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Quantum statistical mechanics of gases in terms of dynamical filling fractions and scattering amplitudes

André LeClair

Newman Laboratory, Cornell University, Ithaca, NY, USA

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Abstract

We develop a finite temperature field theory formalism in any dimension that has the filling fractions as the basic dynamical variables. The formalism efficiently decouples zero temperature dynamics from the quantum statistical sums. The zero temperature ‘data’ are the scattering amplitudes. A saddle-point condition leads to an integral equation which is similar in spirit to the thermodynamic Bethe ansatz for integrable models, and effectively resums infinite classes of diagrams. We present both relativistic and non-relativistic versions.

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1. Introduction

For the investigation of finite temperature quantum field theory, the standard and well-developed formalism is based on the Euclidean field theory with time compactified on a circle of circumference $\beta = 1/T$, where T is the temperature. In practice, this involves the sums over Matsubara frequencies in perturbation theory [1, 2]. Though this formalism is very useful for some problems, such as the finite temperature dependence of the effective potential [3], for other properties, such as the equation of state involving the pressure and density, it would be desirable to have a formalism that more clearly preserves the classical picture of a gas of particles at given density and interacting via collisions.

It helps to realize that at least in principle it is possible to decouple the zero temperature dynamics and the quantum statistical sums. The argument is simple: the computation of the partition function $Z = \text{Tr}(e^{-\beta H})$ is in principle possible from the complete knowledge of the zero temperature eigenstates of the Hamiltonian H . In practice this is rather difficult and one resorts to perturbative methods such as the Matsubara method, which unfortunately entangles the zero temperature dynamics from the quantum statistical mechanics. However, there does exist a beautiful realization of this kind of decoupling for integrable quantum field theories in two spacetime dimensions due to Yang and Yang [4], which is referred to as the thermodynamic Bethe ansatz (TBA). (For the relativistic version, see [5].) In this formalism the decoupling is manifest. The free energy is expressed in terms of a pseudo-energy; in fact

it takes the free field form, and the pseudo-energy is a solution of an integral equation whose kernel depends on the zero temperature S -matrix. In fact, the S -matrix and the free-particle dispersion relation are the only properties of the theory that are needed as input. The TBA is a very powerful tool for tracking RG flows and for computing the conformal central charge at the fixed points, and this was one of the main motivations for this work.¹

Dashen, Ma and Bernstein derived an expression for the partition function in terms of the S -matrix in [6]. The derivation is very general, does not rely on integrability, and is valid in any number of spacetime dimensions². The main result in [6] is rather formal, and a considerable amount of additional work is needed to churn it into a useful computational tool. Though some steps towards further developing the formalism were taken in [6, 8], the program was never completed and appears to be eventually abandoned in favour of the Matsubara approach. As should be clear in our work, some important aspects of the approach were not well understood in the original works.

In this paper, we show that, with a new interpretation, the main formula of Dashen *et al*, can serve as the starting point for a finite temperature formalism based on the physical occupation number densities and zero temperature scattering amplitudes. First, by using the cluster expansion for the S -matrix in a way not exploited in [6], we are able to resolve certain difficulties previously encountered and render the formalism considerably more appealing. Secondly, through a Legendre transformation we are able to formulate the quantum statistical mechanics directly in terms of dynamical filling fractions. By ‘dynamical’ we refer to the property that they are determined from a variational principle, or saddle-point condition, as in the TBA.

We wish to also point out the work of Lee and Yang on quantum statistical mechanics [9] which preceded the TBA work of Yang and Yang. That approach is not based on the S -matrix but rather on matrix elements of $e^{-\beta H}$ itself. Since these matrix elements depend on the temperature, that approach does not disentangle the dynamics from the statistical sums. Nevertheless, we found some of the ideas, in particular diagrammatic description, very useful.

An outline of the paper is the following. In the following section we describe in a completely general way how one formulates quantum statistical mechanics of gases in terms of dynamical filling fractions. In section 3, the main result of [6] is reviewed and some potential difficulties pointed out with so-called type B terms. In section 4, we show how the extensivity of the free energy follows from the cluster decomposition of the S -matrix, however in a delicate way that actually provides some constraints on the interpretation. We argue that the formalism is only consistent with the cluster decomposition if one passes to Euclidean space. This also suggests a possible solution to the problem with the type B terms. In section 5, we present a diagrammatic description of the formalism. It must be stressed that the resulting diagrams have nothing to do with finite temperature Matsubara/Feynman diagrams. In section 6, we show that for the saddle-point construction of section 2, one needs only consider the two-particle irreducible diagrams. The saddle-point equation is an integral equation that automatically resums infinite numbers of diagrams. In section 7, we consider contributions that come only from two-body scattering. Here also the integral equation sums infinite numbers of ‘foam’ diagrams. Though we originally had in mind applications to relativistic field theory at high temperatures, our construction does not assume the underlying theory is Lorentz invariant. In section 8, we develop the non-relativistic case and solve the integral equation for a constant two-body scattering amplitude.

¹ In this 2D context, the central charge c is the coefficient of the conformal free energy $\mathcal{F} = -c\pi T^2/6$ and c is the same c as appears in the Virasoro algebra.

² To our knowledge, a complete derivation of the thermodynamic Bethe ansatz equations from this formalism is not known. Some steps in this direction were taken in [7].

It is well known that in order to obtain sensible results in finite temperature field theory certain resummations of diagrams are necessary (see for instance [1, 2, 10, 11].) Since these resummations are also usually performed with the help of an integral equation, we remark on the relation of some of these formalisms to ours. In the case of a constant scattering amplitude, which is often the case to lowest order, our kernel is constant and the integral equation is quite similar to the self-consistency equations in [1, 2] and the saddle-point equations in [10]. In the non-relativistic case they are very similar to self-consistency equations in Hartree–Fock [12]. Thus, in the two-body approximation our integral equation is a generalization of these methods where the constant kernel is replaced by the full two-body zero-temperature S -matrix. One should also mention the ‘thermo field dynamics’ approach [13], which also is partly based on filling fractions. Since the latter has mainly been developed for finite-temperature correlation functions rather than the partition function and thus involves a doubling of particle species because of its connection with the Schwinger–Keldysh formalism, a direct connection with our formalism is not so straightforward.

In the concluding section, we comment on the potential advantages of our formalism for certain classes of problems.

2. Free energy as a dynamical functional of filling fractions

In the scattering description of quantum statistical mechanics that we will develop, a momentum space description is obviously appropriate. A very physical momentum space description uses the occupation number densities as the basic dynamical variables. In this section we generally describe how this can be done and illustrate it for free particles.

The free-energy density (per volume) \mathcal{F} is defined as

$$\mathcal{F} = -\frac{1}{\beta V} \log Z, \quad Z = \text{Tr} e^{-\beta(H-\mu N)}, \quad (1)$$

where $\beta = 1/T$, μ are the inverse temperature and chemical potential, V is the d -dimensional spacial volume, and H and N are the Hamiltonian and particle number operator. Since $\log Z$ is an extensive quantity, i.e. proportional to the volume, the pressure p of the gas is minus the free-energy density since $p = T \partial \log Z / \partial V = -\mathcal{F}$. For now, let us assume there is one species of bosonic ($s = 1$) or fermionic ($s = -1$) particle. Given $\mathcal{F}(\mu)$, one can compute the thermally averaged number density n :

$$n = -\frac{\partial \mathcal{F}}{\partial \mu} \equiv \int \frac{d^d \mathbf{k}}{(2\pi)^d} f(\mathbf{k}), \quad (2)$$

where \mathbf{k} is the d -dimensional momentum vector. ($D = d + 1$ is the spacetime dimension.) The dimensionless quantities f are sometimes called the filling fractions.

One can express \mathcal{F} as a functional of f (and μ) in a meaningful way with a Legendre transformation. Define

$$G \equiv \mathcal{F}(\mu) + \mu n. \quad (3)$$

Treating f and μ as independent variables, then using equation (2) one has that $\partial_\mu G = 0$, which implies it can be expressed only in terms of f and satisfies $\delta G / \delta f = \mu$.

Inverting the above construction shows that there exists a functional $F(f, \mu)$:

$$F(f, \mu) = G(f) - \mu \int \frac{d^d \mathbf{k}}{(2\pi)^d} f(\mathbf{k}), \quad (4)$$

which satisfies equation (2) and is a stationary point with respect to f :

$$\frac{\delta F}{\delta f} = 0. \quad (5)$$

The above stationary condition is to be viewed as determining f as a function of μ . The physical free energy is then $\mathcal{F} = F$ evaluated at the solution f to the above equation. We will refer to equation (5) as the saddle-point equation since it is suggestive of a saddle-point approximation to a functional integral:

$$Z = \int Df e^{-\beta V F(f)} \approx e^{-\beta V \mathcal{F}}. \quad (6)$$

Let us illustrate these definitions for a free theory, in a way that will be useful in the following. In a free theory, the eigenstates of H are multi-particle Fock space states $|\mathbf{k}_1, \mathbf{k}_2, \dots\rangle$. Let $\omega_{\mathbf{k}}$ denote the one-particle energy as a function of momentum \mathbf{k} . It is well known that the trace over the multi-particle Fock space gives

$$\mathcal{F}_0(\mu) = \frac{s}{\beta} \int \frac{d^d \mathbf{k}}{(2\pi)^d} \log(1 - s e^{-\beta(\omega_{\mathbf{k}} - \mu)}). \quad (7)$$

From the definition equation (2) one finds the filling fractions

$$f(\mathbf{k}) = \frac{1}{e^{\beta(\omega_{\mathbf{k}} - \mu)} - s} \equiv f_0(\mathbf{k}). \quad (8)$$

In order to find the functional $F(f, \mu)$ one first computes G from equation (3) and eliminates μ to express it in terms of f using equation (8). One finds

$$F_0(f, \mu) = \int \frac{d^d \mathbf{k}}{(2\pi)^d} \left((\omega_{\mathbf{k}} - \mu) f - \frac{1}{\beta} [(f + s) \log(1 + sf) - f \log f] \right). \quad (9)$$

One can then easily verify that $\delta F / \delta f = 0$ has the solution $f = f_0$, and plugging this back into equation (9) gives the correct result equation (7) for \mathcal{F}_0 .

There is another way to view the above construction which involves the entropy. Write equation (9) as

$$F = \mathcal{E} - \frac{1}{\beta} \mathcal{S}, \quad (10)$$

where \mathcal{E} is the first $(\omega - \mu)f$ term in equation (9), which is the energy density, and \mathcal{S} is the remaining term in brackets. One can show by a standard counting argument, which involves the statistics of the particles, that \mathcal{S} represents the entropy density of a gas of particles (see for instance [14].)

In the following, it will be convenient to trade the chemical potential variable μ for the variable f_0 :

$$F_0(f, f_0) = -\frac{1}{\beta} \int \frac{d^d \mathbf{k}}{(2\pi)^d} \left(s \log(1 + sf) + f \log \left(\frac{1 + sf}{f} \frac{f_0}{1 + sf_0} \right) \right). \quad (11)$$

In section 6 we will express the corrections to F for an interacting theory in terms of scattering amplitudes.

3. Formal expression for Z in terms of the S -matrix

The trace that defines Z is computed with respect to a complete set of orthogonal states $|\alpha\rangle$:

$$\langle \alpha' | \alpha \rangle = \delta_{\alpha' \alpha}, \quad \mathbf{1} = \sum_{\alpha} |\alpha\rangle \langle \alpha| \implies Z = \sum_{\alpha} \langle \alpha | e^{-\beta(H - \mu N)} | \alpha \rangle. \quad (12)$$

Let us separate H into free (H_0) and interacting (H_1) parts

$$H = H_0 + H_1. \quad (13)$$

Since the states α in equation (12) are not required to be eigenstates of H , let us take the trace over eigenstates of H_0 :

$$H_0|\alpha\rangle = E_\alpha|\alpha\rangle. \tag{14}$$

In the following section we will specialize to plane-wave scattering states, but for the remainder of this section one need not be so specific.

It was shown how to express the thermal trace in terms of the S -matrix in [6]. The necessary algebraic tools are familiar from the formal theory of scattering [15, 16]. There is a simple derivation of what will turn out to be the essential term which goes as follows. For simplicity, we first set the chemical potential μ to zero; it can easily be restored at the end by letting $\omega_{\mathbf{k}} \rightarrow \omega_{\mathbf{k}} - \mu$. Define the resolvent operator

$$G(E) = \frac{1}{E - H + i\varepsilon}, \tag{15}$$

where E is a real variable and ε is small and positive. If H is Hermitian, then in the limit $\varepsilon \rightarrow 0^+$,

$$G(E) - G(E)^\dagger = -2\pi i \delta(E - H). \tag{16}$$

Assuming that the spectrum of H has $E \geq 0$, one then evidently has

$$Z = -\frac{1}{2\pi i} \int_0^\infty dE e^{-\beta E} \text{Tr}(G(E) - G^\dagger(E)). \tag{17}$$

Henceforth, we will not always display that operators depend on the variable E ; all operators depend on E except for H, H_0, H_1 .

In order to obtain an expression that is meaningful when the trace is taken over the free Fock space, one wants to separate out expressions depending on H_0 as much as possible. The resolvent satisfies the equation³

$$G = G_0 + G_0 H_1 G, \tag{18}$$

where $G_0(E) = (E - H_0 + i\varepsilon)^{-1}$. As in standard discussions of scattering (see e.g. [15]), define the operator

$$T(E) = H_1 + H_1 G(E) H_1. \tag{19}$$

It satisfies

$$H_1 G = T G_0, \quad G H_1 = G_0 T. \tag{20}$$

Using equation (20), one now has

$$G = G_0 + G_0 T G_0 \tag{21}$$

and

$$Z = Z_0 - \frac{1}{\pi} \text{Im} \int_0^\infty dE e^{-\beta E} \text{Tr}(G_0 T G_0), \tag{22}$$

where $Z_0 = \text{Tr} e^{-\beta H_0}$ is the partition function of the free theory. Using now the cyclicity of the trace, $\partial_E G_0 = -G_0^2$, an integration by parts, and $\text{Im} G_0 = -\pi \delta(E - H_0)$, one finds

$$Z = Z_0 + Z_A + Z_B, \tag{23}$$

where

$$Z_A \equiv -\beta \text{Re} \left(\int dE e^{-\beta E} \text{Tr}(\delta(E - H_0) T(E)) \right) = -\beta \sum_\alpha e^{-\beta E_\alpha} \text{Re}(T_{\alpha;\alpha}). \tag{24}$$

³ $(A - B)^{-1} = A^{-1}(1 + B(A - B)^{-1}) = (1 + (A - B)^{-1}B)A^{-1}$.

The term Z_B involves $\partial_E T = -T G_0^2 T$ and is thus quadratic in T . The derivation in [6] performs further algebraic manipulations of equation (22) and elegantly expresses the final result for both $Z_{A,B}$ in terms of the S -matrix. The construction is summarized in appendix, where one finds

$$Z = Z_0 + \frac{1}{4\pi i} \int_0^\infty dE e^{-\beta E} \text{Tr}(S^{-1} \overleftrightarrow{\partial}_E S), \tag{25}$$

where $X \overleftrightarrow{\partial}_E Y \equiv X(\partial_E Y) - (\partial_E X)Y$, and $S(E)$ is an operator valued function of E related to the S -matrix⁴. More specifically,

$$\begin{aligned} S(E) &= 1 - 2\pi i \delta(E - H_0)T(E) \\ S^{-1}(E) &= 1 + 2\pi i \delta(E - H_0)T^\dagger(E). \end{aligned} \tag{26}$$

The on-shell matrix elements of $S(E)$ are the usual S -matrix elements

$$\langle \alpha' | S(E) | \alpha \rangle = \langle \alpha' | \alpha \rangle - 2\pi i \delta_{\alpha';\alpha}^{(E)} T_{\alpha';\alpha}, \quad \text{iff } E = E_\alpha, \tag{27}$$

where $\delta_{\alpha';\alpha}^{(E)} \equiv \delta(E_{\alpha'} - E_\alpha)$. The condition ‘iff $E = E_\alpha$ ’ is what is referred to as ‘on-shell’.

A significant amount of work remains in order to obtain a useful calculational tool from equation (25), and this will be the main subject of the following section. For now, note that there are two types of terms (in addition to Z_0) in equation (25) as in equation (23), where

$$\begin{aligned} Z_A &= -\frac{1}{2} \int_0^\infty dE e^{-\beta E} \text{Tr}[\partial_E(\delta(E - H_0)(T + T^\dagger))] \\ Z_B &= -i\pi \int_0^\infty dE e^{-\beta E} \text{Tr}[(\delta(E - H_0)T^\dagger) \overleftrightarrow{\partial}_E(\delta(E - H_0)T)]. \end{aligned} \tag{28}$$

We will refer to these as type A and type B terms. Because of the $\delta(E - H_0)$ factors, we can now trace over eigenstates $|\alpha\rangle$ of H_0 and perform the integral over E . Consider first Z_A . Integrating by parts gives

$$Z_A = -\beta \sum_\alpha e^{-\beta E_\alpha} \text{Re}(T_{\alpha;\alpha}) + \delta^{(E)}(0) \text{Re}(\langle 0|T|0\rangle), \tag{29}$$

where $|0\rangle$ is the free-particle vacuum of zero energy. Assuming the vacuum is stable, $\langle 0|T|0\rangle = 0$ and the $\delta^{(E)}(0)$ term can be dropped and equation (29) agrees with (24). ($\delta^{(E)}(0)$ will be regularized below.)

The type A and B terms are quite different. The type B terms are actually rather peculiar since they may potentially spoil the extensivity of the free energy, since they do not obviously have the same connectivity properties as the type A terms. We will return to this issue in the following section and actually propose that they should be discarded. Z_B can be simplified using the optical theorem, which follows from $S^{-1}S = 1$:

$$T - T^\dagger = -2\pi i T^\dagger \delta(E - H_0)T. \tag{30}$$

Using this, and the cyclicity of the trace, one finds that the terms involving the derivative of the δ -functions vanish. Inserting two complete sets of states one then finds

$$\begin{aligned} Z_B &= -i\pi \sum_{\alpha,\alpha'} e^{-\beta E_\alpha} \delta(E_\alpha - E_{\alpha'}) T_{\alpha';\alpha}^* \overleftrightarrow{\partial}_{E_\alpha} T_{\alpha';\alpha} \\ &= 2\pi \sum_{\alpha,\alpha'} e^{-\beta E_\alpha} \delta(E_\alpha - E_{\alpha'}) \text{Re}(T_{\alpha';\alpha}) \overleftrightarrow{\partial}_{E_\alpha} \text{Im}(T_{\alpha';\alpha}). \end{aligned} \tag{31}$$

Note that the type B terms vanish if $\text{Im } T = 0$.

⁴ Another form of equation (25) is based on the identity $\text{Tr } S^{-1} \overleftrightarrow{\partial}_E S = 2i \text{Im } \text{Tr } \partial_E \log S$, where we have used the on-shell relation $S^{-1} = S^\dagger$. Though this form may be useful to compare with the TBA, we do not use it in this paper.

4. Extensivity of the free energy and the cluster decomposition

In this section, we specialize to a trace over plane wave scattering states and describe some new features that arise. In particular, in infinite volume, the free energy is expected to be extensive, i.e. proportional to the spacial volume V . So, one first must understand how all the various types of terms sum up in a way that can be reorganized as the exponential of something proportional to the volume. Clearly this has to do with properties of connectedness. In the present formalism, this property is essentially a consequence of the cluster decomposition of the S -matrix. The volume factors will arise from the following regularization of the momentum space delta function:

$$(2\pi)^d \delta^{(d)}(0) = \lim_{\mathbf{k}=\mathbf{k}'} \int d^d \mathbf{x} e^{i\mathbf{x}\cdot(\mathbf{k}-\mathbf{k}')} \equiv V. \tag{32}$$

If expression (23) clusters in the expected way, then the free energy $-T \log Z$ can be identified with the sum of all terms with only one power of V . As we will show, *requiring* that the cluster decomposition for (23) leads to a free energy with this property actually provides some constraints on the interpretation of various terms.

4.1. Fock space and S -matrix conventions

Since we are considering a quantum field theory, the Hilbert space of the free theory is a Fock space. Let us now fix our normalizations for the free-particle states and their scattering amplitudes. The creation-annihilation operators satisfy

$$a_{\mathbf{k}} a_{\mathbf{k}'}^\dagger - s a_{\mathbf{k}'}^\dagger a_{\mathbf{k}} = (2\pi)^d \delta^{(d)}(\mathbf{k} - \mathbf{k}'). \tag{33}$$

The Hilbert space is then spanned by the multi-particle states

$$|\mathbf{k}_1 \mathbf{k}_2 \cdots \mathbf{k}_N\rangle = \left(\prod_i \sqrt{2\omega_{\mathbf{k}_i}} \right) a_{\mathbf{k}_1}^\dagger \cdots a_{\mathbf{k}_N}^\dagger |0\rangle \tag{34}$$

satisfying

$$H_0 |\mathbf{k}_1 \mathbf{k}_2 \cdots \mathbf{k}_N\rangle = \left(\sum_i \omega_{\mathbf{k}_i} \right) |\mathbf{k}_1 \mathbf{k}_2 \cdots \mathbf{k}_N\rangle. \tag{35}$$

(The factors $\sqrt{2\omega_{\mathbf{k}}}$ are a matter of convention.) One has the nonzero inner products

$$\langle \mathbf{k}'_1 \cdots \mathbf{k}'_N | \mathbf{k}_1 \cdots \mathbf{k}_N \rangle = (2\pi)^{Nd} \sum_{\mathcal{P}} s^p \prod_{i=1}^N 2\omega_{\mathbf{k}_i} \delta(\mathbf{k}'_i - \mathbf{k}_i), \tag{36}$$

where the sum is over the $N!$ permutations \mathcal{P} of the order of the \mathbf{k}'_i and $p(\mathcal{P})$ is the degree of the permutation such that $p = 0$ ($p = 1$) if \mathcal{P} involves an even (odd) number of pairwise permutations of particles. The above implies the following resolution of the identity:

$$\mathbf{1} = \sum_{N=0}^{\infty} \frac{1}{N!} \int \underline{d\mathbf{k}}_1 \underline{d\mathbf{k}}_2 \cdots \underline{d\mathbf{k}}_N |\mathbf{k}_1 \cdots \mathbf{k}_N\rangle \langle \mathbf{k}_1 \cdots \mathbf{k}_N|, \tag{37}$$

where for convenience we have defined the notation

$$\int \underline{d\mathbf{k}} \equiv \int \frac{d^d \mathbf{k}}{(2\pi)^d} \frac{1}{2\omega_{\mathbf{k}}}. \tag{38}$$

(We have chosen our normalization of states so that the above integration measure over \mathbf{k} is Lorentz invariant. We emphasize however that we are not assuming the theory to be Lorentz invariant; a non-relativistic case is worked out in section 8.)

4.2. Cluster decomposition

In order to simplify the notation, the free-particle states $|\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n\rangle$ will be denoted as $|\mathbf{12} \dots \mathbf{n}\rangle$ and the S -matrix elements as

$$\langle \mathbf{k}'_1, \mathbf{k}'_2, \dots, \mathbf{k}'_n | S | \mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n \rangle = S_{\mathbf{1}'\mathbf{2}' \dots \mathbf{n}' ; \mathbf{12} \dots \mathbf{n}}. \quad (39)$$

For the S -matrix the cluster decomposition is based on the physical requirement that particles that are causally separated cannot scatter (see for instance [16]). The cluster decomposition also ensures that the free energy only depends on connected S -matrix elements. The cluster decomposition may be expressed as follows:

$$\langle \alpha' | S | \alpha \rangle = \sum_{\text{partitions}} s^p S_{\alpha'_1; \alpha_1}^c S_{\alpha'_2; \alpha_2}^c S_{\alpha'_3; \alpha_3}^c \dots, \quad (40)$$

where the sum is over partitions of the state $|\alpha\rangle$ into clusters $|\alpha_1\rangle, |\alpha_2\rangle, \dots$ (The number of particles in $|\alpha_i\rangle$ and $|\alpha'_i\rangle$ is not necessarily the same.) The above formula essentially *defines* what is meant by the connected matrix elements S^c . The particles are assumed to be stable which implies

$$\langle \mathbf{k}'_1 | S | \mathbf{k}_1 \rangle = \langle \mathbf{k}'_1 | \mathbf{k}_1 \rangle = (2\pi)^d 2\omega_{\mathbf{k}_1} \delta^{(d)}(\mathbf{k}'_1 - \mathbf{k}_1) \equiv \delta_{\mathbf{1}'\mathbf{1}}^{(\mathbf{k})}. \quad (41)$$

It will be convenient to express the cluster decomposition in terms of \widehat{T} defined by

$$S = 1 + i\widehat{T}. \quad (42)$$

The cluster decomposition for \widehat{T} is then same as for that of S but without the terms involving only delta functions which come from the '1' in $S = 1 + i\widehat{T}$. (One can show that these additional terms involving only delta functions are what give rise to Z_0 .) The connected matrix elements \widehat{T}^c are characterized as having only a single overall momentum and energy conserving delta function and cannot be factorized into functions of only a subset of the momenta. Below we will need \widehat{T}^c in terms of the conventional scattering amplitudes \mathcal{M} :

$$\widehat{T}_{\alpha'; \alpha}^c = -2\pi \delta_{\alpha'; \alpha}^{(E)} T_{\alpha'; \alpha} = (2\pi)^{d+1} \delta_{\alpha'; \alpha}^{(E)} \delta^{(d)}(\mathbf{k}_\alpha - \mathbf{k}_{\alpha'}) \mathcal{M}_{\alpha'; \alpha}, \quad (43)$$

where $E_\alpha, \mathbf{k}_\alpha$ are the total energy and momentum of the state $|\alpha\rangle$ and $\delta_{\alpha'; \alpha}^{(E)} \equiv \delta^{(E)}(E_{\alpha'} - E_\alpha)$.

For $2 \rightarrow 2$ and $3 \rightarrow 3$ particles the cluster decomposition for \widehat{T} then reads

$$\widehat{T}_{\mathbf{1}'\mathbf{2}'; \mathbf{12}} = \widehat{T}_{\mathbf{1}'\mathbf{2}'; \mathbf{12}}^c \quad \widehat{T}_{\mathbf{1}'\mathbf{2}'\mathbf{3}'; \mathbf{123}} = \widehat{T}_{\mathbf{1}'\mathbf{2}'\mathbf{3}'; \mathbf{123}}^c + [\delta_{\mathbf{1}'\mathbf{1}}^{(\mathbf{k})} \widehat{T}_{\mathbf{2}'\mathbf{3}'; \mathbf{23}}^c \pm \text{perm.}]_9. \quad (44)$$

The subscript '9' indicates the number of permutations within the brace. If the one-particle states were not stable, there would be additional terms. In order to illustrate some important additional features, we will also need the $4 \rightarrow 4$ particle decomposition

$$\begin{aligned} \widehat{T}_{\mathbf{1}'\mathbf{2}'\mathbf{3}'\mathbf{4}'; \mathbf{1234}} &= \widehat{T}_{\mathbf{1}'\mathbf{2}'\mathbf{3}'\mathbf{4}'; \mathbf{1234}}^c + i[\widehat{T}_{\mathbf{1}'\mathbf{2}'; \mathbf{12}}^c \widehat{T}_{\mathbf{3}'\mathbf{4}'; \mathbf{34}}^c \pm \text{perm.}]_{18} + [\delta_{\mathbf{1}'\mathbf{1}}^{(\mathbf{k})} \widehat{T}_{\mathbf{2}'\mathbf{3}'\mathbf{4}'; \mathbf{234}}^c \pm \text{perm.}]_{16} \\ &+ [\delta_{\mathbf{1}'\mathbf{1}}^{(\mathbf{k})} \delta_{\mathbf{2}'\mathbf{2}}^{(\mathbf{k})} \widehat{T}_{\mathbf{3}'\mathbf{4}'; \mathbf{34}}^c \pm \text{perm.}]_{72}. \end{aligned} \quad (45)$$

4.3. One-particle resummation and emergence of filling fractions

To compute the required trace, one must set $\{\mathbf{k}' = \mathbf{k}\}$. This leads to a more specialized cluster decomposition that is suitable to compute Z . For instance, the nine terms in braces in equation (44) separate into 3 + 6 distinct types of terms depending on whether they contain $\delta^{(d)}(0)$:

$$\widehat{T}_{\mathbf{123}; \mathbf{123}} = \widehat{T}_{\mathbf{123}; \mathbf{123}}^c + [(2\pi)^d \delta^{(d)}(0) 2\omega_{\mathbf{k}_1} \widehat{T}_{\mathbf{23}; \mathbf{23}}^c \pm \text{perm.}]_3 + [s \delta_{\mathbf{12}}^{(\mathbf{k})} \widehat{T}_{\mathbf{23}; \mathbf{13}}^c \pm \text{perm.}]_6. \quad (46)$$

In order to illustrate the variety of terms that can arise from the cluster decomposition, let us compute the type A terms for low numbers of particles. For simplicity, we set the chemical potential to zero. For two particles one finds

$$Z_A|_{2 \text{ part.}} = \frac{\beta V}{2} \int \underline{\underline{\mathbf{k}_1}} \underline{\underline{\mathbf{k}_2}} e^{-\beta(\omega_1+\omega_2)} \text{Re}(\mathcal{M}_{12;12}), \tag{47}$$

where we have used equation (32). ($\omega_i \equiv \omega_{\mathbf{k}_i}$)

For three particles one finds

$$Z_A|_{3 \text{ part.}} = \frac{\beta V}{3!} \int \underline{\underline{\mathbf{k}_1}} \underline{\underline{\mathbf{k}_2}} \underline{\underline{\mathbf{k}_3}} e^{-\beta(\omega_1+\omega_2+\omega_3)} \text{Re}(\mathcal{M}_{123;123}) \tag{48}$$

$$+ s \frac{\beta V}{2} \int \underline{\underline{\mathbf{k}_1}} \underline{\underline{\mathbf{k}_2}} e^{-\beta(\omega_1+\omega_2)} (e^{-\beta\omega_1} + e^{-\beta\omega_2}) \text{Re}(\mathcal{M}_{12;12}) \tag{49}$$

$$+ \beta V^2 \left(\int \underline{\underline{\mathbf{k}_1}} \underline{\underline{\mathbf{k}_2}} e^{-\beta(\omega_1+\omega_2)} \text{Re}(\mathcal{M}_{12;12}) \right) \left(\int \frac{d^d \mathbf{k}}{(2\pi)^d} e^{-\beta\omega_{\mathbf{k}}} \right). \tag{50}$$

These terms have the following interpretation. Equation (48) is a new contribution of the same kind as equation (47). Term (49) just modifies the integration measure $\underline{\underline{\mathbf{k}}}$ for the (47) term. The combined measure factors are the first terms in the expansion of the free filling fraction f_0 defined in equation (8). This manner in which the filling fraction emerges was also a feature of one approach to finite temperature correlation functions in [18, 19]. The last term is proportional to V^2 and is thus expected to be a V^2 term in the expression $Z = \exp(-\beta V \mathcal{F})$. One can easily verify that it is the correct combinatorial product of a term from the free contribution \mathcal{F}_0 and another from the two-particle contribution in equation (47).

A simple combinatorial argument shows that one can sum up all the terms that are a product of one \widehat{T}^c and some $\delta_{\mathbf{nm}}^{(\mathbf{k})}$ factors to obtain

$$\mathcal{F} = \mathcal{F}_0 - \sum_{N=2}^{\infty} \frac{1}{N!} \int \left(\prod_{n=1}^N \frac{d^d \mathbf{k}_n}{(2\pi)^d} \frac{f_0(\mathbf{k}_n)}{2\omega_{\mathbf{k}_n}} \right) \text{Re}(\mathcal{M}_{12\dots N;12\dots N}) + \dots \tag{51}$$

Restoring the chemical potential μ , the dependence on it is only through f_0 as given in equation (8).

For a scalar field interacting with potential $V(\phi) = \lambda\phi^4/4!$, to lowest order $\mathcal{M}_{12;12} = -\lambda$ [17] and the two-particle contribution in equation (51) gives the same result to order λ , as the Matsubara approach [1]. (In the latter approach this arises as a two-loop finite temperature Feynman diagram.) The $3 \rightarrow 3$ particle contribution to equation (51) was also shown to agree with the three-loop result in [20].

4.4. The need to continue to Euclidean space

There are additional contributions to \mathcal{F} that come from terms in the cluster expansion that involve more than one \widehat{T}^c factor. They first arise at four particles. The terms in $\widehat{T}_{1234;1234}$ that give new contributions to \mathcal{F} not already included in equation (51) are the following:

$$\widehat{T}_{1234;1234} = i[\widehat{T}_{12;12}^c \widehat{T}_{34;34}^c]_3 + i[s\widehat{T}_{13;12}^c \widehat{T}_{24;34}^c]_{12} + i[\widehat{T}_{12;34}^c \widehat{T}_{34;12}^c]_3 + \dots \tag{52}$$

In order to compute their contribution to Z_A , we start with expression (24) in terms of T . We then obtain the cluster decomposition of T from equation (52) using $\widehat{T}_{\alpha';\alpha} = -2\pi \delta_{\alpha';\alpha}^{(E)} T_{\alpha';\alpha}$. In carrying this out, one sees that one can divide both sides of equation (52) by $\delta^{(E)}(0)$ and

obtain something well defined. Finally, we express the final result in terms of the scattering amplitudes \mathcal{M} . The first term in equation (52) in this way leads to

$$Z_A|_{4\text{part.}} = \dots \frac{\beta V^2}{8} \operatorname{Re} \left[2\pi i \delta^{(E)}(0) \left(\int \underline{d\mathbf{k}}_1 \underline{d\mathbf{k}}_2 e^{-\beta(\omega_1+\omega_2)} \mathcal{M}_{12;12} \right)^2 \right] + \dots \quad (53)$$

Since this is proportional to V^2 it must come from the square of the two-particle term in the expansion of $Z = (1 + \dots) \exp(\beta V/2 \int \operatorname{Re}(\mathcal{M}_{12;12}))$. In attempting to match this with equation (53), one notices a very interesting phenomenon: the two terms can only be identified after one makes the Wick rotation

$$\delta_{\alpha';\alpha}^{(E)} \rightarrow -i\delta_{\alpha';\alpha}^{(E)} \quad (54)$$

One then regularizes the $\delta^{(E)}(0)$ as follows:

$$2\pi \delta^{(E)}(0) \equiv \beta. \quad (55)$$

The above equation can be understood as following from the fact that in the Matsubara approach to finite temperature field theory, one goes to Euclidean space and compactifies the time on a circle of circumference, i.e. volume, β . The above equation is then simply the Euclidean time version of equation (32).

Implementing the rules discussed in the last paragraph, the two additional sets of terms in the cluster decomposition (52) lead to two new contributions to the free energy. In the resummation of one-particle terms, the filling fractions f_0 again emerge. These lead to

$$\mathcal{F} = -\frac{s\beta}{2} \int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{d^d \mathbf{k}_2}{(2\pi)^d} \frac{d^d \mathbf{k}_3}{(2\pi)^d} \frac{f_0(\mathbf{k}_1)}{2\omega_1} \frac{f_0(\mathbf{k}_2)^2}{4\omega_2^2} \frac{f_0(\mathbf{k}_3)}{2\omega_3} \operatorname{Re}(\mathcal{M}_{12;12} \mathcal{M}_{23;23}) \quad (56)$$

$$-\frac{1}{8} \int \frac{d^d \mathbf{k}_1}{(2\pi)^d} \frac{d^d \mathbf{k}_2}{(2\pi)^d} \frac{d^d \mathbf{k}_3}{(2\pi)^d} \left(\prod_{n=1}^4 \frac{f_0(\mathbf{k}_n)}{2\omega_n} \right) 2\pi \delta_{12;34}^{(E)} \operatorname{Re}(\mathcal{M}_{12;34} \mathcal{M}_{34;12}) + \dots, \quad (57)$$

where $\mathbf{k}_4 = \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3$ and $\omega_4 = \omega_{\mathbf{k}_4}$.

4.5. Z_B terms: to B or not to B?

We now return to the issue of the type B terms in equation (31). It is clear from the previous results of this section that the property of the extensivity of the free energy arises in a delicate way from the cluster decomposition. Since $Z = Z_0 + Z_A + Z_B$ and the Z_B terms are quadratic in T , they could very easily spoil the extensivity. We have already shown how $Z_0 + Z_A$ exponentiates to something proportional to the volume, but the way this comes about is quite subtle.

One may argue that the need to go to Euclidean space can potentially cure this problem, at least for relativistic theories. In trying to perform the match discussed in the last subsection, one actually needs a stronger constraint:

$$\beta \left(\int \operatorname{Re}(\mathcal{M}_{12;12}) \right)^2 = \operatorname{Re} \left[2\pi \delta^{(E)}(0) \left(\int \mathcal{M}_{12;12} \right)^2 \right]. \quad (58)$$

That is $\mathcal{M}_{12;12}$ must be real. It is well known that for relativistic theories, the imaginary parts of scattering amplitudes arise through cuts when one is in Minkowski space [17]. In Euclidean space the imaginary part actually vanishes. Since Z_B involves the imaginary part of the amplitude's, this argument would indicate that the Z_B terms can be discarded. However, further checks of the consistency of this argument, in particular with unitarity of the S -matrix, would be helpful.

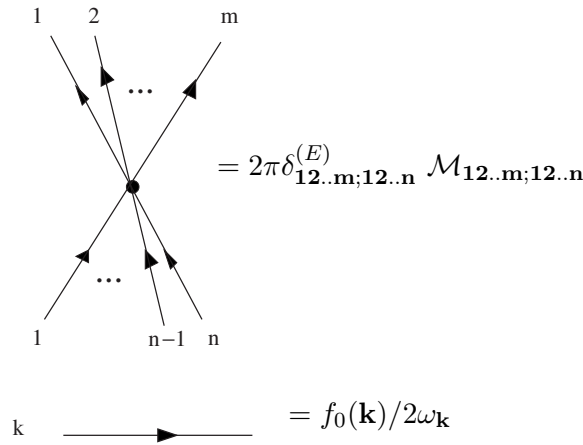


Figure 1. Diagrammatic ingredients.

5. Diagrammatic description

The contributions to \mathcal{F} have a nice diagrammatic description. Let us represent the scattering amplitudes $\mathcal{M}_{\mathbf{12}\dots\mathbf{m};\mathbf{12}\dots\mathbf{n}}$ as a vertex with n incoming and m outgoing lines. We construct a diagram with no external lines by linking the lines of vertices. The rules for computing a contribution to the free-energy density \mathcal{F} are then the following.

- (i) Assign a factor of the scattering amplitude and an energy conserving delta function $2\pi\delta_{\alpha';\alpha}^{(E)}\mathcal{M}_{\alpha';\alpha}$ to each vertex as in figure 1.
- (ii) Assign a factor $f_0(\mathbf{k})/2\omega_{\mathbf{k}}$ to each line as in figure 1.
- (iii) Conserve momentum \mathbf{k} at each vertex and integrate over every unconstrained momentum with $\int d^{(d)}\mathbf{k}/(2\pi)^d$.
- (iv) Identify $2\pi\delta^{(E)}(0) = \beta$.
- (v) Divide by the symmetry factor of the diagram, defined as the number of permutations of the internal lines that do not change the topology of the graph, including relative positions.
- (vi) For fermions determine the overall sign of the diagram: it has an overall factor of s if it arises from an odd permutation of the outgoing state $\langle \mathbf{1}'\mathbf{2}' \dots |$ in the cluster expansion of $\langle \mathbf{1}'\mathbf{2}' \dots | T | \mathbf{12} \dots \rangle$.
- (vii) Divide by $-\beta$.

The terms in equation (51) are then represented by the diagram in figure 2. The two terms in equations (56), (57) are represented as diagrams in figure 3.

The structure of the ‘ring’ diagrams shown in figure 4 is especially simple. We compute the sum of such diagrams in order to illustrate the above rules and also since we will need the result in the following section. Let the diagram in figure 4 be denoted as $\mathcal{F}_{\text{ring}}^{(n)}$. The symmetry factor of this diagram is 2 for $n = 1$ and n for $n \geq 2$. For fermions, the overall sign of the diagram is s^{n+1} . The sum over n then simply gives a log

$$\sum_{n=2}^{\infty} \mathcal{F}_{\text{ring}}^{(n)} = -\frac{1}{\beta} \int \frac{d^d\mathbf{k}}{(2\pi)^d} \left(-\frac{y_0(\mathbf{k})}{2} - s \log(1 - sy_0(\mathbf{k})) \right) \tag{59}$$

$$y_0(\mathbf{k}) \equiv \frac{\beta f_0(\mathbf{k})}{2\omega_{\mathbf{k}}} \int \frac{d^d\mathbf{k}'}{(2\pi)^d} \mathcal{M}_{\mathbf{12};\mathbf{12}}(\mathbf{k}, \mathbf{k}') \frac{f_0(\mathbf{k}')}{2\omega_{\mathbf{k}'}}$$

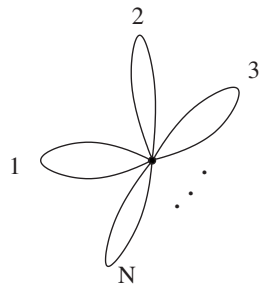


Figure 2. Diagrammatic representation of terms in equation (51).

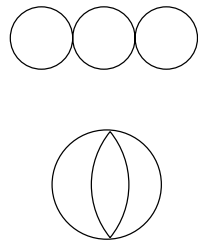


Figure 3. Diagrammatic representation of the two terms in equations (56) and (57) respectively.

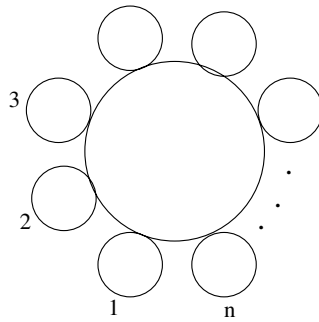


Figure 4. Ring diagrams.

6. F and the saddle-point equations

We now return to including interactions in the free-energy functional F of section 2. Let us write

$$F(f, f_0) = F_0(f, f_0) + F_1, \tag{60}$$

where F_0 is given in equation (11) and we define U as the ‘potential’ which incorporates interactions

$$F_1 = -\frac{1}{\beta} \int \frac{d^d \mathbf{k}}{(2\pi)^d} U(\mathbf{k}). \tag{61}$$

It is not too difficult to understand that F_1 is given by the two-particle irreducible diagrams of the last section. These are defined as diagrams that cannot become disconnected by the cutting of two internal lines. For instance, starting from the $N = 2$ diagram in figure 2, it is clear that the ring diagrams can be generated by attaching additional loops. The ring

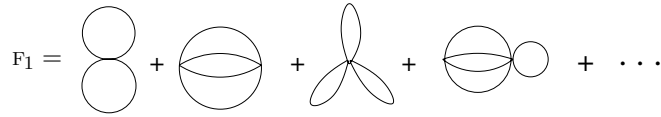


Figure 5. F_1 as the sum of two-particle irreducible diagrams.

diagrams are not two-particle irreducible and should thus not be included in F_1 . A more detailed argument was given by Lee and Yang [9]. We express this explicitly as follows: F_1 is just $\mathcal{F}_{2\text{-part.irred.}}(f_0)$ with f_0 replaced by f :

$$F_1(f) = \sum \mathcal{F}_{2\text{-part.irred.}}(f_0 \rightarrow f). \tag{62}$$

This is shown in figure 4, where it is implicit that the lines have a factor of f rather than f_0 .

Given F , f is determined by the saddle-point equation

$$\log\left(\frac{1+sf}{f}\right) - \log\left(\frac{1+sf_0}{f_0}\right) = -\frac{\partial U}{\partial f}. \tag{63}$$

Substituting the solution of (63) back into F , it can be written in a variety of ways, depending on how one utilizes relation (63). One useful way is

$$\begin{aligned} \mathcal{F} &= -\frac{1}{\beta} \int \frac{d^d \mathbf{k}}{(2\pi)^d} [s \log(1+sf) + (1-f\partial_f)U] \\ &= \mathcal{F}_0 - \frac{1}{\beta} \int \frac{d^d \mathbf{k}}{(2\pi)^d} \left[s \log\left(\frac{1+sf}{1+sf_0}\right) + (1-f\partial_f)U \right]. \end{aligned} \tag{64}$$

It is convenient to define a pseudo-energy ε as the following parameterization of f :

$$f \equiv \frac{1}{e^{\beta\varepsilon} - s}. \tag{65}$$

Then the saddle-point equation and free-energy density take the form

$$\varepsilon = \omega - \mu - \frac{1}{\beta} \frac{\partial U}{\partial f} \tag{66}$$

$$\mathcal{F} = -\frac{1}{\beta} \int \frac{d^d \mathbf{k}}{(2\pi)^d} [-s \log(1 - s e^{-\beta\varepsilon}) + (1-f\partial_f)U]. \tag{67}$$

7. Two-body approximation

If the gas is not too dense, one expects that two-particle scattering will give the most important contribution. This is especially true in the non-relativistic case where scattering preserves the number of particles.

Define the following kernel from the two-particle scattering amplitude:

$$\mathbf{K}(\mathbf{k}, \mathbf{k}') \equiv \frac{1}{4\omega_{\mathbf{k}} \omega_{\mathbf{k}'}} \mathcal{M}_{12;12}(\mathbf{k}, \mathbf{k}') \tag{68}$$

and the convolution

$$(\mathbf{K} * f)(\mathbf{k}) \equiv \int \frac{d^d \mathbf{k}'}{(2\pi)^d} \mathbf{K}(\mathbf{k}, \mathbf{k}') f(\mathbf{k}'). \tag{69}$$

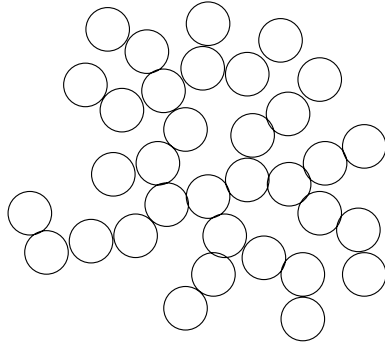


Figure 6. Foam diagrams.

The two-particle contribution to U can then be written as

$$U(\mathbf{k}) = \frac{\beta}{2} f(\mathbf{k})(\mathbf{K} * f)(\mathbf{k}). \tag{70}$$

The saddle-point equation and free energy then take the forms

$$\log\left(\frac{1+sf}{f}\right) - \log\left(\frac{1+sf_0}{f_0}\right) = -\beta\mathbf{K} * f \tag{71}$$

$$\mathcal{F} = -\frac{1}{\beta} \int \frac{d^d\mathbf{k}}{(2\pi)^d} \left[s \log(1+sf) + \frac{f}{2} \log\left(\frac{1+sf}{f} \frac{f_0}{1+sf_0}\right) \right]. \tag{72}$$

In terms of the pseudo-energy

$$\varepsilon = \omega - \mu - \mathbf{K} * \left(\frac{1}{e^{\beta\varepsilon} - s} \right) \tag{73}$$

$$\mathcal{F} = -\frac{1}{\beta} \int \frac{d^d\mathbf{k}}{(2\pi)^d} \left[-s \log(1 - s e^{-\beta\varepsilon}) + \frac{\beta f}{2} (\varepsilon - \omega + \mu) \right]. \tag{74}$$

In this two-body approximation, the integral equation (73) resums all diagrams involving two-body scattering. These ‘foam diagrams’ are of the kind shown in figure 6.

The foam diagrams contain much more than the ring diagrams. As a check, we now show how the ring diagrams are contained in the solution of the integral equation. Let us define y as $\log\left(\frac{1+sf}{1+sf_0}\right) = \log(1+y)$, where

$$y \equiv \frac{f - f_0}{1 + sf_0}. \tag{75}$$

The integral equation (71) can then be expanded in powers of y :

$$y - \frac{(1+2sf_0)}{2f_0} y^2 + \dots = \beta\mathbf{K} * (f_0 + (1+sf_0)y). \tag{76}$$

Now let $y = y_0 + y_1 + \dots$ and plug this into the above equation. Many kinds of terms are generated, but to compare with the ring diagrams we only focus on terms of the type in equation (59). To lowest orders one finds

$$y = y_0 + 2sy_0^2 + \dots, \tag{77}$$

where y_0 is defined in equation (59). Plugging this lowest order solution into equation (72) for the free energy one finds

$$\mathcal{F} - \mathcal{F}_0 = -\frac{1}{\beta} \int \frac{d^d \mathbf{k}}{(2\pi)^d} (y_0 + s y_0^2/2 + \dots), \tag{78}$$

which agrees with the low-order expansion of equation (59).

8. Non-relativistic case: hardcore bosons

We have not assumed the underlying theory is Lorentz invariant in the above construction. However, in the definition equation (34) of the states $|\mathbf{k}_1 \dots \mathbf{k}_n\rangle$ we included factors of $\sqrt{2\omega_{\mathbf{k}}}$ in order that $\underline{d\mathbf{k}}$ in equation (36) is Lorentz invariant. This simplifies the comparison with other approaches for relativistic models, as we did in section 4.3 for the ϕ^4 theory, since then \mathcal{M} are the conventional scattering amplitudes.

8.1. Generalities of the non-relativistic case

For non-relativistic theories, where $\omega_{\mathbf{k}} = \mathbf{k}^2/2m$, it is more conventional to normalize the states as

$$|\mathbf{k}_1 \dots \mathbf{k}_N\rangle = a_{\mathbf{k}_1}^\dagger \dots a_{\mathbf{k}_N}^\dagger |0\rangle. \tag{79}$$

The formulae of the previous sections still apply but with the modification

$$\underline{d\mathbf{k}} = \int \frac{d^d \mathbf{k}}{(2\pi)^d 2\omega_{\mathbf{k}}} \rightarrow \int \frac{d^d \mathbf{k}}{(2\pi)^d}. \tag{80}$$

We will keep the definition equation (43) of \mathcal{M} in terms of \widehat{T} . The formulae for the two-body approximation in section 7 then all apply, but now with

$$\mathbf{K}(\mathbf{k}, \mathbf{k}') \equiv \mathcal{M}_{12,12}(\mathbf{k}, \mathbf{k}'). \tag{81}$$

The above kernel has dimensions of energy \times volume which corresponds to an energy dimension of $1 - d$ (up to velocity factors).

8.2. Hardcore boson model

Consider the two-body potential in position space \mathbf{x} ,

$$V(\mathbf{x}, \mathbf{x}') = \frac{\gamma}{2} \delta^{(d)}(\mathbf{x} - \mathbf{x}'). \tag{82}$$

This leads to the second quantized Hamiltonian

$$H = \int d^d \mathbf{x} \left(\frac{1}{2m} \vec{\nabla} \psi^\dagger \cdot \vec{\nabla} \psi + \frac{\gamma}{4} \psi^\dagger \psi^\dagger \psi \psi \right). \tag{83}$$

To lowest order $T = H_1$ and

$$\langle \alpha' | H_1 | \alpha \rangle = -(2\pi)^d \delta^{(d)}(\mathbf{k}_\alpha - \mathbf{k}_{\alpha'}) \mathcal{M}_{\alpha';\alpha}. \tag{84}$$

Expanding the field in terms of annihilation operators

$$\psi(\mathbf{x}) = \int \frac{d^d \mathbf{k}}{(2\pi)^d} e^{i\mathbf{k}\cdot\mathbf{x}} a_{\mathbf{k}}, \tag{85}$$

then to lowest order one finds

$$M_{12;12} = -\gamma = \mathbf{K}. \tag{86}$$

The coupling constant γ has units of energy \times volume. It can be expressed in terms of a physical scattering length a as follows. To first order in perturbation theory the differential cross section in the centre of mass is

$$\frac{d\sigma}{d\Omega} = \frac{m^2 \gamma^2}{4(2\pi)^{d-1}} k^{d-3}, \quad (87)$$

where k is the magnitude of \mathbf{k} for one of the incoming particles. Since a cross section has dimensions of length ^{$d-1$} , we define a such that the cross section is a^{d-1} when the wavelength of the particle is $2\pi/a$:

$$\left. \frac{d\sigma}{d\Omega} \right|_{k \sim 2\pi/a} \sim a^{d-1}. \quad (88)$$

This leads us to make the definition

$$\frac{\gamma}{(2\pi)^{d/2}} \equiv \frac{a^{d-2}}{m}. \quad (89)$$

8.3. Lowest order solution

It is interesting to carry out our analysis for arbitrary spacial dimension $d > 0$. Integrals over momenta can be traded for integrals over ω :

$$\int \frac{d^d \mathbf{k}}{(2\pi)^d} = \left(\frac{m}{2\pi}\right)^{d/2} \frac{1}{\Gamma(d/2)} \int_0^\infty d\omega \omega^{(d-2)/2}. \quad (90)$$

For a constant kernel $\mathbf{K} = -\gamma$, and $d > 0$, the solution to the integral equation (73) takes the simple form

$$\varepsilon(\mathbf{k}) = \omega_{\mathbf{k}} - \mu + T\delta, \quad (91)$$

where δ is independent of \mathbf{k} and satisfies the equation⁵

$$\delta = h \text{Li}_{d/2}(z_\mu z_\delta), \quad (92)$$

where we have defined the fugacities

$$z_\mu \equiv e^{\beta\mu}, \quad z_\delta = e^{-\delta} \quad (93)$$

and a renormalized thermal coupling h and thermal wavelength λ_T :

$$h \equiv \left(\frac{\sqrt{2\pi}a}{\lambda_T}\right)^{d-2}, \quad \lambda_T \equiv \sqrt{\frac{2\pi}{mT}}. \quad (94)$$

The function $\text{Li}_\nu(z)$ is the standard polylogarithm, defined as the appropriate analytic continuation of

$$\text{Li}_\nu(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^\nu}. \quad (95)$$

Equation (92) is thus seen as non-trivial, transcendental equation that determines δ as a function of μ , T , and the coupling h . Given the solution $\delta(\mu)$ of this equation, using equation (74) the density can be expressed as

$$n(\mu) = \frac{1}{\lambda_T^d} \text{Li}_{d/2}(z_\mu z_\delta) = \frac{T\delta}{\gamma}. \quad (96)$$

⁵ We have used $\int_0^\infty dx x^{\nu-1}/(e^x/z - 1) = \Gamma(\nu)\text{Li}_\nu(z)$ for $\text{Re}(\nu) > 0$.

For $d > 0$, one can integrate by parts and obtain the following expressions for the free energy:

$$\mathcal{F} = -\frac{T}{\lambda_T^d} \left(\text{Li}_{(d+2)/2}(z_\mu z_\delta) + \frac{\delta}{2} \text{Li}_{d/2}(z_\mu z_\delta) \right). \quad (97)$$

The case of $2d$ is interesting since equation (92) then becomes algebraic due to $\text{Li}_1(z) = -\log(1 - z)$. These formulae will be applied to Bose–Einstein condensation, and other problems, in [23].

9. Concluding remarks

In this paper we have mainly focused on developing the formalism in a general way for both relativistic and non-relativistic theories. In the two-body approximation, the main result is summarized in the two formulae equations (73) and (74) and is quite straightforward to implement: one computes, or measures, the two-body forward-scattering kernel \mathbf{K} at zero temperature, solves the integral equation (73), and the free energy is given in terms of this solution in equation (74). For non-constant kernels, one will probably need to solve the equations numerically.

A formalism that efficiently disentangles zero temperature dynamics and quantum statistical sums potentially has many applications, and we discuss some of them in these concluding remarks.

Our formalism is especially well suited for studies of the effects of interactions in Bose–Einstein condensation, since there the filling fractions play a central role. We have already obtained some results on this problem and will publish them elsewhere [23]. The results presented there also give new insights on the Riemann hypothesis.

For high-energy particle physics, our formalism has the following potential advantages over the Matsubara approach. The necessity to renormalize ultraviolet divergences is essentially a zero temperature problem; however, the Matsubara approach again entangles the zero-temperature renormalization with the quantum statistical mechanics and the issue of scheme-dependent results can sometimes be a problem. In our formalism, any need for renormalization is carried out at zero temperature and the S -matrix is expressed in terms of physical quantities at zero temperature, such as particle masses, etc. Our integral equation could also shed some light on the infra-red problems that are common in the Matsubara approach and also require special resummations [1, 2, 10, 11, 21, 22]. We emphasize that since the diagrams in this paper have no relation to finite temperature Feynman diagrams, our type of resummation is entirely different than the resummations carried out in these other works. Some aspects of the relativistic case will be published in [24]. Our formalism may help to study the known results on the free energy of strongly coupled supersymmetric gauge theories [26].

Our formalism may also be well suited to studies of the quark–gluon plasma [25] currently being studied at RHIC, since many of the hadronic cross sections are known.

Acknowledgments

I would like to thank G Mussardo and H Thacker for discussions and for drawing my attention to the work [6].

Appendix

In this appendix, we complete the steps leading to result (25) obtained in [6]. Starting from equation (22), the next step is to try and use the relation $G_0 - G_0^\dagger = -2\pi i \delta(E - H_0)$ so that one can integrate over E . One way to do this is using the operators Ω :

$$\begin{aligned}\Omega(E) &\equiv GG_0^{-1} = 1 + G_0T \\ \Omega^{-1}(E) &= G_0G^{-1} = 1 - G_0H_1.\end{aligned}\tag{A.1}$$

As we show below, Ω is the operator that relates free-particle states to the in-states of scattering theory. Introduce the notation $X \overset{\leftrightarrow}{\partial} Y \equiv X(\partial Y) - (\partial X)Y$. Then, using $\partial_E G_0 = -G_0^2$ and $H_1\Omega = T$ one can readily show that

$$\Omega^{-1} \overset{\leftrightarrow}{\partial}_E \Omega = -2G_0^2T.\tag{A.2}$$

In order to deal with the complex conjugation needed in equation (22), for any operator $X(E)$ define $X^*(E)$ as simply $X(E)$ but with $i\varepsilon$ replaced by $-i\varepsilon$. This definition gives $G^*(E) = G(E)^\dagger$, $\Omega^*(E) = 1 + G^\dagger H_1$ and $(\Omega^{-1})^* = 1 - G_0^\dagger H_1$. One then has

$$(\Omega^{-1})^* \overset{\leftrightarrow}{\partial}_E \Omega^* = -2(G_0^\dagger)^2 T^\dagger.\tag{A.3}$$

The last step is to define

$$S(E) = (\Omega^{-1})^* \Omega(E).\tag{A.4}$$

Using equations (22) and (A.2), and the cyclicity of the trace, one obtains

$$Z = Z_0 + \frac{1}{4\pi i} \int_0^\infty dE e^{-\beta E} \text{Tr}(S^{-1} \overset{\leftrightarrow}{\partial}_E S).\tag{A.5}$$

We now demonstrate that the so-called on-shell matrix elements of the S -operator are the usual S -matrix. Consider first the operator Ω . Inserting a complete set of states $|\alpha'\rangle$ one finds

$$\Omega(E_\alpha)|\alpha\rangle = |\alpha\rangle + \sum_{\alpha'} \frac{1}{E_\alpha - E_{\alpha'} + i\varepsilon} T_{\alpha'\alpha}|\alpha'\rangle,\tag{A.6}$$

where

$$T_{\alpha'\alpha} = \langle\alpha'|T(E)|\alpha\rangle, \quad \text{iff } E = E_\alpha.\tag{A.7}$$

The condition $E = E_\alpha$ is the on-shell condition. Equations (A.6) are the Lippmann–Schwinger equations

$$|\alpha\rangle_{\text{in}} = \Omega(E_\alpha)|\alpha\rangle,\tag{A.8}$$

which arise from attempting to solve $H|\alpha\rangle_{\text{in}} = E_\alpha|\alpha\rangle_{\text{in}}$ for the in-states (which also have energy E_α).

Turning now to the S -operator, using identities given above, one can easily establish

$$\begin{aligned}S(E) &= 1 - 2\pi i \delta(E - H_0)T(E) \\ S^{-1}(E) &= 1 + 2\pi i \delta(E - H_0)T^\dagger(E).\end{aligned}\tag{A.9}$$

The latter implies

$$\langle\alpha'|S(E)|\alpha\rangle = \langle\alpha'|\alpha\rangle - 2\pi i \delta(E_\alpha - E_{\alpha'})T_{\alpha'\alpha}, \quad \text{iff } E = E_\alpha.\tag{A.10}$$

Equation (A.5) together with identification (A.9) of the S -matrix is the main result obtained in [6].

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