of the attractive part of the potential. More specifically, we consider interactions with an asymptotic van der Waals tail $V(r \to \infty) = -C_6/r^6$ and a short range repulsion at $r \lesssim \sigma$ whose detailed behavior is not important except for the constraint that the potential increases more rapidly than $1/r^3$. A standard example is provided by the Lennard-Jones potential $V(r) = 4\epsilon \left[ (\sigma/r)^{12} - (\sigma/r)^6 \right]$ where the short distance scale $\sigma$ and the depth $\epsilon$ are connected with the strength of the van der Waals tail via $C_6 = 4\epsilon \sigma^6$. Independent of their precise form, the class of potentials which obey equation (2) lead to a well defined many-body ground state, whose energy $E_0(N) = u N + \ldots$ scales linearly with the particle number. In the regime $\Lambda_{\text{dB}} > \Lambda_{\text{dB}}^*$ of a gaseous ground state, the repulsive part of the interaction dominates and the scattering length $a$ is positive. Introducing $g = 4\pi \hbar^2 a/m > 0$, both the energy per particle $u(n) \to gn/2 = \sqrt{gp/2}$ and the density $n(p) \to \sqrt{2p/g}$ then vanish in the zero pressure limit. By contrast, a liquid ground state has a finite density $\bar{n}$ at vanishing pressure. As a result, $u(\bar{n})$ is finite and negative. Specifically, this is the case for $^4\text{He}$, where $\Lambda_{\text{dB}} \simeq 0.4$. The attractive part of the two-body interaction is then just barely sufficient to give rise to a bound state with a binding energy $B_2 \simeq k_B \cdot 1.7\text{ mK}$. It is tiny compared with the ground state energy per particle $u \simeq -k_B \cdot 7\text{ K}$ in the bulk liquid at zero pressure and dimensionless density $\bar{n} \sigma^4 \simeq 0.364$ [1, 30].

At the level of just two particles, determining the spectrum of $\hat{H}_2$ is an elementary problem in quantum mechanics. In the standard regime $\Lambda_{\text{dB}} \ll 1$, there is a large number $N_{\ell} \simeq 1/(\pi \Lambda_{\text{dB}}) \gg 1$ of s-wave bound states. Upon reduction of the strength of the attractive interaction, their number decreases and eventually reaches zero at a critical value of the de Boer parameter. In physical terms, this happens when the van der Waals length $\ell_{\text{vdW}} = (mC_6/\hbar^2)^{1/4}/2$, which is determined solely by the asymptotic form $-C_6/r^6$ of the interatomic interaction, has decreased to a value of the order of the short distance scale $\sigma$. For the specific case of a Lennard-Jones potential, where the scattering length can be determined with high precision (see e.g. Gómez and Sesma [31]), the limit beyond which the two-body Hamiltonian $H_2$ no longer has a bound state is reached at $\Lambda_{\text{dB}}^*(N = 2) = 0.423 \ldots$ or $\ell_{\text{vdW}} = 1.09 \sigma$. At this point, the scattering length jumps form $+\infty$ to $-\infty$ and the last two-body bound state unbinds. Upon further increasing the de Boer parameter, the scattering length increases monotonically from $-\infty$ towards zero, which is reached at some critical value $\Lambda_{\text{dB}}^c$. Specifically, one finds $\Lambda_{\text{dB}}^c = 0.679 \ldots$ for a Lennard-Jones potential, corresponding to a van der Waals length $\ell_{\text{vdW}} \simeq 0.86 \sigma$. Increasing $\Lambda_{\text{dB}}$ beyond its critical value, the interaction turns into a dominantly repulsive one, and the scattering length stays positive. An analytical expression is obtained for the pure $4\epsilon (\sigma/r)^{12}$ part of the Lennard-Jones potential, where

\[1\]
Quantum-unbinding near a zero temperature liquid–gas transition

\[ \Lambda_{dB}^*(3) = \frac{\Gamma(0.9)}{\Gamma(1.1)} \left( 8 \Lambda_{dB}^{3/2} / 5 \right)^{1/5} \]

which is of order \( \ell_{vdW} \simeq \sigma \) for realistic values of \( \Lambda_{dB} \simeq 1 \). The qualitative dependence of the scattering length on the de Boer parameter in the regime of interest is sketched in figure 2. In the vicinity of the last zero crossing near \( \Lambda_{dB}^* \), the scattering length vanishes linearly

\[ a(\Lambda_{dB}) = a_A \ell_{vdW} (\Lambda_{dB} - \Lambda_{dB}^*) + \ldots \]

with a numerical constant \( a_A \) of order one. This result is expected to hold quite generally for the class of potentials considered here.

The three-body problem for short range potentials with a van der Waals tail can be solved numerically. For the specific case of a Lennard-Jones interaction and in the regime of a shallow potential well, where no two-body bound state is present, this has been investigated by Mestrom et al [33] using the hyperspherical approach. It turns out that the last three-body bound state disappears beyond a critical value \( \Lambda_{dB}^* \) of the Boer parameter. Expressed in terms of the scattering length, this corresponds to \( a_-(3) = -9.6 \ell_{vdW} \) [33]. The order of magnitude \( a_-(3)/\ell_{vdW} \simeq -9 \) of this ratio is generic for interactions involving a van der Waals tail at large distances, independent of the short range scale \( \sigma \). For single channel potentials with a large number \( N_b \gg 1 \) of s-wave bound states, the ratio \( a_-(3)/\ell_{vdW} \) has in fact a universal value in the absence of three-body forces, as shown by Wang et al [34]. In practice, a change in the scattering length relies on the use of Feshbach resonances. A nearly universal value of the ratio \( a_-(3)/\ell_{vdW} \simeq -9 \) then appears only in the open-channel dominated limit [13].
Moreover, even in this regime, the experimentally observed ratio \( a_-(3)/\ell_{\text{vdW}} \) varies within a range between \(-8\) and \(-10\), a spread which is likely to be caused by different strengths of repulsive short-range three-body forces, see Langmack et al [35].

As discussed in the introduction, bound states exist also for larger particle numbers. Based on the numerical results obtained by von Stecher [20, 21], the magnitudes \(|a_-(N)|\) of the threshold scattering lengths below which no \( N \)-body bound state exists, form a monotonically decreasing sequence. By Seiringer’s theorem mentioned above, this sequence has \( a_0 = 0 \) as a lower limit which, as will be shown in section 4 below, is approached in a power law form as \( N \gg 1 \). For a study of \( N \)-body bound states in the limit of large \( N \), it is therefore sufficient to consider the regime of small, negative scattering lengths \(|a| \ll \ell_{\text{vdW}} \simeq \sigma\). Fine tuning of the interaction to the special value \( \Lambda_{\text{dB}} = \Lambda_{\text{c dB}} \), where the scattering length vanishes, is naively expected to realize an ideal Bose gas. This is not true, however, because a vanishing scattering length does not imply that the interactions have disappeared completely. Indeed, two-body interactions are still present in relative angular momenta \( l = 2, 4, \ldots \). For interactions with an attractive van der Waals behavior \(-C_6/r^6\), the leading \( d \)-wave contribution to the two-body scattering amplitude \( f(k, \theta) \) for identical bosons at low relative momenta \( k \) is2

\[
f(k, \theta)|_{a=0} = \frac{64\pi}{63} \ell_{\text{vdW}} (k\ell_{\text{vdW}})^3 P_2(\cos \theta) + \ldots
\]

In order to understand in more detail the limit of bosons with nearly vanishing scattering length, it is instructive to consider the two- and three-body problems in a cubic box of size \( L \) with periodic boundary conditions. For just two particles, the three leading terms of the associated ground state energy

\[
E_0(2|L) = \frac{g}{L^3} \left[ 1 + 2.837 \ldots \left( \frac{a}{L} \right) + 6.375 \ldots \left( \frac{a}{L} \right)^2 \right] + \mathcal{O}(L^{-6})
\]

only depend on the scattering length, as was shown by Lüscher [36] in the context of finite size scaling for quantum field theories on a lattice. If the scattering length is zero, the first non-vanishing contribution to the two-particle ground state energy therefore scales like \( L^{-6} \), i.e. like the square of the effective density \( n \simeq 1/L^3 \). In fact, such a dependence appears as the leading term at \( a = 0 \) in the extension of the result (7) to three particles, which has been derived by Tan [27]. Specifically, the ground state energy of three bosons with vanishing two-body scattering length in a box with periodic boundary conditions turns out to be [27]

\[
E_0(3|L)|_{a=0} = \frac{\hbar^2 D}{mL^6} + \mathcal{O}(L^{-8})
\]

The associated parameter \( D \) has been called the three-body scattering hypervolume by Tan [27]. It has dimension (length)\(^4\) and characterizes the strength of three-body interactions. In analogy to the definition of the scattering length via the asymptotic behavior \( \psi_{E=0}(x_1, x_2) = 1 - a/r_{12} \) of the two-body wave function at zero energy, the three-body scattering hypervolume \( D \) can alternatively be defined by the asymptotic behavior

\[2\] Note that the van der Waals interaction decays too slowly to guarantee the standard power law \( f_l(k \to 0) \sim k^{2l} \) for the behavior of the \( l \)-wave scattering amplitude at low momenta in the leading \( l = 2 \) contribution.
of the three-body wave function at zero energy and vanishing scattering length \cite{27}. Moreover, the position of the three-body bound states is determined by the poles of the hypervolume \( D \). Decreasing the de Boer parameter from its critical value \( \Lambda_{\text{dB}}^c \) to \( \Lambda_{\text{dB}}^c(3) \), the three-body scattering hypervolume \( D \) thus approaches minus infinity. In the regime \( \Lambda_{\text{dB}} < \Lambda_{\text{dB}}^c(3) \) where three-body bound states exist, it also acquires a finite imaginary part. Indeed, as shown by Zhu and Tan \cite{37}, the imaginary part of \( D \) describes the three-body loss rate via

\[
\Gamma_3 = -\dot{N}_{3\text{-body}}/N = L_3 n^2 = -\frac{\hbar}{m} \text{Im}(D) n^2. 
\]

In the following, we are interested in the regime \( \Lambda_{\text{dB}}^c(3) < \Lambda_{\text{dB}} \lesssim \Lambda_{\text{dB}}^c \) close to vanishing scattering length, where no three-body bound states exist and the parameter \( D \) is real. Our fundamental assumption is that \( D > 0 \) is positive in a finite range of scattering lengths near \( a = 0 \), where it must be of order \( \sigma^4 \sim \ell_{\text{vdW}}^4 \) by dimensional analysis. This assumption is supported by the numerical results for the many-body problem by Miller \textit{et al} \cite{28}, as will be discussed in more detail in the context of equation (19) below. It is also consistent with an explicit calculation of the three-body scattering hypervolume for a Gaussian potential \( V(r) \sim v_0 \exp(-r^2/r_0^2) \) by Zhu and Tan \cite{37}. Indeed, they find \( D > 0 \) not only in the purely repulsive case \( v_0 > 0 \) but also in a finite range of attractive interactions as long as the magnitude of the associated negative scattering length obeys \( |a| \lesssim r_0 \). Since their interaction vanishes identically at \( a = 0 \), one trivially finds \( D = 0 \) at the zero crossing of the scattering length. This is an artefact, however, of an interaction which is either purely repulsive or attractive and is not expected to apply for potentials e.g. of the Lennard Jones type near \( \Lambda_{\text{dB}}^c \). It is important to note that a positive value of \( D \) near vanishing scattering length may also arise from repulsive three-body forces which were studied in connection with the unexpectedly wide range of the observed ratio \( a_-(3)/\ell_{\text{vdW}} \) by Langmack \textit{et al} \cite{35}. The property \( D(a = 0) > 0 \) is not guaranteed however, for the full class of two-body interactions which obey the stability criterion (2). Indeed, as shown by Baumgartner \cite{39}, it is possible to construct interactions which obey (2) but they exhibit a three-body bound state even in the regime of positive scattering lengths. In contrast to the expected gaseous BEC, which is indeed found in the physically relevant example of spin-polarized hydrogen \cite{40}, the non-monotonic interactions considered by Baumgartner lead to a crystalline ground state. In practice, this is the case for \( \Lambda_{\text{dB}} < \Lambda_{\text{dB}}^c \approx 0.37 \) \cite{41}. By contrast, here we consider the situation near \( \Lambda_{\text{dB}}^c \approx 0.7 \) where the ground state above \( \Lambda_{\text{dB}}^c \) is a gas. A positive scattering length in the absence of any two-body bound state then implies the absence of bound states for all \( N > 2 \).

A crucial consequence of the assumption of a positive value \( D > 0 \) of the three-body scattering hypervolume near \( a = 0 \) is that, at finite density, the energy per particle \( u(n) = (\hbar^2 D/6m) \cdot n^2 \) scales quadratically with \( n \) \cite{27}. At vanishing scattering length, therefore, the many-body Bose fluid is stabilized by repulsive three-body interactions. The relation between pressure and chemical potential right at \( a = 0 \) is then of the form

\[
\psi_{E=0}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)\big|_{a=0} = 1 - \frac{\sqrt{3} D}{2\pi^2(r_{12}^2 + r_{13}^2 + r_{23}^2)^{3/2}} + \ldots
\]

3 see also the related recent work by Mestrom \textit{et al} \cite{38} for a square well potential.
Quantum-unbinding near a zero temperature liquid–gas transition

\[ p(\mu)|_{a=0} = \left( \frac{8m}{9\hbar^2 D} \right)^{1/2} \cdot \mu^{3/2} \rightarrow \mu(n)|_{a=0} = \frac{\hbar^2 D}{2m} \cdot n^2. \] (11)

As a result, the density \( n(\mu) = \partial p / \partial \mu \) scales with the square root of the chemical potential rather than the linear behavior found for positive scattering lengths. This is a consequence of the non-standard critical exponent \( \beta = 1/4 \) associated with the appearance of a finite order parameter \( |\psi(\mu)| \sim \mu^\beta \) at a tricritical point, which will be discussed in more detail below. The associated compressibility \( \tilde{\kappa} = \partial n / \partial \mu \) exhibits a weak power law divergence

\[ \tilde{\kappa}(p)|_{a=0} = 3 \left( \frac{m}{9\hbar^2 D} \right)^{2/3} \cdot p^{-1/3} \] (12)

in the limit of vanishing pressure, instead of approaching a constant \( \tilde{\kappa}(p \to 0) = 1/g \) for finite, positive values of the scattering length. The relation (12) provides a possible experimental tool to verify the presence of three-body interactions in a Bose gas at vanishing scattering length and to determine the associated three-body scattering hypervolume \( D \). Indeed, as shown by Ku et al [42] for Fermi gases at unitarity and by Desbuquois et al [43] for Bose gases in two dimensions, the function \( \tilde{\kappa}(p) \) is accessible from precision measurements of in-situ density profiles in a harmonic trap. In the following we will show that the stabilization of the gas right at zero scattering length due to three-body interactions is sufficient to determine the universal behavior near the quantum tricritical point which separates the liquid ground state in the regime \( a < 0 \) from the situation at \( a > 0 \), where the ground state is a gas and the phase diagram at finite temperature has the form shown in figure 1.

3. Zero temperature phase diagram and quantum tricritical point

In order to derive an effective field theory of the zero temperature gas–liquid transition in the many-body problem at a finite density \( n \), we start from the microscopic action of a Bose system with pure two-body interactions as described by equation (1). The associated generating functional \( Z[J] = \int D\psi \exp \left( -S[\psi] / \hbar + \int J\psi \right) \) for the correlation functions of the complex scalar field \( \psi(\tau, x) \) can formally be expressed as a functional integral with action

\[ S = \int_\tau \int_x \left\{ \psi^*(\tau, x) \left( \hbar \partial_\tau - \frac{\hbar^2}{2m} \nabla^2 - \mu \right) \psi(\tau, x) + \frac{1}{2} |\psi(\tau, x)|^2 \int_{x'} V(x - x') |\psi(\tau, x')|^2 \right\} = S_0 + S_{\text{int}}. \] (13)

At the mean field level, the effective potential for a field configuration with no dependence on the time and spatial variables \( \tau \) and \( x \), where \( |\psi|^2 = n \) can be identified with the particle density, has the form \( V_{\text{eff}}^{(0)} = -\mu n + (g/2)n^2 \). The coefficient \( g = 4\pi\hbar^2 a/m > 0 \) is fixed by the two-body scattering length in vacuum\(^4\), which is positive in the regime

\(^4\) In the naïve mean field approach, \( g \) contains the scattering length in the Born approximation, which is ill-defined for potentials which increase more strongly than \( 1/r^3 \) at short distances. This problem is eliminated only in a full treatment of the two-body problem which is contained in the formulation in terms of an effective potential in equation (17) below.
\[ \Lambda_{\text{dB}} > \Lambda_{\text{dB}}^c \] where the two-body interactions are dominantly repulsive. The onset transition from the vacuum to a low density superfluid gas is then well understood in terms of a Gross–Pitaevskii description. In particular, the density of bosons \( n(\mu) = \mu/g + \ldots \) rises linearly to lowest order as \( \mu \to 0^+ \), while \( n(\mu) \equiv 0 \) vanishes for negative values of the chemical potential. Thus, \( \mu = 0, g > 0 \) is a line of quantum critical points which separates the vacuum state from a superfluid gas at finite density [4]. Despite the finite jump in the compressibility from \( \tilde{\kappa} = 0 \) to \( \tilde{\kappa} = 1/g > 0 \), the vacuum to superfluid transition is a continuous one. Indeed, approaching the line \( \mu = 0 \) from positive values, the correlation length is the well known healing length \( \xi = \hbar/\sqrt{2m\mu} = (8\pi a)^{-1/2} \) of a weakly interacting Bose–Einstein condensate. It is large compared to the average interparticle spacing since \( na^3 \ll 1 \) in the low density limit. Moreover, using the zero temperature Gibbs–Duhem relation \( \mu = u + p/n \) which connects the chemical potential and the pressure to the energy \( u \) per particle, one has \( u(n) = gn/2 = \sqrt{gp/2} \to 0 \) in the limit of vanishing density or pressure.

The endpoint at \( g = 0 \) of the line \( \mu \equiv 0 \) is a quantum tricritical point (see figure 3). It separates the continuous onset transition from the vacuum to a gaseous state in the regime \( g > 0 \) from a first order transition at \( \mu_c < 0 \) between the vacuum and a liquid for negative values of the scattering length. Now, as shown by Son and Wingate [44], the leading order effective field theory describing any finite density superfluid is completely fixed by the relation between the pressure and the chemical potential. Specifically, using (11), the Lagrange density (expressed in real time) of the superfluid just above the quantum tricritical point reads

\[
\mathcal{L}_{\text{eff}}|_{g=0} = \left( \frac{8m}{9\hbar^2 D} \right)^{1/2} \left( \hbar \partial_t \theta - \frac{\hbar^2}{2m} (\nabla \theta)^2 \right)^{3/2} \to p(\mu)|_{g=0} = n(\mu) \hbar \partial_t \varphi \\
+ \frac{\tilde{\kappa}(\mu)}{2} (\hbar \partial_t \varphi)^2 - \frac{\hbar^2 n(\mu)}{2m} (\nabla \varphi)^2 + \ldots
\]

Upon expansion to quadratic order in small gradients of the variable \( \theta = \mu t/\hbar - \varphi(t, x) \), it gives rise to the standard quantum hydrodynamic description of a superfluid in terms of a time and space dependent phase variable \( \varphi(t, x) \), see e.g. [45]. The velocity \( c_s \) of the resulting phonon-like excitations is determined from

\[
m c_s^2 = n/\tilde{\kappa} \to 2 \mu = \frac{\hbar^2 D}{m} n^2(\mu) \quad \text{at} \quad g = 0.
\]

In a superfluid gas at vanishing scattering length, therefore, the velocity \( c_s \) depends linearly on the density rather than the standard square root behavior found for positive scattering lengths \( g > 0 \).

A more complex situation arises for \( \Lambda_{\text{dB}} < \Lambda_{\text{dB}}^c \) where the scattering length is negative. In order to properly deal with the regime \( g < 0 \), where the ground state at vanishing pressure is a finite density liquid, it is necessary to include the quantum fluctuations of the field \( \psi(\tau, x) \) to all orders. On a formal level, this can be expressed in terms of an effective potential
\[ \Gamma[\psi] = \sum_{N=1}^{\infty} \frac{1}{N!} \int_{p_1 \ldots q_N} \Gamma_N(p_1 \ldots p_N, q_1 \ldots q_N) \psi^*(p_1) \ldots \psi^*(p_N) \psi(q_1) \ldots \psi(q_N) \]

\[ = \int_{\tau, x} \left\{ V_{\text{eff}}[\psi] + \psi^* \tilde{D} \psi + \ldots \right\} \]

(16)

which is defined via a Legendre transform \( \Gamma[\psi] = \ln \{ Z[J]/Z[0] \} - \int J \psi \) of the generating functional \( Z[J] \) associated with the action (13). It contains the exact vertex functions \( \Gamma_N \) at arbitrary orders, which are essentially the amplitudes for scattering processes with \( N \) incoming and \( N \) outgoing particles. Knowledge of the \( \Gamma_N \), including their dependence on the \( 2N \) momentum variables \( p_1 \ldots q_N \) which are constrained only by translation invariance in space and time \( p_1 + \ldots + p_N = q_1 + \ldots + q_N \), therefore requires a complete solution of the \( N \)-body problem. This is clearly impossible. Fortunately, however, for the discussion of the behavior near the quantum tricritical point, which is a zero density fixed point, we need only the leading non-vanishing terms in the expansion of the effective potential

\[ V_{\text{eff}}[\psi] = -\mu |\psi|^2 + \frac{g}{2} |\psi|^4 + \frac{\lambda_3}{3} |\psi|^6 + \ldots \]

(17)

associated with a time and space independent ‘classical’ field \( \psi \). Here, the coefficient \( \lambda_3 = \hbar^2 D/2m \) of the contribution \( \sim |\psi|^6 \) arises from the zero momentum limit \( \Gamma_3(0) = \hbar^2 D/m \) of the vertex function which is associated with effective three-body

\[ \text{Figure 3.} \] Zero temperature phase diagram as a function of the chemical potential \( \mu \) and the deviation \( g \sim \Lambda_{\text{dB}} - \Lambda_{\text{dB}}^c \) of the de Boer parameter from its critical value. The gaseous ground state in the regime \( g > 0 \) arises from the vacuum at \( \mu < 0 \) via a continuous transition. For \( g < 0 \), the ground state is a liquid. It is separated from the vacuum by a first order transition at \( \mu_c < 0 \). The point \( \mu = g = 0 \) is a quantum tricritical point.

\[ \text{\footnotesize Footnote 5:} \] Due to Galilei invariance, derivatives can only appear in the covariant form \( \tilde{D} = \hbar \partial_t - \hbar^2 \nabla^2/2m \).
interactions. It is fixed by the hypervolume $D$ discussed above and may in principle be calculated for a given two-body potential by solving for the three-body wave function at zero energy, as specified in equation (9). In the regime $g < 0$, the symmetry broken phase with a finite density $n(\mu) = |\psi|^2 \neq 0$ appears already beyond a negative value
\begin{equation}
\mu_c = -3g^2/(16\lambda_3) = -6\pi^2 \hbar^2 a^2/(mD)
\end{equation}
of the chemical potential, which vanishes with the square of the distance from the quantum tricritical point as indicated in figure 3. Remarkably, this behavior is identical to that found in the numerical approach to the bosonic many-body problem near $\Lambda_{dib}^c$ by Miller et al [28]. Specifically, they have determined the dimensionless curvature
\begin{equation}
\bar{u}''_c := \frac{1}{4\epsilon} \left. \frac{d^2 u(p = 0)}{d\Lambda_{dib}^2} \right|_{c} = -3\pi^2 a^2 \sigma^2 \frac{\ell_{dW}^2}{D}
\end{equation}
of the energy per particle $u(p = 0)$ right at the critical point. By the Gibbs–Duhem relation, $u(p = 0) = \mu$, coincides with the critical chemical potential since the pressure vanishes along the line separating the vacuum from the finite density liquid. In equation (19), $u(p = 0)$ has been normalized by the zero point energy $\epsilon_\sigma = \hbar^2/ma^2$ at the scale $\sigma$, while $a_\Lambda$ is the numerical constant which appears in equation (5). Recalling that for a Lennard-Jones interaction one has $\epsilon_{dW} = 0.86D$ at zero scattering length, the numerical result $\bar{u}''_c \simeq -6.547$ of [28] for the dimensionless critical curvature leads to an associated three-body scattering hypervolume $D(a = 0) \simeq 3.34 a_\Lambda^4\sigma^4$. The assumption of a positive value of the three-body scattering hypervolume near $a = 0$ for interactions which are strongly repulsive below a short distance scale $\sigma$ is therefore supported implicitly by the numerical results of Miller et al [28]. They did not realize, however, the connection between $\Lambda_{dib}^c$ and the zero of the scattering length nor the relation between the finite curvature (19) and the three-body problem through the associated scattering hypervolume. The extraction above of its specific value near $a = 0$ from numerical results of a many-body calculation thus obscures the fact that the parameter $D$ is fully determined by solving a three-body problem. Since $u(p = 0) \equiv 0$ in the regime of positive scattering lengths, the second derivative of $u(p = 0)$ with respect to $\Lambda_{dib}$ exhibits a jump at the quantum tricritical point. In physical terms, this gives rise to a jump in the derivative of the kinetic energy per particle $u_{kin} = (\Lambda_{dib}/2)du/d\Lambda_{dib}$, which has been interpreted as a signature for a conventional second order transition [28]. This conclusion, however, hides the presence of the underlying quantum tricritical point, whose critical exponents differ from those in standard Landau theory. Moreover, the virial theorem along the zero pressure line $\mu = \mu_c$, which takes the simple form $u_{kin} + 6u_{12} - 3u_6 = 0$ for the specific example of a Lennard-Jones interaction [28], becomes trivial at the quantum tricritical point because it is a zero density fixed point where both $u_{kin}$ and $u_{int}$ vanish.

Right on the line $\mu = \mu_c$, the density jumps from zero in the vacuum state $\mu < \mu_c$ to a finite value
\begin{equation}
\bar{n} = n(\mu_c) = 3|g|/(4\lambda_3) = 6\pi |a|/D \rightarrow \bar{n}\sigma^3 = 6\pi |a|\sigma^3/D = \frac{2|\bar{u}''_c|}{0.86 \pi a_\Lambda} (\Lambda_{dib}^c - \Lambda_{dib}) .
\end{equation}
The dimensionless product $\bar{n}\sigma^3$ therefore approaches zero linearly with the deviation from the quantum tricritical point, with a numerical prefactor of order one. Despite
Quantum-unbinding near a zero temperature liquid–gas transition

the large deviation $\Lambda_{\text{dB}}^c - \Lambda_{\text{dB}} \simeq 0.28$ of the de Boer parameter from its critical value, one might naively try to use equation (20) for a rough estimate of the density at zero pressure in $^4$He, whose empirical value is $\tilde{n}_0 \sigma^3 = 0.364$. Such an estimate is misleading, however, because the $^4$He interaction supports a two-body bound state and thus the relation (5) underlying this estimate does not apply. Quite generally, the equation of state in the liquid is of the form

$$p(\mu) = -V_{\text{eff}}[n(\mu)] = \tilde{n}(\mu - \mu_c) + \tilde{\kappa}_c (\mu - \mu_c)^2 / 2 + \ldots \Theta(\mu - \mu_c).$$

(21)

Since the compressibility $\tilde{\kappa} = \partial^2 p / \partial \mu^2$ is positive, $p(\mu)$ is a convex function of the chemical potential which must vanish identically in the vacuum regime $\mu < \mu_c$. Here, a constant in (17) has been added to guarantee $V_{\text{eff}}[\tilde{n}] = 0$. Moreover, there is a minus sign in comparison with the effective Lagrange density of equation (14) since the latter is expressed in real time $t$ rather than the imaginary time variable $\tau$ used in equation (16).

The density profile at a liquid-to-vacuum boundary with an effective potential of the form (17) has been calculated by Bulgac [46]. It has the form $n(z) = \tilde{n}/ (1 + \exp(2\kappa_0 z))$ with a healing length $1/\kappa_0 = \hbar / \sqrt{2m|\mu_c|} \simeq \sqrt{D}/|a|$ which diverges linearly with the distance from the quantum tricritical point. As a result, the surface tension derived in [46],

$$\tilde{\sigma} = \frac{\lambda_3 \tilde{n}^3}{6 \kappa_0} \simeq \frac{\hbar^2 a^2}{m D^{3/2}}$$

vanishes quadratically $\tilde{\sigma} \sim (\Lambda_{\text{dB}}^c - \Lambda_{\text{dB}})^2$, consistent with a scaling relation due to Widom [48] which connects the exponent of the surface tension $\tilde{\sigma} \sim 1/\xi^{d-1}$ with that of the correlation length. This result will play a crucial role in the following section, where we discuss the shift of the zero temperature liquid–gas transition for finite particle numbers.

Finally, we mention that within the microscopic model defined by equation (13), there are in fact two separate quantum phase transitions which occur as a function of the de Boer parameter $\Lambda_{\text{dB}}$. The first one, discussed here, appears between a gaseous and a liquid ground state at a critical value $\Lambda_{\text{dB}}^c \simeq 0.7$ where the scattering length crosses zero. Decreasing the de Boer parameter further below values $\Lambda_{\text{dB}} \simeq 0.4$ characteristic for $^4$He, the liquid ground state will eventually turn into a solid via a first order quantum phase transition. On the basis of a variational Ansatz for the ground state wave function, the associated critical de Boer parameter for bosons has been estimated to be around $\Lambda_{\text{dB}}^{\text{solid}} \simeq 0.37$ by Nosanow et al [41]. In the case of Fermions $\Lambda_{\text{dB}}^{\text{solid}} \simeq 0.42$ is substantially larger because Fermions prefer to stay localized near a discrete set of lattice sites even for larger values of the zero point motion. Note that, in contrast to the gas–liquid transition studied here, these critical values cannot be determined from two-body physics.

---

6 We use a bar in the surface tension $\tilde{\sigma}$ to distinguish it from the short distance length scale $\sigma$. Note also that the exponent $\kappa_0 = \nu_1/\phi_1 = 1$ for the divergence of the correlation length $1/\kappa_0$ along the first-order transition line $\mu = \mu_c$ is a subsidiary tricritical exponent in the notation of Griffiths [47]. The relevant crossover exponent $\phi_1 = 1/2$ is determined by the quadratic behavior (18) of the chemical potential near the quantum tricritical point.

https://doi.org/10.1088/1742-5468/ab3ccc
4. Quantum unbinding for finite particle numbers

In the regime \( \lambda_{dIB} < \lambda_{dIB}^c \) of negative scattering lengths, the ground state at vanishing pressure is a superfluid liquid. By the Gibbs–Duhem relation, the energy per particle \( u(p = 0) = \mu_c < 0 \) is negative. A given number \( N \) of particles thus has an extensive binding energy \( B_N = |u(p = 0)|N \). Moreover, since the liquid has a finite density \( \bar{n} \) at zero pressure, the radius of the associated bound state scales like \( R_N \simeq (N/\bar{n})^{1/3} \). In the limit where the scattering length approaches zero, both \( u(p = 0) \) and \( \bar{n} \) vanish. The zero pressure liquid thus evaporates into a gas precisely at the quantum tricritical point. This is true, however, only in the thermodynamic limit. For finite particle numbers, the binding energy \( B_N \) is reduced because particles on the surface of the associated cluster are less bound than those in the bulk. For the specific case of a Lennard-Jones interaction, this has been studied numerically for small clusters by Meierovich et al [6] and by Sevryuk et al [7]. In particular, it has been found that, at finite \( N \), quantum unbinding appears at values \( \lambda_{dIB}^c(N) < \lambda_{dIB}^c = 0.679 \) of the de Boer parameter which are considerably lower than what is expected in the thermodynamic limit. This observation can be understood by including a finite, positive surface energy \( f_s \) per particle in the liquid phase, which also accounts for the essentially flat radial density distributions found numerically near \( \lambda_{dIB}^c \) [7]. The surface energy is defined by the subleading term in the expansion

\[
E_0(N) = u \, N + f_s \, N^{2/3} + \ldots
\]

of the \( N \)-body ground state energy for \( N \gg 1 \). In practice, this expansion requires particle numbers larger than \( N \simeq 10 \). In fact, numerical studies of small helium clusters, where the scattering length is close to infinity rather than \( a \simeq 0 \) as studied here, yield \( E_0(N) \sim N^2 \) up to \( N = 10 \), see e.g. Yan and Blume [49]. Based on the finite size generalization of the liquid ground state energy in equation (23), the unbinding condition \( E_0(N + 1) = E_0(N) \) of a vanishing single particle addition energy \( \mu(N) = E_0(N + 1) - E_0(N) = 0 \) can be written in the form

\[
\frac{-3}{2f_s} [\lambda_{dIB}^*(N)] = N^{-1/3}.
\]

The finite size scaling of the deviation \( \lambda_{dIB}^c - \lambda_{dIB}^*(N) \) for \( N \gg 1 \) is thus determined by the dependence of the bulk energy \( u \) and the surface energy \( f_s \) per particle on the de Boer parameter. In [7] it has been assumed that \( u(\lambda_{dIB}) \) vanishes linearly near \( \lambda_{dIB}^c = \lambda_{dIB}^*(\infty) \). This leads to \( \lambda_{dIB}^*(\infty) - \lambda_{dIB}^*(N) \sim N^{-1/3} \) provided \( f_s \) is finite at the quantum tricritical point. This is clearly not the case, however, because the ground state at \( g = 0 \) is a gas, which has vanishing surface energy. In order to determine the proper scaling for large \( N \), we use the result (18) derived above. It shows that the energy per particle \( u(p = 0) = \mu_c \) on the zero pressure line separating the vacuum from the finite density liquid vanishes like the square of the deviation from the quantum tricritical point. Indeed, the quadratic dependence near \( \lambda_{dIB}^c \) agrees quite well with the numerically calculated ground state energy of Miller et al [28] (see their figure 4). It also provides a much better extrapolation towards the critical point of the data shown in figures 2(b) and 10 of [7] than the assumption of a linear behavior. To determine how the surface energy \( f_s \) per particle vanishes near \( \lambda_{dIB}^c \), we follow an argument due to...
Bulgac [46], who has used the expansion (23) to discuss Bose droplets with $N$ particles in the vicinity of the scattering lengths where the three-body scattering hypervolume $D$ diverges. For the conceptually quite different situation of small negative scattering lengths and no three-body bound states discussed here, the results (20) for the average interparticle spacing $\bar{n}^{-1/3}$ and (22) for the surface tension imply that the surface energy $f_s \simeq 4\pi \bar{n}^{-2/3} \cdot \tilde{\sigma} \sim |\Lambda_{dB}^c - \Lambda_{dB}^s|^{4/3}$ vanishes with a nontrivial power law near the quantum tricritical point. Based on equations (24) and (18), the threshold values $\Lambda_{dB}^c(N)$ of the de Boer parameter beyond which $N$-body bound states disappear therefore approach the critical value $\Lambda_{dB}^s$ of the bulk liquid–gas transition according to

$$\Lambda_{dB}^c - \Lambda_{dB}^s(N) \sim N^{-1/2}.$$  \hspace{1cm} (25)

Moreover, in view of equation (5), this leads immediately to a power law behavior

$$-a_-(N \gg 1) \simeq \left(\frac{\sqrt{D}}{N}\right)^{1/2}$$  \hspace{1cm} (26)

of the associated scattering lengths. Together with the basic conceptual structure of the phase diagram shown in figure 3, the result (26) is a major prediction of the present work. It has the remarkable feature that the three-body scattering hypervolume $D(a = 0)$ at vanishing scattering length sets the scale for the unbinding of $N$-body bound states in the asymptotic limit $N \gg 1$. This is a consequence of the fact that $D$ appears in the leading term $\sim D |\psi|^6$ in equation (17) which stabilizes the superfluid at both vanishing and small negative scattering lengths, while higher order contributions are negligible near the quantum tricritical point, where $\bar{n} \to 0$.

5. Conclusion

To conclude, we have discussed the quantum phase transition between a liquid and a gaseous phase of bosons with increasing strength of the zero point motion. A major result is encoded in figure 3 which shows that, at vanishing pressure, these two phases are separated by a quantum tricritical point. Its location is determined by the condition $a(\Lambda_{dB}^c) = 0$ of a vanishing scattering length. Note that a similar type of phase diagram was found previously by Nikolic and Sachdev [51] for Fermi gases near unitarity. In this case, the boundary between the vacuum and a superfluid phase at finite density exhibits a quantum multicritical point where two lines of fixed points with continuous transitions meet. The present approach for dealing with the zero temperature liquid–gas transition for bosons is complementary to the early work on this problem by Miller et al [28], which was based on microscopic model calculations. As a result, the underlying universality and in particular the connections of the many-body problem with two- and three-body physics was not realized. Indeed, apart from the fact that the location of the quantum critical point is determined by two-body physics, it is a unique feature of the

---

7 In [7], a power law with an exponent 1/3 has been fitted to the data for particle numbers between $N = 2$ and $N = 40$. In view of the restricted range in $N^{1/3}$ the agreement found there is still consistent with the different asymptotic behavior predicted here. The result (25) also differs from an earlier analysis of the quantum unbinding problem by Hanna and Blume [50], where numerical results on Helium clusters were extrapolated assuming a much faster approach $\Lambda_{dB}^c - \Lambda_{dB}^s(N) \sim 1/N$ to the critical de Boer parameter.
present problem that even the universal behavior in its vicinity is fixed by the parameter $D$ which is fully determined by solving a three-body problem. In practice, the only two systems where the physics discussed here is applicable in direct form are $^4$He and spin-polarized hydrogen. In the latter case, the ground state is a superfluid gas with a finite temperature phase diagram as shown in figure 1. In turn, the $^4$He ground state is a superfluid liquid which, as noted above, is unfortunately quite far from a system with small negative scattering length. Our results are of direct relevance, however, for numerical studies of Bose clusters near $\Lambda_{dB}^c$, as performed by Meierovich et al [6] and by Sevryuk et al [7]. In particular, a systematic study of larger particle numbers should reveal the finite size scaling (25) and also the associated dependence $-u(\Lambda_{dB}^c(N)) \sim 1/N$ of the negative shift in energy per particle where clusters unbind at finite $N$, which is based on our analysis of the ratio $u/f_s$ as a function of $\Lambda_{dB}$. From a mathematical point of view, an open problem is to specify precisely the class of two-body interactions $V(x)$ for which the three-body scattering hypervolume $D$ is positive near the zero of the scattering length where no two-body bound states are present.

A promising but more complex case for an application of the present ideas appears in ultracold gases, where the scattering length and thus the effective de Boer parameter can be changed externally via Feshbach resonances [8]. In particular, it is straightforward to tune an ultracold Bose gas to zero scattering length. In contrast to the situation discussed in the context of figure 2, however, the three-body scattering hypervolume now has a finite imaginary part associated with three-body losses via the relation (10). Moreover, since the de Boer parameter $\Lambda_{dB}$ associated with the full two-body interaction is much less than one, one has $\ell_{vdW} \gg \sigma$ and a true ground state which is a solid for both signs of the scattering length. Yet, in the regime of non-negative scattering lengths $a \geq 0$, dilute ultracold Bose gases stay in an effectively thermalized gaseous phase on time scales shorter than the inverse three-body loss rate $\Gamma_3^{-1}$. In particular, provided that the real part of the three-body scattering hypervolume $D$ is positive near the relevant zero crossing of the scattering length, the equation of state is dominated by three-body interactions. The gas at finite density is thus described by an effective potential of the form (17) with $g = 0$. As a result, it will exhibit a non-trivial relation (12) between compressibility and pressure and a sound velocity which depends linearly on density, as derived in equation (15). These relations provide a means to determine the parameter $D$ and it would obviously be of interest to check these predictions experimentally. A first step in this direction has been taken by Shotan et al [52], who have measured the recombination length $L_m$ in Im $D \simeq L_m^4$ near a zero crossing of the scattering length at $B \simeq 850$G in $^7$Li. Consistent with the dimensional argument above in the context of the purely real value $D \simeq (\ell_{vdW})^4$ of the three-body scattering hypervolume near the zero crossing of the scattering length where no two-body bound state exists, the observed recombination length near $a = 0$ turns out to be of order $L_m \simeq 4 \ell_{vdW}$ [52]. For negative scattering lengths, the true ground state of single component ultracold Bose gases is a solid. The finite density liquid discussed in connection with equation (20) in the regime near the critical de Boer parameter $\Lambda_{dB}^c$ is therefore not accessible. However, as shown by Petrov [53], a possible realization of a dilute liquid phase of bosons at negative scattering length which is stabilized by repulsive three-body interactions may be achieved in a situation where two internal states $|\uparrow\rangle$ and $|\downarrow\rangle$ are coupled by an rf-field. By varying the effective Rabi coupling,
the scattering length in the symmetric configuration \(|\uparrow\rangle + |\downarrow\rangle|/\sqrt{2}\) can be tuned to zero. The associated three-body scattering hypervolume \(D(a = 0) \approx a_{\uparrow\uparrow}^3/\xi\) is large and positive provided \(\xi = (a_{\uparrow\downarrow} + a_{\uparrow\uparrow})/(a_{\uparrow\downarrow} - a_{\uparrow\uparrow}) \ll 1\). In particular, it is a factor \(1/\xi \gg 1\) larger than the characteristic magnitude \(\text{Im} D \approx a_{\uparrow\uparrow}^4\) of its imaginary part, which determines the standard scaling of the three-body loss rate. Neglecting losses, the resulting effective potential (17) gives rise to a dilute Bose liquid in the regime where \(a < 0\). Its dimensionless density \(\bar{n}a_{\uparrow\uparrow}^3 \approx \xi |a|/a_{\uparrow\uparrow}\) vanishes linearly with the effective scattering length as in equation (20) and—moreover—is small enough to be accessible in the extremely dilute regime of ultracold gases. In fact, this type of liquid is a three-body interaction analog of self-bound droplets in two component Bose gases which are stabilized by the Lee–Huang–Yang contribution to the interaction energy, as predicted by Petrov [54] and observed experimentally by Cabrera [55]. A study of the unbinding of such droplets in the limit \(a \to 0^-\) might open the possibility to verify the predictions from the finite size scaling analysis of the disappearance of \(N\)-body bound states in section 4, complementary to the quite challenging extension of experimental data on loss features beyond \(N = 5\) [19].

**Acknowledgments**

It is a pleasure to thank Sergej Moroz, Richard Schmidt and Robert Seiringer for constructive comments. I am particularly grateful to Dmitry Petrov for pointing out the paper by Bulgac [46] and an inconsistency in the definition of the correlation length and the associated surface energy in the original version of the manuscript. Moreover, I would like to acknowledge Philippe Nozières, whose Lecture Notes on ‘Liquides et Solides Quantique’ from a course at the Collège de France in 1983 have provided an important part of the motivation for this project. The work has been completed during a stay at Nordita in a program on ‘Effective Theories of Quantum Phases of Matter’ whose support is gratefully acknowledged.

**References**

[1] Ceperley D M 1995 *Rev. Mod. Phys.* 67 279
[2] Boninsegni M, Pollet L, Prokof’ev N and Svistunov B 2012 *Phys. Rev. Lett.* 109 025302
[3] Leggett A 1973 *Phys. Rep.* 8 125
[4] Sachdev S 2011 *Quantum Phase Transitions* 2nd edn (Cambridge: Cambridge University Press)
[5] De Boer J 1948 *Physica* 14 139
[6] Mierovich M, Mushinski A and Nightingale M 1996 *J. Chem. Phys.* 105 6498
[7] Sevryuk M, Toennies J and Ceperley D 2010 *J. Chem. Phys.* 133 064505
[8] Chin C, Grimm R, Julienne P and Tiesinga E 2010 *Rev. Mod. Phys.* 82 1225
[9] Efimov V 1970 *Phys. Lett. B* 33 563
[10] Kraemer T et al 2006 *Nature* 440 315
[11] Braaten E and Hammer H-W 2006 *Phys. Rep.* 428 259
[12] Huang B, Sidorenkov I A, Grimm R and Hutson J M 2014 *Phys. Rev. Lett.* 112 190401
[13] Schmidt R, Rath S P and Zwerger W 2012 *Eur. Phys. J. B* 85 386
[14] Hammer H-W and Platter L 2007 *Eur. Phys. J. A* 32 113
[15] von Stecher J, D’Incao J P and Greene C H 2009 *Nat. Phys.* 5 417
[16] Schmidt R and Moroz S 2010 *Phys. Rev. A* 81 052709
[17] Deltuva A 2012 *Phys. Rev. A* 85 012708

https://doi.org/10.1088/1742-5468/ab3ccc
Quantum-unbinding near a zero temperature liquid–gas transition

19https://doi.org/10.1088/1742-5468/ab3ccc

J. Stat. Mech. (2019) 103104

[18] Ferlaino F, Knoop S, Berninger M, Harm W, D’Incao J P, Nägerl H-C and Grimm R 2009 Phys. Rev. Lett. 102 140401
[19] Zenesini A, Huang B, Berninger M, Besler S, Nägerl H-C, Ferlaino F, Grimm R, Greene C H and von Stecher J 2013 New J. Phys. 15 043040
[20] von Stecher J 2010 J. Phys. B 43 101002
[21] von Stecher J 2011 Phys. Rev. Lett. 107 200402
[22] Seiringer R 2012 J. Spec. Theo. 2 321
[23] Hammer H-W and Son D T 2004 Phys. Rev. Lett. 93 250408
[24] Bazak B and Petrov D S 2018 New J. Phys. 20 023045
[25] Kolomeisky E B, Qi X and Timmins M 2003 Phys. Rev. B 67 165407
[26] Herzog C, Olshanii M and Castin Y 2014 C. R. Phys. 15 285
[27] Tan S 2008 Phys. Rev. A 78 013636
[28] Miller M D, Nosanow L H and Parish L J 1977 Phys. Rev. B 15 214
[29] Fisher M E 1964 Arch. Ration. Mech. Anal. 17 377
[30] Kalos M H, Lee M A, Whitlock P A and Chester G V 1981 Phys. Rev. B 24 115
[31] Gómez F and Sesma J 2012 Eur. Phys. J. D 66 6
[32] Stwalley W and Nosanow L 1976 Phys. Rev. Lett. 36 910
[33] Mestrom P M A, Wang J, Greene C H and D’Incao J P 2017 Phys. Rev. A 95 032707
[34] Wang J, D’Incao J P, Esry B D and Greene C H 2012 Phys. Rev. Lett. 108 263001
[35] Langmack C, Schmidt R and Zwerger W 2018 Phys. Rev. A 97 033623
[36] Lüscher M 1986 Commun. Math. Phys. 105 153
[37] Zhu S and Tan S 2017 Three-body scattering hypervolumes of particles with short-range interactions (arXiv:1710.04147)
[38] Mestrom P M, Colussi V E, Secker T and Kokkelmans S J M F 2019 (arxiv:1905.07205)
[39] Baumgartner B 1997 J. Phys. A: Math. Gen. 30 L741
[40] Fried D, Killian T, Willmann L, Landhuis D, Moss S, Kleppner D and Greytak T 1998 Phys. Rev. Lett. 81 3811
[41] Nosanow L H, Parish L J and Pinski F J 1975 Phys. Rev. B 11 191
[42] Ku M J H, Sommer A T, Cheuk L W and Zwierlein M W 2012 Science 333 563
[43] Desbuquois R, Yefsah T, Chomaz L, Weitenberg C, Corman L, Nascimbène S and Dalibard J 2014 Phys. Rev. Lett. 113 020404
[44] Son D T and Wingate M 2006 Ann. Phys., NY 321 197
[45] Pitaevskii L and Stringari S 2016 Bose–Einstein Condensation and Superfluidity (Oxford: Oxford University Press)
[46] Bulgac A 2002 Phys. Rev. Lett. 89 050402
[47] Griffiths R B 1973 Phys. Rev. B 7 545
[48] Widom B 1965 J. Chem. Phys. 43 3892
[49] Yan Y and Blume D 2015 Phys. Rev. A 92 033626
[50] Hanna G J and Blume D 2006 Phys. Rev. A 74 063604
[51] Nikolic P and Sachdev S 2007 Phys. Rev. A 75 033608
[52] Shotan Z, Machtet O, Kokkelmans S and Khaykovich L 2014 Phys. Rev. Lett. 113 053202
[53] Petrov D S 2014 Phys. Rev. Lett. 112 103201
[54] Petrov D S 2015 Phys. Rev. Lett. 115 155302
[55] Cabrera C R, Tanzi L, Sanz J, Naylor B, Thomas P, Cheiney P and Tarruell L 2018 Science 359 301