Detecting phase transitions from the high-temperature phase in systems with a small physical parameter

P. Pieri, G. C. Strinati, and I. Tifrea*

Dipartimento di Matematica e Fisica, Sezione INFM, Università di Camerino, I-62032 Camerino, Italy

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The critical temperature of a dilute Bose gas is obtained in terms of the associated small gas parameter, by a unifying approach which treats three *and* two spatial dimensions on equal footing, even though the superfluid phase transition is known to be driven by different mechanisms in three and two dimensions. Good agreement is found with the critical temperature obtained by recent Monte Carlo data in three dimensions and by previous analytic methods in two dimensions, respectively. This approach is expected to apply more generally to systems where the many-body theory is controlled by a small physical parameter in the high-temperature phase.

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Phase transitions at a critical temperature T_c can be theoretically detected by (i) Determining the vanishing of an order parameter upon approaching T_c from below. This approach is, however, not applicable when an order parameter cannot be identified. (ii) Selecting a specific mode (regarded to be physically relevant) and looking for divergences in the associated susceptibility upon lowering the temperature (e.g., Thouless criterion for superconductivity and Stoner criterion for magnetism).

Starting from the normal phase, the occurrence of a phase transition can also be detected when perturbation theory in terms of the bare coupling constant breaks down upon lowering the temperature (Ginzburg criterion). This originally phenomenological criterion can be turned to have deeper significance for detecting phase transitions, when considering systems for which physical quantities in the high-temperature phase can be expressed in terms of a *small physical parameter p*. These systems include, for instance, the dilute Bose gas (for which p is the gas diluteness parameter) and magnetic systems with N spin components (for which $p=1/N$). The aim of this Brief Report is to generalize the Ginzburg criterion to cases for which a small physical parameter exists. By implementing this idea specifically for the dilute Bose gas in three ($D=3$) as well as in two ($D=2$) spatial dimensions, we are able to treat *on equal footing* two noticeably distinct cases for which the phase transition can ($D=3$) or cannot ($D=2$) be associated with the existence of an order parameter below T_c.

When the many-body diagrammatic theory in the high-temperature phase can be organized in powers of a small parameter p, certain contributions are retained and others are discarded at a given order in p. The relative importance of these contributions is, however, expected to be temperature dependent. Upon lowering the temperature, it may thus happen that contributions which were originally discarded become comparable with the ones retained, so that the whole classification scheme in terms of p no longer holds. When this happens, an *absolute* temperature scale $T_L(p)$ can be identified, below which the organization of the diagrammatic theory in terms of p breaks down. This temperature scale thus signals the occurrence of a phase transition, in the sense that $T_L(p)$ represents the *upper boundary of the critical region* about the critical temperature $T_c(p)$. Since the two temperatures T_L and T_c are expected on physical grounds to have the same functional dependence on p (apart for a numerical coefficient of order unity), determining $T_L(p)$ should also give a reasonable estimate of $T_c(p)$. This expectation will be explicitly verified by the examples considered below. It should be emphasized that no phenomenological parameter is involved in this procedure, which in addition holds irrespective of the kind of order parameter that may be identified below T_c. Accordingly, one is able in this way to detect the *occurrence* of a phase transition but not to identify its nature.

The dilute Bose gas in *three dimensions* has been of much interest in the past several years, especially after Bose condensation has been achieved experimentally in dilute gases of alkali atoms[1] and in atomic hydrogen.[2] The inclusion of interaction effects on the critical temperature (over and above the noninteracting Bose-Einstein value $T_{\mathrm{BE}}=3.31n^{2/3}/m$, where n is the density and m the boson mass) has, in particular, been much debated, with alternative approaches yielding different dependences of $(T_c-T_{\mathrm{BE}})/T_{\mathrm{BE}}$ on the diluteness parameter $p=n^{1/3}a$ (a being the scattering length), e.g., of the type p (cf. Refs. 3–6), $p^{1/2}$ (cf. Ref. 7), and $p^{2/3}$ (cf. Ref. 8). Only recently, Monte Carlo simulations for the 3D hard-core Bose gas in the dilute limit have settled the issue, yielding the linear dependence $(T_c-T_{\mathrm{BE}})/T_{\mathrm{BE}}\propto p$ (cf. Refs. 9 and 10). We will show below that our approach, when applied to the 3D Bose gas, yields precisely the linear dependence $(T_L-T_{\mathrm{BE}})/T_{\mathrm{BE}}\propto p$ obtained by Monte Carlo data, even with the right proportionality coefficient.[10]

The dilute Bose gas in *two dimensions*, on the other hand, has been investigated to a lesser extent. In two dimensions, Bose-Einstein condensation is known not to occur at finite temperature for the ideal and interacting boson systems; nevertheless, the lack of a condensate does not necessarily imply the absence of a phase transition to the superfluid state for an interacting 2D Bose system.[11] In particular, predictions on the dependence of the critical temperature on the diluteness parameter $p=1/\ln[1/(nr_0^2)]$ (where r_0 represents the interaction range) have been made by Popov using a functional integral approach in the superfluid phase,[12] and by Fisher and

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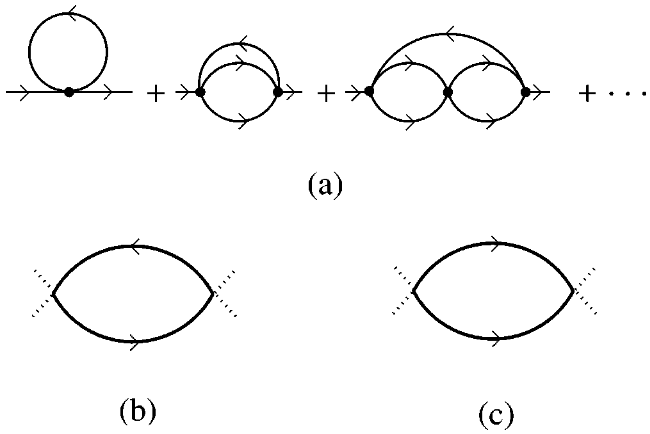

FIG. 1. (a) *t*-matrix approximation for the self-energy of an interacting Bose gas; (b) particle-hole bubble; (c) particle-particle bubble.

Hohenberg using a renormalization group approach in the normal phase,[13] finding in both cases $T_c \propto 1/|\ln p|$. We will show below that our approach is also able to recover the same functional dependence for T_L on p.

We consider a bosonic system interacting via a repulsive short-range two-body potential of range r_0 (which becomes a δ-function when $r_0 \to 0$ both in 3D and 2D), and with given Fourier transform v_0 at zero wave vector.

For the Bose gas, a characteristic temperature T_n can be identified which relates the thermal wavelength $\lambda = \sqrt{2\pi/(mT)}$ to the density n, via the relation $\lambda^D n = 1$ (we set $\hbar = k_B = 1$ throughout). In 3D this temperature corresponds to the Bose-Einstein temperature $T_{\rm BE}$ (apart from a factor of order unity), while in 2D it marks the occurrence of quantum effects.[14] For the (interacting) dilute Bose gas, when $T \sim T_n$ many-body diagrammatic theory can be organized in powers of p. It turns out that the classification scheme is formally the same in 3D and in 2D, with every additional cycle (defined as a closed path constructed with bare bosonic propagators sharing a common internal wave vector and Matsubara frequency integration) introducing a factor of p in a given diagram.

At the leading order in the diluteness parameter, the self-energy is thus given by the *t*-matrix approximation Σ_t depicted in Fig. 1(a), where every diagram contains one cycle only. When estimating higher-order diagrams, the *t*-matrix itself replaces the bare potential (renormalized perturbation theory) and every additional cycle introduces a factor $t_0 \Pi_{\rm ph}(0) = t_0(\partial n/\partial\mu) \propto p$ for $T \sim T_n$. Here, t_0 and $\Pi_{\rm ph}(0)$ are the zero frequency and wave vector values of the *t*-matrix and of the particle-hole bubble [Fig. 1(b)], respectively, with t_0^{-1} being, in turn, proportional to the particle-particle bubble depicted in Fig. 1(c), as it will be shown below. Note that, when evaluating $\Pi_{\rm ph}(0)$, a wave vector cutoff of the order of $T^{1/2}$ emerges naturally from the Bose function originating from a Matsubara frequency sum. This contrasts previous approaches where only the contribution from the zero Matsubara frequency was retained.[5]

The single-particle propagators entering the diagrams of Fig. 1 correspond, in principle, to free bosons. The classification scheme can, however, be improved by including self-energy insertions [corresponding to the *t*-matrix approximation of Fig. 1(a)] in the single-particle propagators. Quite generally, self-energy insertions in the single-particle propagators become relevant upon approaching the phase transition,[5] especially because they modify the value of the chemical potential just where it would be vanishingly small. In our case, making the propagators self-consistent will enable us to approach the temperature of interest T_L below T_n.

Calculation of the *t*-matrix self-energy of Fig. 1(a) requires two steps, namely, summing the repeated particle-particle diagrams which define the *t*-matrix and performing the remaining convolution with the single-particle propagator closing the cycle. Both steps cannot be performed in a complete analytic way. Simplifying features can be introduced by parametrizing the short-range interaction potential by a separable potential in wave vector space, i.e., $v(\mathbf{k}-\mathbf{k}') \to v_0 w(\mathbf{k}) w(\mathbf{k}')$ with $w(\mathbf{k}) = \theta(k_0 - |\mathbf{k}|)$ and $k_0 = r_0^{-1}$. Another simplifying feature is the assumption that the wave vector and frequency dependence of Σ_t, which enters in a self-consistent way the single-particle propagators of Fig. 1(a) defining Σ_t itself, can be neglected. Since this additional assumption is crucial to the following argument, we will explicitly verify it by showing that the wave vector and frequency dependence of the self-energy of Fig. 1(a) is irrelevant to the calculation of physical quantities in the dilute limit.

With this assumption, the relation between the chemical potential and the particle density reads

$$\mu - \Sigma_t(0) = \mu_0, \tag{1}$$

where $\Sigma_t(0)$ is the zero-wave vector and frequency value of the *t*-matrix self-energy and $\mu_0 = \mu_0(n,T)$ is the chemical potential of the ideal Bose gas.[15] The net effect of these approximations is thus to replace $\mu - \Sigma_t(0)$ by μ_0, whenever this combination appears in the single-particle propagators. The ensuing *t*-matrix then reads

$$t(\mathbf{k},\mathbf{k}';K) = w(\mathbf{k}) w(\mathbf{k}') t(K), \tag{2}$$

with the four-vector notation $K = (\mathbf{K}, \Omega_\nu)$ [$\Omega_\nu = 2\pi\nu T$ (ν integer) being a bosonic Matsubara frequency] and where

$$t^{-1}(K) = \frac{1}{v_0} + \frac{m}{4\pi} \ln\left[\frac{k_0^2/m - 2\mu_0 + \mathbf{K}^2/(4m) - i\Omega_\nu}{-2\mu_0 + \mathbf{K}^2/(4m) - i\Omega_\nu}\right] \tag{3}$$

for $D=2$, and

$$t^{-1}(K) = \frac{1}{v_0} + \frac{m}{2\pi^2}\left[k_0 - m^{1/2}\sqrt{-2\mu_0 + \frac{\mathbf{K}^2}{4m} - i\Omega_\nu} \times \arctan\frac{k_0/m^{1/2}}{\sqrt{-2\mu_0 + \frac{\mathbf{K}^2}{4m} - i\Omega_\nu}}\right] \tag{4}$$

for $D=3$, in the limit $n r_0^D \ll 1$.

Calculation of the self-energy from the t-matrix (3) and (4) requires an additional sum over a four-vector. In particular, the sum over the Matsubara frequency can be performed by a contour integration, leading two distinct contributions from an isolated pole and from a cut along the real axis. We have verified numerically that the contribution from the cut becomes negligibly small in the limit $nr_0^D \ll 1$ (for instance, when $T=T_n$ the contribution from the cut to $\Sigma_t(0)$ is less than 5% in 2D when $nr_0^2 \lesssim 10^{-4}$, and less than 2% in 3D when $nr_0^3 \lesssim 10^{-4}$). We thus arrive to the expressions (which also hold asymptotically in the limit $nr_0^D \ll 1$)

$$\frac{\Sigma_t(k)}{2n} = w^2\left(\frac{\mathbf{k}}{2}\right) \times \left\{ \frac{1}{v_0} + \frac{m}{4\pi} \ln\left[\frac{k_0^2/m - \mu_0 + \mathbf{k}^2/(4m) - i\omega_\nu}{-\mu_0 + \mathbf{k}^2/(4m) - i\omega_\nu} \right] \right\}^{-1} \tag{5}$$

for $D=2$, and

$$\frac{\Sigma_t(k)}{2n} = w^2\left(\frac{\mathbf{k}}{2}\right) \left[\frac{1}{v_0} + \frac{m}{2\pi^2} \left(k_0 - \sqrt{-\mu_0 + \frac{\mathbf{k}^2}{4m} - i\omega_\nu} \times m^{1/2} \arctan \frac{k_0/m^{1/2}}{\sqrt{-\mu_0 + \frac{\mathbf{k}^2}{4m} - i\omega_\nu}} \right) \right]^{-1} \tag{6}$$

for $D=3$.

The above expressions for the self-energy can be used to explicitly verify that, when evaluating physical quantities (such as the density n), the wave vector and frequency dependence of $\Sigma_t(k)$ is actually irrelevant. To this end, we observe that in 3D the wave vector and frequency dependence of $\Sigma_t(k)$ is appreciable only over the scales k_0 and $k_0^2/(2m)$, respectively, k_0 being much larger than the cutoff introduced by the temperature. In 2D, on the other hand, the scale is set by $|\mu_0|$, but the presence of the logarithm in Eq. (5) makes the dependence of $\Sigma_T(k)$ on k rather slow. In both cases, the approximation $\Sigma_t(k) \approx \Sigma_t(0)$ is justified over a large portion of k space and can be exploited to evaluate physical quantities. In particular, for $T=T_n$ we have verified numerically that the relative error when evaluating $n = -T\Sigma_\nu \int [d^D\mathbf{k}/(2\pi)^D] G(k)$ alternatively with $G(k) = [i\omega_\nu - \mathbf{k}^2/(2m) + \mu - \Sigma_t(k)]^{-1}$ and with $G(k) \to G_0(k) = [i\omega_\nu - \mathbf{k}^2/(2m) + \mu - \Sigma_t(0)]^{-1}$ is less than 1% for $nr_0^2 \lesssim 10^{-2}$ in 2D and for $nr_0^3 \lesssim 5\times 10^{-3}$ in 3D, the error decreasing further for decreasing nr_0^D.

Having established the approximations required to implement the diagrammatic theory for the ($D=2,3$) dilute Bose gas at temperatures $T \sim T_n$, we can now determine down to which temperature $T_L(p) < T_n$ the leading diagrams still dominate over the subleading ones. To this end, it is enough to compare the particle-hole bubble $\Pi_{\text{ph}}(0) (= \partial n/\partial\mu)$ at zero wave vector and frequency with its particle-particle counterpart $\Pi_{\text{pp}}(0) \simeq t_0^{-1}$. The value of the ratio $\Pi_{\text{ph}}(0)/\Pi_{\text{pp}}(0)$ (which defines the small parameter p when $T \sim T_n$) becomes temperature dependent below T_n, thus making the effective coupling of renormalized perturbation theory increasing for decreasing T. The temperature $T_L(p)$ at which this coupling equals unity [i.e., when $\Pi_{\text{ph}}(0) = \Pi_{\text{pp}}(0)$] is determined by evaluating $\partial n/\partial\mu$ in the limit $|\mu_0| \ll T$.

In $D=3$ one obtains aymptotically[15]

$$\frac{\partial n}{\partial\mu} = \frac{2\,m\,n^{1/3}}{3\zeta(3/2)^{4/3}} \frac{T_{\text{BE}}}{T - T_{\text{BE}}}, \tag{7}$$

where $\zeta(3/2) \simeq 2.612$ is the Riemann zeta function of argument 3/2, as well as

$$\Pi_{\text{pp}}(0) = \frac{m}{2\pi^2 r_0} = \frac{m}{4\pi a}, \tag{8}$$

from which it readily follows that

$$\frac{T_L(p) - T_{\text{BE}}}{T_{\text{BE}}} = \frac{8\pi}{3\zeta(3/2)^{4/3}} p \simeq 2.33\,p, \tag{9}$$

with $p = n^{1/3}a$. Note that Eq. (8) has been obtained under the assumption $v_0^{-1} \ll m/(2\pi^2 r_0)$ [cf. Eq. (4)], which can always be satisfied in the limit $r_0 \to 0$. Note also that the *linear dependence* on p of the temperature shift (9) has been directly related to the quadratic dependence of the free-boson chemical potential on $(T - T_{\text{BE}})$ near T_{BE} in 3D. The result (9) is in excellent agreement with Monte Carlo simulations[10] for the critical temperature of the 3D dilute Bose gas, which yields $[T_c(p) - T_{\text{BE}}]/T_{\text{BE}} = (2.3 \pm 0.25)p$, and coincides with the result of Ref. 6 obtained by a completely different analytic approach (large-N expansion). The upper temperature T_L thus turns out to be *extremely* close to the actual critical temperature T_c.[16] Recently, Monte Carlo calculations[17] have provided the value 1.3 instead of 2.3. This discrepancy has been attributed in Ref. 18 to the presence of negative subleading contributions, which act to reduce the coefficient from the upper value 2.3 of Ref. 10 when the asymptotic dilute limit is not yet reached. This gives further support to our estimate (9) for T_L in 3D.

In $D=2$ one instead obtains[15]

$$\frac{\partial n}{\partial\mu} = \frac{m}{2\pi} \frac{e^{\mu_0/T}}{1 - e^{\mu_0/T}} = \frac{m}{2\pi} \frac{T}{|\mu_0|}, \tag{10}$$

where the last expression holds in the limit $|\mu_0| \ll T$, as well as

$$\Pi_{\text{pp}}(0) = \frac{m}{4\pi} \ln\left(\frac{1}{2m|\mu_0| r_0^2} \right) \tag{11}$$

[under the assumption that v_0^{-1} can be neglected in Eq. (3) when $k_0^2/(m|\mu_0|) \gg 1$]. Comparison of Eqs. (10) and (11) then identifies the temperature T_L:

$$\frac{1}{2}\ln\frac{1}{2m|\mu_0|r_0^2}=\frac{T_L}{|\mu_0|}. \quad (12)$$

Entering in Eq. (12) the asymptotic expression $\mu_0 = -Te^{-T_n/T}$ (which holds in the limit $T \ll T_n \equiv 2\pi n/m$) yields

$$\ln[1/(nr_0^2)]+\ln[T_n/(4\pi T_L)]+T_n/T_L=2e^{T_n/T_L}. \quad (13)$$

Provided further that $\ln[1/(nr_0^2)] \gg T_n/T_L$ (which is consistently verified by the solution for T_L below) and that $\ln\ln[1/(nr_0^2)] \gg 1$ (which *defines* the ‘‘diluteness condition’’ in 2D), Eq. (13) is readily solved to give $T_L = T_n/|\ln p|$, with $p=1/\ln[1/(nr_0^2)]$. This expression coincides with the estimates given by Popov[12] and by Fisher and Hohenberg[13] for the critical temperature of the 2D dilute Bose gas. Note that the *double-log dependence* of T_L on nr_0^2 originates, on the one hand, from the log dependence of $\Pi_{pp}(0)$ on $|\mu_0|$ and, on the other hand, from the exponential dependence of μ_0 on T at low temperatures.

In the above treatment, we have exploited the fact that the compressibility $\partial n/\partial\mu$ increases upon lowering the temperature both in $D=3$ and $D=2$. From a *physical* point of view, $\partial n/\partial\mu$ embodies the collective behavior of the Bose gas, which becomes dominant over the two-particle property (represented by Π_{pp}) when approaching the transition. In this context, it is interesting to mention that higher derivatives of n with respect to μ become even more singular than $\partial n/\partial\mu$ upon lowering the temperature. As these higher-order derivatives can be associated with multiple self-energy insertions into the single-particle propagators, there would be no way of determining T_L unless t-matrix self-energy insertions are properly resummed in *all* possible ways, as we have consistently done with the replacement (1).

In conclusion, we have shown that, with an appropriate generalization of the Ginzburg criterion for systems (such as the dilute Bose gas in $D=2$ and $D=3$) for which a small *physical* parameter p exists, the occurrence of a phase transition from the normal phase can be detected by determining the temperature at which the diagrammatic structure organized in terms of p breaks down (irrespective of the nature of the transition itself). Even though we have applied specifically our method to the dilute Bose gas, we expect that it can be generalized to other systems, for which the many-body diagrammatic theory in the high-temperature phase can be organized in terms of a small physical parameter.

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*Permanent address: Dept. of Theoretical Physics, ‘‘Babes-Bolyai’’ University, 3400 Cluj, Rumania.

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