Diagrammatic methods within the path integral representation for quantum systems

A Alastuey

1 Laboratoire de Physique, ENS Lyon/CNRS, 69364 Lyon Cedex 07, France
E-mail: angel.alastuey@ens-lyon.fr

Abstract The path integral representation has been successfully applied to the study of equilibrium properties of quantum systems for a long time. In particular, such a representation allowed Ginibre to prove the convergence of the low-fugacity expansions for systems with short-range interactions. First, I will show that the crucial trick underlying Ginibre’s proof is the introduction of an equivalent classical system made with loops. Within the Feynman-Kac formula for the density matrix, such loops naturally emerge by collecting together the paths followed by particles exchanged in a given cyclic permutation. Two loops interact via an average of two-body genuine interactions between particles belonging to different loops, while the interactions between particles inside a given loop are accounted for in a loop fugacity. It turns out that the grand-partition function of the genuine quantum system exactly reduces to its classical counterpart for the gas of loops. The corresponding so-called magic formula can be combined with standard Mayer diagrammatics for the classical gas of loops. This provides low-density representations for the quantum correlations or thermodynamical functions, which are quite useful when collective effects must be taken into account properly. Indeed, resummations and or reorganizations of Mayer graphs can be performed by exploiting their remarkable topological and combinatorial properties, while statistical weights and bonds are purely c-numbers. The interest of that method will be illustrated through a brief description of its application to two long-standing problems, namely recombination in Coulomb systems and condensation in the interacting Bose gas.

1 Introduction

The standard formalism for studying the equilibrium properties of interacting quantum systems is the many-body perturbation theory [1]. Thermodynamic quantities are systematically expanded in powers of the interactions, and any contribution in the corresponding series can be represented by a Feynman graph built with loops describing free propagation, which are connected at vertices by interaction lines. The structure of Feynman graphs is determined by well-defined topological
rules, while their contributions follow from conservation laws prescriptions at the vertices. The many-body perturbation theory is well-suited when interactions can be indeed treated as weak perturbations. This occurs for instance at high temperatures, or at high densities for fermions since the corresponding Fermi kinetic energy then becomes quite large.

In this paper, we will present another formalism, based on the Feynman path integral representation of quantum mechanics [2]. Within that representation, one can introduce an equivalent classical gas made of loops with interactions generated by imaginary-time averages of the genuine particle interactions along the paths defining the shapes of the loops. Interestingly, standard methods of classical statistical mechanics can be straightforwardly extended to the gas of loops, in particular the familiar Mayer series which are quite useful at low densities. Furthermore, the classical nature of the loops allows one to proceed to systematic reorganizations and resummations of the diagrammatical series, which are crucial for taking into account collective effects. Eventually, we stress that interactions are not treated perturbatively, an essential feature for dealing with phenomena like recombination for instance.

The usefulness of the loop formalism will be illustrated here through its applications to two long-standing problems in statistical mechanics of quantum systems. First, we will study recombination into atoms or molecules in a quantum plasma made with nuclei and electrons (see e.g. Ref. [3]). The second problem concerns the existence of Bose-Einstein (BE) condensation in an interacting Bose gas in the absence of external fields (see ch.2 in Ref. [4]).

The paper is organized as follows. In Section 2, we define the Hamiltonian of the general non-relativistic models with two-body interactions which can be studied within the path integral formalism. Then, we present the two examples considered further, namely the hydrogen plasma and an interacting Bose gas. In Section 3, after introducing the Feynman-Kac representation in the simple case of a single particle submitted to an external potential, we sketch the main steps of the transformations which lead to the introduction of a gas made with classical loops, which displays a grand-partition function identical to that of the genuine quantum system of interest. According to the corresponding so-called magic formula, we show that the equilibrium quantities of the quantum system can be represented by Mayer-like series for the equivalent gas of loops. The formalism is first applied to the hydrogen plasma in Section 4, where further resummations and reorganizations of Mayer series provide a series representations in terms of graphs made with particle clusters. The corresponding Screened Cluster Representation allows us to define and compute unambiguously the contributions of any recombined chemical species at finite temperatures. We turn to the second application in Section 5, namely the study of condensation in an interacting Bose gas. We show that, within the celebrated Kac scaling, the mean-field results can be readily retrieved from Mayer-like series. Contributions of fluctuations are also determined, but far from the critical region where a condensate might emerge. Eventually, we give some concluding comments in Section 6.
2 Non-relativistic quantum systems with two-body interactions

2.1 The model

In many situations encountered on Earth or in Astrophysics, a suitable description relies on the introduction of a quantum system made of point particles with Hamiltonian

$$H_N = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_{\alpha_i}} \Delta_i + \frac{1}{2} \sum_{i \neq j} u_{\alpha_i,\alpha_j}(|x_i - x_j|).$$

(1)

Here, $\alpha_i$ denotes the species of the $i$th particle, while $\Delta_i$ is the Laplacian with respect to its position $x_i$. In addition to the non-relativistic kinetic energy, the total potential energy is a sum of pairwise two-body instantaneous interactions $u_{\alpha_i,\alpha_j}(|x_i - x_j|)$ which only depend on the relative distance $|x_i - x_j|$ between particles. Notice that the non-relativistic Hamiltonian (1) does not depend on the spins $\sigma_{\alpha_i}$ of the particles, which only determine their bosonic or fermionic nature.

2.2 Examples

A first example is the hydrogen plasma, which can be viewed, within the so-called physical picture, as a mixture of quantum point particles which are either protons or electrons, interacting via the instantaneous Coulomb potential. Protons and electrons have respective charges, masses, and spins, $e_p = e$ and $e_e = -e$, $m_p$ and $m_e$, $\sigma_p = \sigma_e = 1/2$, while the two-body interaction reduces to

$$u_{\alpha_i,\alpha_j}(|x_i - x_j|) = e_{\alpha_i} e_{\alpha_j} v(|x_i - x_j|)$$

(2)

with $v(r) = 1/r$. Here both species are fermions, and the two-body Coulomb interaction is long-ranged.

A second example is an atomic gas described as a system of neutral point particles with mass $m$ and spin $\sigma = 0$. The corresponding two-body interaction potential $u(r)$ includes, in general, both a short-range repulsive part and a long-range attractive part, like the familiar Lennard-Jones potential. Now, the particles are bosons.

Notice that, at a more fundamental level, the atomic system should be also viewed as a quantum plasma made of point nuclei and point electrons with two-body Coulomb interactions, similarly to the case of the Hydrogen plasma. Nevertheless, the more phenomenological description in terms of an interacting Bose gas, is a priori sufficient at rather low temperatures and low densities. In fact, the difficult questions about recombination and effective interactions would be precisely investigated for the Hydrogen plasma.

3 Path integral representation and the equivalent gas of loops

3.1 The Feynman-Kac formula

For the sake of pedagogy, we introduce the path integral representation in the simple case of a single particle with mass $m$ submitted to a potential $V(r)$. Its Hamiltonian reads

$$H = -\frac{\hbar^2}{2m} \Delta + V(r).$$

(3)
The corresponding density matrix at a given temperature \( T \), namely the matrix element of Gibbs operator \( \exp(-\beta H) \), is exactly given by Feynman-Kac formula\[5, 6, 7, 8\]

\[
\langle r_b | \exp(-\beta H) | r_a \rangle = \frac{\exp[-(r_b - r_a)^2/(2\lambda^2)]}{(2\pi\lambda^2)^{3/2}} \int D(\xi) 
\times \exp[-\beta \int_0^1 ds \ V((1-s) r_a + s r_b + \lambda \xi(s))], \tag{4}
\]

with thermal de Broglie wavelength \( \lambda = (\beta \hbar^2/m)^{1/2} \). In the r.h.s. of (4), \( \xi(s) \) is a dimensionless Brownian bridge which starts from the origin at dimensionless time \( s = 0 \) and comes back at the origin at dimensionless time \( s = 1 \), i.e. \( \xi(0) = \xi(1) = 0 \). Functional measure \( D(\xi) \) is the normalized Gaussian Wiener measure which characterizes the Brownian process, and it is entirely defined by its covariance

\[
\int D(\xi) \xi_\mu(s) \xi_\nu(t) = \delta_{\mu\nu} \inf(s,t) (1 - \sup(s,t)). \tag{5}
\]

The corresponding functional integration is performed over all Brownian bridges \( \xi(s) \). Representation (4) is the proper mathematical formulation of genuine Feynman’s idea, which amounts to express the density matrix as a sum over all possible paths going from \( r_a \) to \( r_b \) in a time \( \beta \hbar \), of weighting factors \( \exp(-S/\hbar) \) where \( S \) is the classical action of a given path computed in potential \(-V\). Here, such paths are parametrized according to

\[
\omega_{ab}(s\beta \hbar) = (1-s) r_a + s r_b + \lambda \xi(s), \tag{6}
\]

where \( (1-s) r_a + s r_b \) describes the straight uniform path connecting \( r_a \) to \( r_b \). An example of path is shown in Fig. 1. Also, weighting factor \( \exp(-S/\hbar) \) is split into the product of three terms. The first term, which arises from the kinetic energy of the straight uniform path, reduces to the Gaussian prefactor in front of the functional integral. The second term, associated with the kinetic contribution of the Brownian part of the path, is a Gaussian functional of \( \xi(s) \) embedded in Wiener measure \( D(\xi) \). The third and last term is rewritten as the Boltzmann-like factor associated with time average

\[
\int_0^1 ds \ V(\omega_{ab}(s\beta \hbar)) \tag{7}
\]

of potential \( V \) along the considered path \( \omega_{ab} \). We stress that, independently of the rather poetic introduction of path integrals by Feynman\[2\], representation (4) can be derived in a straightforward way by starting from the obvious identity \( \exp(-\beta H) = [\exp(-\beta H/N)]^N \) combined with a suitable insertion of \( (N-1) \) closure relations in position-space (see e.g. Ref.\[9\]). Feynman-Kac formula (4) then follows by taking the limit \( N \to \infty \), as it has been proved for a wide class of potentials\[5\].

Feynman-Kac (FK) representation (4) perfectly illustrates the intrusion of dynamical features in equilibrium static quantities for quantum systems. Let us consider the diagonal density matrix \( \langle r_a | \exp(-\beta H) | r_a \rangle \). Because of the non-commutativity of the kinetic and potential parts of \( H \), that matrix element does not reduce to its classical counterpart

\[
\frac{\exp(-\beta V(r_a))}{(2\pi\lambda^2)^{3/2}}, \tag{8}
\]
so it is not entirely determined by $V(r_a)$. In fact, according to formula (4) specified to $r_b = r_a$, \[ \langle r_a | \exp(-\beta H) | r_a \rangle \] now depends on the potential landscape in some neighbourhood of $r_a$ with size $\lambda$, which is explored in time-average (7) thanks to Brownian motion. Therefore, $\langle r_a | \exp(-\beta H) | r_a \rangle$ appears to be indeed generated by a dynamical process. Not surprisingly, particle mass $m$ controls the importance of the corresponding dynamical effects. In particular, in the limit of an infinitely heavy particle $m \to \infty$, $\lambda = (\beta \hbar^2 / m)^{1/2}$ vanishes and $\langle r_a | \exp(-\beta H) | r_a \rangle$ obviously tends to its classical counterpart (8) : dynamical effects do not intervene anymore in the potential contribution which takes its purely static form. Quantum corrections to classical formula (8) can be expanded in powers of $\hbar^2$ according to the well-known Wigner-Kirkwood expansion [10, 11, 12]. That expansion can be easily retrieved within FK representation (4), by expanding time-average (7) in power series of $\lambda \xi$ and by applying Wick theorem to the calculation of the resulting moments of $\xi$. Notice that the present dynamical considerations are the manifestation, in the framework of path integrals, of the Heisenberg uncertainty principle which prevents the particle to stay at $r_a$. Hence, Brownian paths can be interpreted as describing intrinsic quantum fluctuations of position.

Remarkably, FK representation (4) involves only classical objects and c-numbers, so the operatorial structure of quantum mechanics is, in some sense, erased. That feature turns out to be particularly useful in the framework of the many-body problem, as described further. However, the intrinsic complexity of quantum mechanics is now hidden in the functional integration over all Brownian bridges, which remains a formidable task. In fact, explicit calculations can be performed in a few number of cases, as reviewed in Ref. [8]. Also, asymptotic Wigner-Kirkwood expansions of $\langle r_a | \exp(-\beta H) | r_a \rangle$ around the classical formula (8), can be derived for situations where $\lambda$ becomes small compared to the characteristic length $[|\nabla V(r_a)|/|V(r_a)|]^{-1}$ of variation of $V(r)$ in the neighbourhood of $r_a$. Such situations occur for very heavy particles or for high temperatures, and also at large distances for potentials which decay as power laws at infinity. In the opposite limit where $\lambda$ diverges, direct estimations of FK functional integral become rather cumbersome. Notice that, if $H$ has a single isolated boundstate with energy $E_0$ and wavefunction $\psi_0$, in the zero-temperature limit, the asymptotic behaviour of $\langle r_a | \exp(-\beta H) | r_a \rangle$ is merely extracted from its spectral representation, i.e.

\[ \langle r_a | \exp(-\beta H) | r_a \rangle \sim |\psi_0(r_a)|^2 \exp(-\beta E_0) \quad \text{when} \quad T \to 0 . \]
As argued in Ref. [13], the relevant paths which provide the low-temperature behaviour (9) occupy a small piece of the whole functional phase space, and they are quite different from the typical paths with divergent size $\lambda$. Consequently, an exact direct estimation of their contribution remains an open problem in general.

### 3.2 The density matrix

Let us come back now to the many-body problem in the framework of the grand-canonical ensemble. The system is enclosed in a box with volume $\Lambda$, in contact with a thermostat at temperature $T$ and a reservoir of particles that fixes the chemical potentials $\mu_\alpha$ of the various species. The corresponding grand-partition function reads

$$\Xi_\Lambda = \text{Tr}_\Lambda \exp \left( -\beta (H_N - \sum_\alpha \mu_\alpha N_\alpha) \right).$$

The trace $\text{Tr}_\Lambda$ is taken over a complete basis of $N$-body wavefunctions, which are symmetrized according to the statistics of each species, and satisfy Dirichlet boundary conditions at the surface of the box, while particle numbers $N_\alpha$ vary from 0 to $\infty$. The grand-partition function (10) can be expressed in the basis of positions and spins, where a given state is the suitably symmetrized Slater sum of products of one-body states $|x_\sigma^z_\alpha\rangle$. This provides a sum of diagonal and off-diagonal matrix elements of $\exp(-\beta H_N)$.

In the case of the hydrogen plasma, an example of above density matrix elements involved in the expression of the grand-partition function, is

$$\langle R_1 R_3 R_2 R_4 | \exp(-\beta H_{3,4}) | R_1 R_2 R_3 R_4 \rangle,$$

for the Hamiltonian $H_{3,4}$ of 3 protons and 4 electrons. Here, the positions of two protons are exchanged, as well as those of three electrons. Contributions of spins are factored out in simple degeneracy factors because the Coulomb Hamiltonian does not depend on the spins. For matrix element (11), that multiplying degeneracy factor is $2^4$, because the spin-states of the exchanged particles are necessarily identical.

The FK representation for each of the matrix elements of $\exp(-\beta H_N)$ takes a form similar to formula (4), with $N_\alpha$ paths $\omega^\alpha$ for each species $\alpha$, as well as a Boltzmann-like factor associated with the time average of the potential part of $H_N$. The paths associated with matrix element (11) can be collected into loops. In fact, that property holds for any matrix element of $\exp(-\beta H_N)$, because any permutation can always be decomposed as a product of cyclic permutations. A loop $L$ is constructed by collecting $q$ paths associated with $q$ particles exchanged in a cyclic permutation. Accordingly, $L$ is characterized by its position $X$, which can be arbitrarily chosen among the extremities of paths $\omega^\alpha$, and several internal degrees of freedom which are particle species ($\alpha$), number $q$ of exchanged particles, and shape $\lambda, \eta$ obtained as the union of the $q$ paths $\omega^\alpha$. It turns out that $\eta(s)$ is itself a Brownian bridge with flight time $q$, i.e. $\eta(0) = \eta(q) = 0$, distributed with the corresponding Wiener measure $D(\eta)$.

In the FK representation, the time-average of the total interaction potential can be obviously rewritten as a sum of two-body interactions $V$ between loops, plus a sum of loop self-energies $U$, namely

$$\frac{1}{2} \sum_{i \neq j} V(L_i, L_j) + \sum_i U(L_i),$$

(12)
where loops associated with the considered matrix element are labelled as $\mathcal{L}_i$ with index $i$ running from 1 to their total number $N$. For instance, four loops can be identified in the FK representation of matrix element (11), as shown in Fig. 2. Two-body potential $V(\mathcal{L}_i, \mathcal{L}_j)$ between loops $\mathcal{L}_i$ and $\mathcal{L}_j$ reduces to a time-average along their respective shapes of the genuine two-body particle interaction $v((X_i + \lambda_\alpha \eta_i(s) - X_j - \lambda_\alpha \eta_j(t)))$ evaluated at times which differ by an integer value. Self-energy $\mathcal{U}(\mathcal{L}_i)$ for loop $\mathcal{L}_i$ is given by a similar average along its own shape of $v((\lambda_\alpha \eta_i(s) - \lambda_\alpha \eta_i(t)))$ evaluated at times which differ by a non-zero integer value, with a prefactor $1/2$ which avoids double counting of genuine interactions between two exchanged particles.

### 3.3 The magic formula

At this stage, grand-partition function (10) is rewritten as a sum of Boltzmann-like factors associated with energies (12) multiplied by combinatorial factors and particle fugacities $z_\alpha/(2\pi \lambda_\alpha^2)^{3/2}$ with $z_\alpha = \exp(\beta \mu_\alpha)$, which have to be integrated over positions and shapes of the involved loops. It turns out that the whole sum can be rewritten as the grand-partition function of a classical gas of undistinguishable loops with suitable activities $z(\mathcal{L})$, namely

$$\Xi_\Lambda = \Xi^{(\text{loop})}_\Lambda = \sum_{N=0}^{\infty} \frac{1}{N!} \int \prod_{i=1}^{N} d\mathcal{L}_i \ z(\mathcal{L}_i) \prod_{i<j} \exp(-\beta V(\mathcal{L}_i, \mathcal{L}_j)) \ . \quad (13)$$

Phase space measure $d\mathcal{L}$ in the world of loops, involves discrete summations over species index $\alpha$ and exchanged-particle number $q$, spatial integration over position $X$ inside $\Lambda$, and functional integration over shapes $\eta$ with Wiener measure $D(\eta)$ restricted to shapes such that $X + \lambda_\alpha \eta(s)$ remains inside $\Lambda$. Loop fugacity reads

$$z(\mathcal{L}) = (\pm 1)^{q-1} \frac{(2\sigma_\alpha + 1) z_\alpha^q}{q(2\pi q \lambda_\alpha^2)^{3/2}} \exp(-\beta \mathcal{U}(\mathcal{L})) \ , \quad (14)$$
the structure of which is easily interpreted as follows. For bosons, the sign is + and the fugacity is always positive. For fermions, the sign is − and factor \((-1)^{q-1}\) is the signature of a cyclic permutation of \(q\) objects, which is negative for \(q\) even. In front of the obvious particle-activity contribution \(z_0^q\), factor \((2\sigma_\alpha + 1)\) is the number of configurations of exchanged-particles spins which are all identical. Factor \(q\) in front of \((2\pi q \lambda_\alpha^2)^{3/2}\) is related to the \(q\) possible choices of position \(X\) among that of the \(q\) exchanged particles. The other factor \(q\) in front of \(\lambda_\alpha^2\), arises from the absorption of the remaining \((q-1)\) integrations over particle positions together with the \(q\) functional integrations over Brownian bridges into the single measure \(\mathcal{D}(\eta)\). Notice that \(q\lambda_\alpha^2\) is nothing but the square of de Broglie wavelength for inverse temperature \(q\beta\). 

We stress that identity (13) proceeds from remarkable combinatorial properties. For instance, in the case of the hydrogen plasma, there are various contributions in term \(N = 4\) of \(\Xi^{(\text{loop})}_\Lambda\), which are identical to that of matrix element (11) in the Slater expansion of \(\Xi_\Lambda\). Such contributions arise from the explicitation of the 4 phase-space measures \(d\mathcal{L}_i\) \((i = 1, 2, 3, 4)\) where 2 protonic loops and 2 electronic loops, carrying respectively 2 or 1 protons and 3 or 1 electrons, have to be chosen among 4 labelled loops. Also, there are several matrix elements in the Slater expansion of \(\Xi_\Lambda\), involving 3 protons and 4 electrons, which provide identical contributions to that of matrix element (11). Thanks to a rather fortunate arrangement between both counting factors, the full respective contributions in both \(\Xi^{(\text{loop})}_\Lambda\) and \(\Xi_\Lambda\) are indeed identical! According to those considerations, and also because of its synthetical form, identity (13) is often called the magic formula. 

Historically, Ginibre [14] was the first to introduce the notion of loops when studying the convergence of Mayer series for quantum gases with short-range forces. However, he did not write explicitly formula (13), which has been derived later by Cornu [15]. Recently, Martin [16] proposed an elegant and shorter derivation of that formula. Notice that identity (13) is valid for any kind of two-body interactions, and an arbitrary number of species with Fermi or Bose statistics. 

Of course, and as quoted in the simple case of a single particle in an external potential, the intrinsic difficulty of quantum mechanics is now hidden in the functional integrations over loop shapes, so an exact calculation of loop grand-partition function remains far beyond human abilities...Nevertheless, magic formula (13) is quite useful because standard tools of classical statistical mechanics can be applied, as well as various transformations relying on simple properties of classical Boltzmann factors.

### 3.4 Mayer-like graphs

The structure of loop grand-partition (13) is identical to that of an ordinary classical system made of point particles with two-body interactions. Therefore, equilibrium quantities of loops can be represented by Mayer-like diagrammatical series, where points are replaced by loops. This provides Mayer series for particle quantities, like particle density \(\rho_\alpha\) which reads

\[
\rho_\alpha = \sum_{\mathcal{G}} \frac{1}{S(\mathcal{G})} \sum_{q_0=1}^{\infty} \int \mathcal{D}(\eta_0) \ z(\mathcal{L}_0) \int \prod_{i=1}^{n} d\mathcal{L}_i \ z(\mathcal{L}_i) \left[ \prod_{f} f \right]_{\mathcal{G}} .
\]

(15)

Each graph \(\mathcal{G}\) is constructed according to the standard Mayer rules [17, 18], It is made with \((n + 1)\) loops \(\mathcal{L}_i\), \(i = 0, ..., n\). Two loops \(i\) and \(j\) are connected at most by a single bond

\[
f_{ij} = \exp(-\beta V(\mathcal{L}_i, \mathcal{L}_j)) - 1 ,
\]

(16)
Figure 3: An example of graph $\mathcal{G}$ with the root loop $\mathcal{L}_0$ connected to two loops $\mathcal{L}_1$ and $\mathcal{L}_2$ via Mayer bonds $f_{01}$ and $f_{02}$. The shapes of the loops are drawn inside bubbles, while the Mayer bonds are represented by thick straight lines connecting the bubbles.

and $[\prod f]_{\mathcal{G}}$ denotes the product of such bonds. Also, graph $\mathcal{G}$ is simply connected, namely it cannot be separated into two parts which are not connected by at least one bond $f$. Symmetry factor $S(\mathcal{G})$ is the number of permutations of black loops $\mathcal{L}_i$ with $i \geq 1$, which leave $[\prod f]_{\mathcal{G}}$ unchanged. Each loop is weighted by its fugacity $z(\mathcal{L}_i)$. The contribution of graph $\mathcal{G}$ is obtained by integrating over all degrees of freedom of black loops embedded in measure $d\mathcal{L}_i$, while the position and species index of root loop $\mathcal{L}_0$ are fixed and only its shape and particle number are integrated over. The species index $\alpha_0$ of root loop $\mathcal{L}_0$ is set equal to $\alpha_i$. Eventually, $\sum_{\mathcal{G}}$ is performed over all topologically different unlabelled graphs $\mathcal{G}$. For instance, the contribution of graph $\mathcal{G}$ made with two field loops $\mathcal{L}_1$ and $\mathcal{L}_2$ only connected to root loop $\mathcal{L}_0$ (see Fig. 3), reads

$$
\frac{1}{2} \sum_{q_0=1}^{\infty} \int D(\eta_0) \frac{q_0}{z(\mathcal{L}_0)} \int d\mathcal{L}_1 d\mathcal{L}_2 \frac{z(\mathcal{L}_1) z(\mathcal{L}_2)}{f_{01} f_{02}} .
$$

(17)

Let us first consider a short-range particle interaction $u_{\alpha_i \alpha_j}(|X_i - X_j|)$ which decays faster than some exponential when $|X_i - X_j| \to \infty$. Since the sizes of the loops are distributed with a Gaussian law, the loop-loop interaction potential $\mathcal{V}(\mathcal{L}_i, \mathcal{L}_j)$ is then bounded by an exponential decaying function of $|X_i - X_j|$. Since Mayer-like series (15) exhibit the same topological structure as their classical counterparts, the analysis of their convergence then becomes similar to that for classical systems with short-range interactions. This was exploited by Ginibre [14] who indeed proved the convergence at sufficiently low fugacities and high temperatures.

If the particle interaction is long ranged, the loop-loop interaction is also long ranged. In particular, for the hydrogen plasma or any Coulomb system, $\mathcal{V}(\mathcal{L}_i, \mathcal{L}_j)$ decays like the genuine Coulomb potential itself at large distances, for most of the loops which have a finite size controlled by the de Broglie wavelengths, namely

$$
\mathcal{V}(\mathcal{L}_i, \mathcal{L}_j) \sim \frac{q_i e_\alpha q_j e_\alpha}{|X_i - X_j|} \quad \text{when} \quad |X_i - X_j| \to \infty .
$$

(18)

Indeed, at large distances, loops can be shrunk to point charges, and further corrections to the monopolar term (18) can be expanded in multipolar power series of $\lambda_\alpha / |X_i - X_j|$ and $\lambda_\alpha / |X_i - X_j|$. 


Like in the case of purely Coulombic interactions, the long-range nature of $V(L_i, L_j)$ induces divergences in every Mayer-like graph because Mayer bonds behave as $-\beta V(L_i, L_j)$ at large distances. Such divergences are removed via systematic chain resummations as exposed further.

4 Emergence of chemical species in the hydrogen plasma

In this Section, we consider the hydrogen plasma in contact with a thermostat at temperature $T$ and a reservoir of particles that fixes the chemical potentials equal to $\mu_p$ and $\mu_e$ for protons and electrons respectively. Because the infinite system maintains local neutrality $\rho_p = \rho_e$ in any fluid phase, the bulk equilibrium quantities depend in fact solely on the mean

$$\mu = (\mu_p + \mu_e)/2,$$

while the difference $\nu = (\mu_e - \mu_p)/2$ is not relevant, as rigorously proved in Ref. [19]. Consequently, the common particle density $\rho = \rho_p = \rho_e$ depends only on $T$ and $\mu$.

We are interested in the emergence of usual chemical species, like atoms H or molecules $H_2$ within the grand-canonical description of the hydrogen plasma, namely the so-called physical picture. First, we provide rough estimations which allow us to identify their contributions at vanishing temperatures in the grand-partition function. Then, we introduce the well-known problem of estimating such contributions at finite temperature which has to face the divergent contributions of Rydberg states. The proper answer to that longstanding question requires a simultaneous and consistent treatment of both recombination and screening. We show that this can be achieved through a suitable reorganization of Mayer-like series. The corresponding screened cluster representation provides an unambiguous definition of finite-$T$ internal partition functions for any chemical species without introducing arbitrary regularizations or adjustable parameters.

4.1 Rough estimations in the zero-temperature limit

In the zero-temperature limit at fixed negative chemical potential $\mu$, the relative importance of the contributions of chemical species to $\Xi_A$ given by the trace (10), follows from the entropy-energy balance between

- Exponentially vanishing fugacity factors $\exp(\beta \mu)$
- Exponentially growing Boltzmann factors $\exp(-\beta E^{(0)}_{H_{np},N_e})$

where $E^{(0)}_{H_{np},N_e}$ is the groundstate energy of $H_{np,N_e}$. For instance, leading contributions of atoms H or molecules $H_2$ obviously arise from $H_{1,1}$ and $H_{2,2}$ with respective groundstate energies $E^{(0)}_{1,1} = E_H = -e^2/(2a_B)$ and $E^{(0)}_{2,2} = E_{H_2}$. The corresponding relative abundance of atoms and molecules depend not only on the relative values of the groundstate energies, but also on the chemical potential $\mu$. In fact, thanks to the inequality

$$3E_H < E_{H_2} < 2E_H,$$
the atomic weight \( \exp(2\beta\mu) \exp(-\beta E_H) \) dominates the molecular weight \( \exp(4\beta\mu) \exp(-\beta E_{H2}) \) if we choose \( \mu \) sufficiently close to \( E_H \). This suggests that an atomic phase should prevail under such conditions, in agreement with the chemical ionization equilibrium introduced by Saha [20].

Above rough estimations can be rigorously controlled within a suitable scaling low-temperature limit (SLT), \( T \to 0 \) with \( \mu \to E_H \), introduced by Macris and Martin [21], who extended the pioneering work by Fefferman [22]. Those authors proved that, within the SLT which properly defines the so-called Saha regime, the hydrogen plasma becomes an ideal mixture of ionized protons, ionized electrons, and hydrogen atoms in their groundstate. The next important question is related to finite temperature effects: what about the contributions of excited atomic states and of other chemical species?

4.2 Divergence of internal partition functions at finite temperature

At finite temperatures, not only the atomic groundstate contributes to thermodynamic quantities, but also excited states. When \( T \) vanishes, an atom can be considered as frozen in its groundstate because of the finite gap between \( E_H \) and the first excited level \( E_H/4 \). This explains why the corresponding contribution to equilibrium quantities merely involves Boltzmann factor \( \exp(-\beta E_H) \) as noticed just above. At finite temperatures, contributions of excited states must also be taken into account. For that purpose, it is natural to introduce the internal atomic partition function in the vacuum

\[
Z_H^{(\text{vac})} = 4 \sum_{n=1}^{\infty} n^2 \exp(-\beta E_H/n^2). \tag{21}
\]

In that definition, factor 4 arises from proton and electron spins degeneracy, factor \( n^2 \) accounts for orbital degeneracy of the level \( n \) with energy \( E_H/n^2 \), and summation extends over all boundstates up to \( n = \infty \).

Obviously \( Z_H^{(\text{vac})} \) diverges because of the contributions of Rydberg states with \( n \to \infty \). Similar divergences would occur in a naive description of recombination into molecules \( H_2 \), ions \( H^- \) and \( H^+ \), and also more complex entities like \( H_2^- \), \( H_3^+ \), \( H_3^- \), etc... In the literature, for atomic contributions, such divergences are removed within phenomenological prescriptions, in particular those leading to the so-called Brillouin-Planck-Larkin formula [23], [24], as described in the review [3] and commented in Ref. [25],

\[
Z_{\text{BPL}} = 4 \sum_{n=2}^{\infty} n^2 [\exp(-\beta E_H/n^2) - 1 + \beta E_H/n^2]. \tag{22}
\]

If the substracted terms in the expression (22) do ensure the convergence of the sum over \( n \), their physical signification is not clear. In fact, the physical idea underlying that phenomenological approach, is that the divergent contributions of Rydberg states are screened by the free charges present in the system. Inside an Hydrogen atom, the proton-electron potential decays faster than \( 1/r \) at distances \( r \) larger than screening length \( \lambda_s \). Thus, there is no accumulation of atomic boundstates near the continuum edge at \( E = 0 \), and all Rydberg states with \( n \) sufficiently large are suppressed. This gives some physical meaning to Brillouin-Planck-Larkin formula (22). At the same time, it suggests to introduce another phenomenological expression for the internal atomic
Figure 4: A convolution chain connecting two loops $\mathcal{L}_a$ and $\mathcal{L}_b$ via 3 intermediary loops. For convenience, the loops are schematically represented by disks, while the potential bonds $-\beta V$ connecting two successive loops in the chain are represented by straight lines.

partition function, namely

$$Z_H^{(scr)} = 4 \sum_{n=1}^{p_S} n^2 \exp(-\beta E_H/n^2), \quad (23)$$

which explicitly accounts for screening effects by setting $p_S \sim \sqrt{\lambda S/a_B}$.

According to above considerations, the estimation of contributions from recombined entities cannot be disentangled from that of screened interactions between ionized charges. Thus, a fully consistent treatment of many-body effects is required, where the interplay between recombination and screening is properly taken into account. As described further, the Mayer-like series for the equivalent gas of loops turns out to be a suitable tool for that purpose. That formalism provides well-behaved prescriptions for computing the contributions of any recombined entity, not only those of atoms but also, for instance, those of molecules $\text{H}_2$ and ions $\text{H}^-$, $\text{H}_2^+$. 

4.3 Recombination and screening within Mayer diagrammatical series

As mentioned previously, all Mayer-like graphs for the gas of loops diverge because of the long range nature of the loop interaction potential $V(\mathcal{L}_i, \mathcal{L}_j)$. In order to account for the collective effects which remove those divergences, as well as for the recombination processes which leads to the formation of chemical species, we proceed to successive resummations and reorganizations which have been derived in detail in Ref. [27]. Here we only sketch the main steps of the method.

- **Introduction of a screened effective potential**

  The first step consists in removing Coulomb divergences. All Mayer bonds $f$ are first expanded in Taylor series (TS) with respect to $(-\beta V)$. This transforms the whole series (15) into a new set of analogous graphs $G^{(TS)}$ where two loops can be connected by bonds which are either $-\beta V$, or $(\beta V)^2/2$ or $-\beta V^3/6$, etc... Now, let us consider a graph $G^{(TS)}_{ab}$ where two given loops $\mathcal{L}_a$ and $\mathcal{L}_b$ are connected by the bond $-\beta V(\mathcal{L}_a, \mathcal{L}_b)$. Such loops may be black loops or one of them may reduce to the root loop $\mathcal{L}_0$. Then, we consider all the other graphs $G^{(TS)}_{ab,n}$ identical to $G^{(TS)}_{ab}$ except that the direct simple bond $-\beta V(\mathcal{L}_a, \mathcal{L}_b)$ between the two loops $\mathcal{L}_a$ and $\mathcal{L}_b$ is now replaced by a convolution chain of $(n + 1)$ bonds $-\beta V$ connecting $n$ intermediary loops $\mathcal{L}_i$, as shown in Fig. 4.

  Thanks to remarkable combinatorial properties [27], the summation of the contributions of graphs $G^{(TS)}_{ab,n}$ to that of graph $G^{(TS)}_{ab}$, can be carried out at the local level, namely considering only loops $\mathcal{L}_a$ and $\mathcal{L}_b$ with the intermediary loops involved in the considered convolution chain. The result of that resummation does not depend on the global structures of the considered graphs, which
Emergence of Boltzmann factors associated with the screened effective potential

The previous result is readily extended to any genuine bond \((-\beta V)^n/n!\), which gives rise to \([-\beta e_{\alpha \beta} e_{\alpha \beta}(L_a, L_b)]^n/n!\) once all chain resummations have been performed. Then, the further summation of all bonds \([-\beta e_{\alpha \beta} e_{\alpha \beta}(L_a, L_b)]^n/n!\) between two given loops \(L_a\) and \(L_b\) makes Boltzmann factors \(\exp(-\beta e_{\alpha \beta} e_{\alpha \beta}(L_a, L_b))\) emerge. As mentioned previously, all those resummations and reexponentiations can be performed independently of the global structures of the considered graphs [27].

Introduction of renormalized fugacities

Chain resummations also apply to other substructures of graphs \(G^{(TS)}\), where to a given loop \(L_a\) are attached one or more rings made with convolution chains of bonds \((-\beta V)\) (see Fig. 6). The summation over all \(n\) intermediary loops inside a given convolution ring with \(n\) varying from 1 to \(\infty\) provides \(I_R(L_a) = \beta(V(L_a, L_a) - e_{\alpha \alpha}^2 \phi(L_a, L_a))\). The sum over all numbers of ring attached to \(L_a\) transform its fugacity \(z(L_a)\) into the renormalized one \(z_R(L_a) = z(L_a) \exp(I_R(L_a)/2)\).

**Convergent prototype graphs**

The topological structure of genuine Mayer graphs \(G\) is conserved through all the previous chain resummations and reexponentiations. Accordingly, we obtain a new set of prototype graphs \(\mathcal{P}\), with
Figure 5: Three examples of double convolution chains connecting two loops $\mathcal{L}_a$ and $\mathcal{L}_b$: (1) chains reduce to the genuine direct bond $[\beta\mathcal{V}(\mathcal{L}_a, \mathcal{L}_b)]^2$ (2) one chain reduces to the direct bond $-\beta\mathcal{V}(\mathcal{L}_a, \mathcal{L}_b)$, while the other one involves 2 intermediary loops (3) both chains involve respectively 3 and 2 intermediary loops. The notations are the same as in Fig. 4.

Figure 6: An example of three ring chains attached to a loop $\mathcal{L}_a$, involving respectively 1, 2 and 3 intermediary loops. The notations are the same as in Fig. 4.
a topological structure identical to that of the genuine Mayer graphs. The bonds are now Mayer bonds associated with the effective potential $\phi$, while the statistical weights are the renormalized fugacities $z_R$, with specific restrictions to avoid double counting generated by the various chain and ring resummations [27].

Similarly to what happens in the classical case, collective effects embedded in the effective potential are expected to screen the bare loop-loop interaction. In fact, the static part $q_a e_a q_b e_b / |X_a - X_b|$ of $\mathcal{V}(L_a, L_b)$, which does not depend on loop shapes, is exponentially screened. On the contrary, the multipolar parts of $\mathcal{V}(L_a, L_b)$ which depend on loop shapes, are not exponentially screened. The resulting effective potential decays only as a dipolar interaction at large distances, namely [26]

$$\phi(L_a, L_b) \sim \frac{A_{a \alpha b}(\eta_a, \eta_b)}{|X_a - X_b|^3} \quad \text{when} \quad |X_a - X_b| \to \infty ,$$  \hspace{1cm} (26)

where $A_{a \alpha b}(\eta_a, \eta_b)$ is an amplitude which depends only on loop species and shapes. The decay of $\phi(L_a, L_b)$ is at the border line for integrability at large distances. However, if loop shapes are first integrated over, all dangerous $1/R^2$-terms vanish. Thus, within that prescription for the order of integrations involved in measures $dL_i$, all long range Coulomb divergences are removed in the prototype graphs which provide convergent contributions.

- Introduction of particle clusters

The final step of the transformations consists in rewriting the prototyope graphs $\mathcal{P}$ built with loops, as graphs $G$ built with particle clusters. For that purpose, we first identify sets of loops $\mathcal{E}_L = \{L_i\}$ such that all the effective interactions between loops inside $\mathcal{E}_L$ are present in the product of Boltzmann factors $\exp(-\beta e_{a \alpha} \phi(L_i, L_j))$. The explicitation of phase-space measures $dL_i$ as sums over species index and particle numbers allow us to identify particle clusters $C(N_p, N_e)$ in a given set $\mathcal{E}_L$. The corresponding statistical weights $Z_{\phi}(C)$ account non-perturbatively for interactions between the particles through the presence of Boltzmann factors $\exp(-\beta e_{a \alpha} \phi(L_i, L_j))$, so all recombination processes are exactly taken into account.

Once particle clusters have been identified, we proceed to subtracting and adding counter terms to their statistical weights $Z_{\phi}(C)$. This defines truncated statistical weights $Z_{\phi}^T(C)$, which are well suited for studying the zero-density limit because they still provide finite contributions when $\phi$ is replaced by the bare Coulomb-like loop potential $\mathcal{V}$. The added counter terms define bonds $F_\phi$ built with powers of $\phi$. They account for the resummation of a priori divergent long-ranged Coulomb contributions, which are ultimately finite thanks to the screening effects embedded in $\phi$.

4.4 The screened cluster representation

The resummation machinery described above amounts to perform an exact transformation of the whole series (15), which can be rewritten as the Screened Cluster Representation (SCR),

$$\rho_a = \sum_G \frac{1}{S(G)} \int dC_0 \; q_a \; Z_{\phi}^T(C_0) \int \prod_{i=1}^n dC_i \; Z_{\phi}^T(C_i) \left[ \prod F_\phi \right]_G ,$$  \hspace{1cm} (27)

where graphs $G$ have the same topological structure as usual Mayer graphs. Now, ordinary points are replaced by particle clusters $C_i$, weighted by factors $Z_{\phi}^T(C_i)$. Two clusters are connected by
Figure 7: An example of graph \( G \) which contributes to the proton density \( \rho_p \). The two clusters are represented by large grey disks. The bond \( \beta^2 \Phi^2/2! \) connecting the two clusters is represented by a double thick straight line. Inside the root cluster \( C_0(1,1) \), the position of the proton, represented by a white disk, is fixed. The positions of the other proton inside \( C_1(1,1) \) and of the electrons, represented by black disks, are integrated over.

at most one bond \( F_\phi \) which can be either \( -\beta \Phi \), \( \beta^2 \Phi^2/2! \) or \( -\beta^3 \Phi^3/3! \) with \( \Phi \) the total effective potential between both clusters. Graphs \( G \) are simply connected, and symmetry factor \( S(G) \) is computed as usual. Phase-space measure \( dC_i \) reduces to integrations over positions and shapes of loops belonging to set \( E_L \) associated with cluster \( C_i \), whereas in \( dC_0 \) position of root particle \( \alpha \) is not integrated over. Eventually, \( \sum_G \) is performed over all topologically different graphs with some simple restrictions, in part avoiding double-counting of genuine particle interactions [27]. For instance, the contribution of graph \( G \) made with two clusters \( C_0 = C(1,1) \) and \( C_1 = C_1(1,1) \) connected by a bond \( \beta^2 \Phi^2/2! \) (see Fig. 7), reads

\[
\int dC_0 \ Z^T_\phi(C_0) \int dC_1 \ Z^T_\phi(C_1) \ \frac{\beta^2 \Phi^2(C,C_1)}{2},
\]

since \( S(G) = 1 \) and \( q_0 = 1 \). That graph arises from the introduction of the truncated weight \( Z^T_\phi(C(2,2)) \) for a cluster made with 2 protons and 2 electrons, according to the substraction and addition of counter terms to the full statistical weight \( Z_\phi(C(2,2)) \) as described above.

Remarkably, not only the genuine structure of Mayer graphs is conserved by the resummation machinery, but both statistical weights \( Z^T_\phi(C) \) and bonds \( F_\phi \) depend on the sole effective potential \( \phi \). Thanks to the sufficient fast decay of \( \phi \), all large-distances divergences are removed in every graph \( G \), which does provide a finite contribution. The presence of complete interactions inside a given cluster \( C(N_p, N_e) \) ensures that chemical species made with \( N_p \) protons and \( N_e \) electrons do emerge at low densities. Both features are detailed below. Notice that the physical ideas underlying the SCR, are close to those involved in the construction of the so-called ACTEX approach by Rogers [28].

Contrarily to Feynman graphs involved in standard many-body perturbation theory [1], graphs \( G \) in SCR account for non-perturbative effects in the Coulomb potential which are essential for a proper description of recombination. In fact, that representation provides the contributions, at finite temperature and finite density, of all chemical species and of their mutual interactions, without
introducing arbitrary regularizations or adjustable parameters. Hence the SCR has been used for different purposes like

- The derivation of exact asymptotic expansions beyond Saha theory in the SLT regime [29]
- The analysis of the cross-over regime between molecular and atomic hydrogen [30]

In the next paragraph, we describe the structure of the contributions of the simplest chemical species like atoms $H$, molecules $H_2$, ions $H^-$ and $H_2^+$, which are key ingredients in the previous works.

4.5 Contributions of chemical species at finite temperature

The ideal-like contribution of a given chemical species made with $N_p$ protons and $N_e$ electrons, emerges in the simple SCR diagram made with the single corresponding particle cluster. Indeed, at low densities, $\phi \rightarrow V$, and $Z(T(C_0))$ gives rise to the cluster partition function

$$Z(N_p, N_e) = (2\pi \lambda_{N_p,N_e}^2)^{3/2} \lim_{\Lambda \rightarrow \infty} \frac{1}{\Lambda} \text{Tr}[\exp(-\beta H_{N_p,N_e})]^{T \text{Mayer}}$$

where $\lambda_{N_p,N_e} = (\beta \hbar^2 / (N_p m_p + N_e m_e))^{1/2}$ is the thermal de Broglie wavelength of the cluster. That partition function is defined in terms of bare Coulomb Hamiltonians, so it depends only on temperature and fundamental constants. It is finite thanks to the truncation procedure defining $\exp(-\beta H_{N_p,N_e})^{T \text{Mayer}}$ and inherited from the procedure of subtracting and adding counter-terms involved in the resummation machinery. The own contributions of subtracted counter terms arise in other SCR diagrams built with several particle clusters connected by bonds $F_\phi$. Such contributions are indeed finite thanks to the screened nature of $\phi$. We stress that, as far as thermodynamical properties are concerned, only the full contribution of $Z(N_p, N_e)$ and of its related screened counter terms makes an unambiguous sense. This illustrates the interplay between recombination and screening devices above on heuristic grounds.

Remarkably, the familiar chemical species naturally emerge from cluster partition function $Z(N_p, N_e)$, which is intrinsic to the considered cluster in the vacuum. A given chemical species made with $N_p$ protons and $N_e$ electrons, is associated with bound states of bare Hamiltonian $H_{N_p,N_e}$. In the zero-temperature limit, it provides the leading contribution to $Z(N_p, N_e)$ which behaves as

$$\exp(-\beta E_{N_p,N_e}^{(0)})$$

apart from possible integer degeneracy factors. At finite temperatures, $Z(N_p, N_e)$ involves not only contributions from thermally excited bound states, but also contributions from diffusive states describing the dissociation into various chemical species which cannot be disentangled. For instance $Z(2,2)$ involves not only a molecular part, but it also includes the contributions of atom-atom interactions at short distances. Notice that the long range part of such atom-atom interactions, i.e. the familiar van der Waals interactions, are embedded in the contributions of graph $G$ shown in Fig. 7.

Cluster partition functions $Z(N_p, N_e)$ can be viewed as generalizations of Ebeling virial coefficients [31] introduced for dealing with contributions from two-particle clusters. Notice that $Z(1,1)$ does not reduce exactly to the heuristic BPL partition function $Z_{\text{BPL}}$, although both quantities are close at low temperatures [32]. Eventually, notice that the contributions of interactions between
chemical species can be expressed also in terms of cluster functions similar to $Z(N_p, N_e)$, like that of graph $G$ shown in Fig. 7. Thus, all contributions related to the formation of complex entities are properly taken into account.

5 Condensation in an interacting Bose gas

In this Section, we consider an interacting Bose gas made of a single species with zero spin, as described in Section 2. First, we recall the familiar criterion introduced for the ideal gas, namely the macroscopic condensation of particles in the same quantum state with zero momentum. We also present an equivalent criterion which is more suited for dealing with interactions, and provides the order parameter of the BE transition. Within the path integral representation in terms of the loop gas, that criterion is shown to be related to the behaviour of the density of open loops with large arbitrary sizes. Then, we turn to the Kac prescription, which amounts to consider the limit of an infinitely weak interaction potential with an infinite range. At leading order, such prescription provides a mean-field theory which predicts that the BE persists. Eventually, we show that Mayer-like series provide interesting preliminary results on the effects of fluctuations beyond that mean-field limit.

5.1 Order parameter of the Bose-Einstein condensation

The appearance of Bose condensate has been first derived for a perfect gas (for a thorough review see [33] and references given therein) showing that this phenomenon does not require any interaction. In the framework of the grand-canonical ensemble, where the given thermodynamical parameters are temperature $T$ and chemical potential $\mu$, the corresponding particle density $\rho$ reads

$$\rho = \rho_0(\beta, \mu) = \frac{1}{(2\pi)^3} \int \frac{1}{\exp(\beta(\epsilon(k)) - \mu) - 1}. \quad (31)$$

Formula (31) describes the perfect gas thermodynamic function $\rho_0(\beta, \mu)$ for any $\rho < \rho_{0,c}(\beta)$ where

$$\rho_{0,c}(\beta) = \frac{1}{(2\pi)^3} \int \frac{1}{\exp(\beta\epsilon(k)) - 1} \quad (32)$$

is the critical density. For $\rho > \rho_{0,c}(\beta)$, a macroscopic condensation of particles in state $k = 0$ takes place.

It is well-known that the Bose-Einstein condensation is directly related to the appearance of off-diagonal long-range order (ODLRO) in the one-body density matrix, which can be viewed as the relevant order-parameter for that transition in the interacting system (see e.g. [33]). In the ideal case, it has been shown that

$$\lim_{|r-r'| \to \infty} \langle r | \mathcal{D}_0^{(1)} | r' \rangle = 0 \quad \text{for} \quad \rho < \rho_{0,c}(\beta) \quad (33)$$

and

$$\lim_{|r-r'| \to \infty} \langle r | \mathcal{D}_0^{(1)} | r' \rangle = \rho - \rho_{0,c}(\beta) \quad \text{for} \quad \rho > \rho_{0,c}(\beta), \quad (34)$$
where $D_0^{(1)}$ is the ideal one-body density matrix. For the interacting system, the eigenstates of the Hamiltonian no longer reduce to tensorial products of one-body states, so the possible persistence of the BE condensation has to be related to the existence of ODLRO for the one-body density matrix $\langle r | D_0^{(1)} | r' \rangle$ above some critical density.

Within the equivalent gas of loops, the off-diagonal matrix element $\langle r | D_0^{(1)} | r' \rangle$ reads [34]

$$\langle r | D_0^{(1)} | r' \rangle = \sum_{q=1}^{\infty} \int D(\eta) q \exp[-(r-r')^2/(2q\lambda^2)]\rho(L_{r,r'}) .$$

Here $\rho(L_{r,r'})$ is the density of open loops $L_{r,r'}$ starting from $r$ and going to $r'$ along a Brownian path

$$(1 - (s/q)) r + (s/q) r' + \lambda \eta(s) ,$$

with $s$ varying from 0 to $q$. Accordingly, $\langle r | D_0^{(1)} | r' \rangle$ can be represented by Mayer-like graphs analogous to those appearing in series (15) for the particle density where now the root loop $L_0$ is replaced by the open loop $L_{r,r'}$. The emergence of ODLRO is related to the behaviour of $\rho(L_{r,r'})$ for large open loops with large values of $q$.

### 5.2 The mean-field Kac limit

Let us introduce a family of two-body potentials $u_\gamma(r)$ defined by the following parametrization

$$u_\gamma(r) = \gamma^3 v(\gamma r)$$

where $\gamma$ is a real positive parameter and $v(r)$ is a given positive, integrable, and spherically symmetric pair potential. When dimensionless parameter $\gamma$ approaches zero, the potential $v(\gamma r)$ becomes weak and long range, whereas the value of the integral

$$\int dr u_\gamma(r) = 4\pi \int_0^\infty dr r^2 v(r) = a > 0$$

remains constant.

In the strict limit $\gamma = 0$, one can expects that particles feel a mean-field constant potential $a\rho$. In other words, the system should then be driven by the so-called mean-field Hamiltonian [35]. That heuristic prediction has been rigorously proved by Pulé and Zagrebnov [36]. More precisely, ODLRO still persists, while the ideal critical density remains unchanged. Furthermore, below $\rho_{0,c}(\beta)$, the density is the unique solution of the self-consistent equation

$$\rho = \rho_0(\beta, \mu - a\rho) = \frac{1}{(2\pi)^3} \int dk \frac{1}{\exp(\beta(\epsilon(k) + a\rho - \mu)) - 1} .$$

which defines the mean-field equation of state $\rho = \rho_{0,\text{eff}}(\beta, \mu)$. For $\rho > \rho_{0,c}(\beta)$, that equation reduces to the simple linear law $\rho = \mu/a$. Notice the simple shift $a\rho$ in the one-body energy spectrum involved in the right hand side of formula (39), in agreement with the mean-field Hamiltonian picture.

Interestingly, the Mayer-like series (15) for $\rho$ provide a self-consistent equation which takes the general form ([37])

$$\rho = F_\gamma(\beta, \mu - a\rho)$$

(40)
where function $F_{\gamma}(\beta, \nu)$ is defined by a series of multiconnected Mayer graphs, which do converge for $\nu$ sufficiently negative, and uniformly with respect to $\gamma$. For $\gamma = 0$, $F_0$ reduces to the sum of tree graphs, which is nothing but the ideal density function $\rho_0(\beta, \nu)$, so relation (40) does coincide with equation (39) as it should.

### 5.3 Contributions of fluctuations beyond the mean-field limit

Now the central question concerns the effects of fluctuations beyond the mean-field limit, and in particular their influence on the possible emergence of ODLRO. The answer requires to study the case of $\gamma$ small but finite. Such a program has been partially accomplished by using the Mayer-like series for the equivalent gas of loops. For finite negative values of $\nu$, $F_{\gamma}(\beta, \nu)$ can be expanded in powers of $\gamma^3$. The first correction to $F_0(\beta, \nu)$ of order $\gamma^3$, is non-trivial, because various resummations of infinite sets of graphs have to be performed in order to properly take into account collective effects arising from the long range nature of the two-body potential $u_\gamma(r)$.

The correction reduces to the sum of contributions from tree and ring graphs \[34\],

\[
\gamma^3 [F_{\text{tree}}^{(1)} + F_{\text{ring}}^{(1)}] \tag{41}
\]

with

\[
F_{\text{tree}}^{(1)} = \frac{\beta v(0)}{2} [f^{(1)}(\nu) - f^{(2)}(\nu)], \tag{42}
\]

\[
F_{\text{ring}}^{(1)} = \frac{\beta^2}{2(2\pi)^3} \int dq \int D(\eta) \exp(-\beta U(L)) \bigg[ f^{(1)}(\nu) f^{(2)}(\nu) \bigg]. \tag{43}
\]

and

\[
f^{(1)}(\nu) = \beta^{-1} \frac{\partial \rho_0}{\partial \nu}(\beta, \nu), \quad f^{(2)}(\nu) = \beta^{-2} \frac{\partial^2 \rho_0}{\partial \nu^2}(\beta, \nu). \tag{44}
\]

Inserting the correction (41) into the self-consistent equation (40), one can compute the $\gamma^3$ corrections to the mean-field equation of state for fixed strictly negative values of $\nu = \mu - \alpha$. Unfortunately, the coefficients of the $\gamma^3$-terms diverges when $\nu \rightarrow 0$, i.e. when one approaches the critical region where a condensate might emerge. Thus, the above perturbative expansion in powers of $\gamma^3$ does not allow one to answer the question of existence of condensation for an arbitrarily small but fixed value of $\gamma$ \[38\].

In order to analyze the behaviours of interest in the critical region for $\gamma$ small but finite, various strategies using Mayer-like series for the equivalent loop gas have been proposed. A first insight should be gained by investigating an approximate version of the self-consistent equation (40), where $F_{\gamma}(\beta, \nu)$ is replaced by the contributions of tree graphs only,

\[
F_{\gamma}(\beta, \nu) = \frac{1}{(2\pi \lambda^2)^{3/2}} \sum_{q=1}^{\infty} \frac{\exp(\beta q \nu)}{q} \int D(\eta) \exp(-\beta U(L)). \tag{45}
\]

The central problem would then be to determine the behaviour, for simultaneously large values of $q$ and small values of $\gamma$, of the average over all loop shapes $\eta$ of the Bolzmann factor associated with the self-energy $U(L)$ of loop $L$ made with $q$ exchanged particles. Another strategy, more ambitious, would be to analyze exactly the possible emergence of ODLRO within formula (35). In that approach, one would have to determine the behaviour of the density of open loops $\rho(L,r,r')$, for both large values of $|r - r'|$ and $q$, and small values of $\gamma$. 


6 Concluding remarks and perspectives

The classical nature of the loop gas allows one to perform exact and useful reorganizations of diagrammatical series with:

- Non-perturbative treatment of interactions
- Incorporation of collective effects
- Systematic account of fluctuations beyond mean-field approaches

Various applications are actually in progress. First, the ionic and molecular internal partition functions for hydrogen are determined within Quantum Monte Carlo numerical computations of their path integral representations. Furthermore, the Screened Cluster Representation will be applied to the hydrogen-helium mixture in order to study the corresponding equation of state at low temperatures and low densities. For the interacting Bose gas, the preliminary results described in Section 5 are promising, and there is some reasonable hope to estimate contributions of large loops, by analogy with the exact results derived for self-repelling closed polymers. However, we notice that there exist alternative methods, like that based on the analysis of the hierarchy equations for the imaginary-time Green functions [39] which might be more efficient.

References

[1] Fetter A L and Walecka J D 1971 Quantum theory of many particle systems (McGraw-Hill, New York)
[2] Feynman R P and Hibbs A R 1965 Quantum mechanics and path integrals (McGraw-Hill, New York)
[3] Ebeling W, Kraeft D and Roepke G 2012 Ann. Phys. 524 311
[4] Seiringer R 2010 Hot topics in cold gases XVIth International Congress on Mathematical Physics (Ed. Pavel Exner, World Scientific, Prague) pp 231-245.
[5] Simon B 1979 Functional Integration and Quantum Physics (Academic, New York)
[6] Schulman L S 1981 Techniques and Applications of Path Integrals (Wiley, New York)
[7] Roepstorff G 1994 Path Integral Approach to Quantum Physics (Springer, Berlin)
[8] Kleinert H 2004 Path Integrals in Quantum Mechanics, Statistics, Polymer Physics and Financial Markets (World Scientific)
[9] Alastuey A, Magro M and Pujol P 2008 Physique et outils mathématiques : méthodes et exemples (EDP Sciences, CNRS Editions)
[10] Wigner E P 1932 Phys. Rev. 40 749
[11] Kirkwood J G 1934 Phys. Rev. 45 116
[12] Landau L D and Lifchitz E M 1958 *Quantum mechanics* vol.5 of the course of Theoretical Physics (Pergamon Press, Oxford)

[13] Paulin S, Alastuey A and Dauxois T 2007 *J. Stat. Phys.* **128** 1391

[14] Ginibre J 1971 *Statistical Mechanics and Quantum Field Theory* edited by C. DeWitt and R. Stora (les Houches, Gordon and Breach)

[15] Cornu F 1996 *Phys. Rev. E* **53** 4562

[16] Martin P A 2003 *Acta Physica Polonica B* **34** 3629

[17] Mayer J E and Montroll E W 1941 *J. Chem. Phys.* **9** 2

[18] Hansen J P and Mc Donald I R 1986 *Theory of simple liquids* (Academic Press, London)

[19] Lieb E and Lebowitz J 1972 *Adv. Math.* **9** 316

[20] Saha M 1920 *Philos. Mag.* **40** 472

[21] Macris N and Martin P A 1990 *J. Stat. Phys.* **60** 619

[22] Fefferman C 1985 *Rev. Math. Iberoamericana* **1** 1

[23] Brillouin L 1930 *Les Statistiques Quantiques et leurs Applications* (Presse Univ. de France, Paris)

[24] Larkin A I 1960 *Zh. exp. teor. Fiz.* **38** 1896

[25] Ballenegger V. 2012 *Ann. Phys.* **524** 103

[26] Ballenegger V, Martin P A and Alastuey A 2002 *J. Stat. Phys.* **108** 169

[27] Alastuey A, Ballenegger V, Cornu F and Martin P A 2003 *J. Stat. Phys.* **113** 455

[28] Rogers F J 1974 *Phys. Rev. A* **10** 2441

[29] Alastuey A, Ballenegger V, Cornu F and Martin P A 2008 *J. Stat. Phys.* **130** 1119

[30] Alastuey A and Ballenegger V 2012 *Cont. Plasma. Phys.* **52** 95

[31] Ebeling W 1967 *Ann. Phys. Leipzig* **19** 104

[32] Alastuey A and Ballenegger V 2012 *Phys. Rev. E* **86** 066402

[33] Ziff R M, Uhlenbeck G E and Kac M 1977 *Physics Reports* **32C** 169

[34] Martin P A and Piasecki J 2005 *Phys. Rev. E* **71** 016109

[35] Lewis J T 1986 *Lecture Notes on Physics* **257** pp 234 (Springer, New York)

[36] Pulé J V and Zagrebnov V A 2004 *J. Phys. A: Math. Gen.* **37** 8929
[37] Martin P A and Piasecki J 2003 Phys. Rev. E 68 016113
[38] Martin P A 2005 International Journal of Theoretical Physics 44 2021
[39] Alastuey A and Piasecki J 2011 Phys. Rev. E 84 041122