Introduction to statistical field theory: from a toy model to a one-component plasma

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Received 29 July 2015
Accepted for publication 4 September 2015
Published 14 October 2015

Abstract
Working with a toy model whose partition function consists of a discrete summation, we introduce the statistical field theory methodology by transforming a partition function via a formal Gaussian integral relation (the Hubbard–Stratonovich transformation). We then consider Gaussian-type approximations, wherein correlational contributions enter as harmonic fluctuations around the saddle-point solution. This work focuses on how to arrive at a self-consistent, non-perturbative approximation without recourse to a standard variational construction based on the Gibbs–Bogolyubov–Feynman inequality that is inapplicable to a complex action. To address this problem, we propose a construction based on selective satisfaction of a set of exact relations generated by considering a dual representation of a partition function, in its original and transformed form.

Keywords: statistical field theory, Gaussian approximation, electrostatics, variational construction

(Some figures may appear in colour only in the online journal)

1. Introduction

The treatment of electrostatics beyond the mean-field in recent years has been dominated by the field theoretical formalism [1–7] based on the Hubbard–Stratonovich transformation of a partition function into a functional integral over an auxiliary field. The saddle-point of an effective Hamiltonian (or an action) within the transformed formulation corresponds to the mean-field solution (given by the Poisson–Boltzmann equation), while the harmonic fluctuations around the saddle-point constitute the random phase approximation treatment of
correlations [8, 9]. Given the charges’ omnipresence in soft-matter systems and the interest in electrostatics by workers of diverse backgrounds (to whom the language and formalism of field theory is neither familiar nor intuitive) it is worthwhile and even desirable to present the field theoretic formalism on a simplified model, where all the steps are transparent, and to point out various challenges that arise within the field-theoretical framework.

In addition to the goal of clarity, the present article focuses on the problem of how to obtain a self-consistent set of equations for a non-perturbative approach, avoiding the standard variational construction based on the Gibbs–Bogolyubov–Feynman (GBF) inequality, inapplicable to a complex action, which turns out to be the case for electrostatic systems. The construction we propose is based on the hierarchy of exact relations extracted from a dual representation of the partition function in different phase-spaces (the physical and the auxiliary phase-space). The two fitting parameters of a Gaussian reference system, the saddle-point and the covariance matrix, are then chosen to satisfy any two relations of the hierarchy. It turns out that the first two relations within the hierarchy are automatically satisfied using the variational construction based on the GBF inequality. Furthermore, our method opens a broader interpretation of the notion of self-consistency. In principle, one can freely chose from the hierarchy any two equations, leading to a different type of self-consistency and, consequently, to a different approximation. Thus for a two parameter Gaussian reference system there is no unique approximation.

The article is organized as follows. In section 2 we consider in detail a one-component toy model for which we develop all the relevant methodology. In section 3 we generalize the model to a multicomponent system, appropriately modifying each step. Finally, in section 4, we consider a realistic partition function for a one-component plasma (a one-component system of charges in an external potential) and derive the relevant equations.

2. The model

A grand-canonical ensemble of a toy model that we choose to work with is given by a discrete summation

$$\Xi = \sum_{N=0}^{\infty} \frac{\lambda^N}{N!} e^{-\varepsilon N^2/2}.$$  \hspace{1cm} (1)

The crucial term in the summation is a pair interaction between particles whose strength is regulated by the dimensionless coupling constant $\varepsilon$. Interactions render the exact analytical solution unavailable. The simple interaction term represents interactions in general, and it yields equations with similar mathematical structure that match well with those obtained for a real system. $\lambda$ in equation (1) represents a generalized fugacity and combines the chemical and any external potential, as well as over-counting of self-interactions in the interaction term, $\lambda = e^{\beta} e^{-\beta U_{ext}} e^{\varepsilon N^2/2}$. Via the application of a formal identity of a Gaussian integral,

$$e^{-\varepsilon N^2/2} = \frac{1}{\sqrt{2\pi \varepsilon}} \int_{-\infty}^{\infty} dx \ e^{-x^2/2\varepsilon} e^{i\alpha N},$$  \hspace{1cm} (2)

the summation is transformed into an integral

$$\Xi = \frac{1}{\sqrt{2\pi \varepsilon}} \int_{-\infty}^{\infty} dx \ e^{-S(x)}.$$  \hspace{1cm} (3)
where the ‘action’

\[ S(x) = \frac{x^2}{2\varepsilon} - \lambda e^{ix}, \]  

(4)

is a complex function, \( S = S_R + iS_I \) with \( S_R = \frac{x^2}{2\varepsilon} - \lambda \cos x \), and \( S_I = -\lambda \sin x \), and the resulting Boltzmann factor is a complex quantity, \( e^{-S} = e^{-S_R} \cos S_I + ie^{-S_R} \sin S_I \), and as such eludes interpretation as a probability measure. Instead a sort of ‘exotic’ probability emerges with imaginary and negative values. The failure of a Boltzmann factor to fulfill the criteria of a probability measure renders the application of a Monte Carlo sampling, used for generating various expectation values [10, 11], no longer feasible. In the literature this is better known as the ‘sign’ problem.

Because the imaginary counterpart of the Boltzmann factor does not contribute to the value of a partition function, which is real, we write

\[ \Xi = \frac{1}{\sqrt{2\pi\varepsilon}} \int_{-\infty}^{\infty} dx \ e^{-S_R(x)} \cos S_I(x). \]  

(5)

In principle, all quantities can be obtained directly from a partition function, without the contribution of imaginary functions. On the other hand, quantities obtained as expectation values may require the imaginary part of the Boltzmann factor. Let us take as an example

\[ -(ix) = \frac{\int_{-\infty}^{\infty} dx \ e^{-S_R(x)} \sin S_I(x)}{\Xi}. \]  

(6)

More generally, any physical expectation value admits a general form

\[ A(x) = A_{\text{even}}(x) - iA_{\text{odd}}(x). \]  

(7)

As a complex integral does not depend on an integration path (contour), and its value depends on endpoints only, we are free to select an integration path \( C \),

\[ \Xi = \frac{1}{\sqrt{2\pi\varepsilon}} \oint_C dz \ e^{-S(z)}, \]  

(8)

in which case \( S \) becomes a function of a complex variable, \( z = x + iy \),

\[ S_R(x, y) = \frac{x^2 - y^2}{2\varepsilon} - \lambda e^{-y} \cos x, \]  

(9)

and

\[ S_I(x, y) = \frac{xy}{\varepsilon} - \lambda e^{-y} \sin x. \]  

(10)

2.1. The saddle-point approximation

A preferred integration contour should have small or no oscillations of a Boltzmann factor. Along such a contour the imaginary part (or phase) of an action should be suppressed, \( S_I(x) \rightarrow 0 \). If a contour satisfies

\[ S_I(z) = 0, \]  

(11)
for every $z \in C$, the partition function can be written as
\[ \Xi = \int_C dz \ e^{-S_I}. \] 
(12)
From equation (10), the constraint $S_I(z) = 0$ leads to the equation
\[ y = \varepsilon \lambda e^{-\frac{\sin x}{x}} \] 
(13)
where the solution is
\[ y(x) = W\left(\frac{\varepsilon \lambda \sin x}{x}\right) \] 
(14)
and where $W(x)$ is the Lambert function. We plot $W(\varepsilon \lambda \sin x/x)$ for $\varepsilon \lambda = 1$ in figure 1. Oscillations quenched in the Boltzmann factor come back in the contour.
A simpler path, with reduced oscillations in the action, is a path parallel to the real axis but displaced along the imaginary axis to include the saddle-point
\[ \frac{\partial S}{\partial z} \bigg|_{z_0} = 0. \]  

The condition of stationarity yields

\[ y_0 = \lambda z e^{-y_0}. \]  

In figure (2) we plot \( \text{Re}[e^{-S}] \) for contours parallel to the real axis and displaced along the imaginary axis by \( y = 0 \) and \( y = y_0 \). The contour that includes the saddle-point displays reduced oscillations.

A physical interpretation of the saddle-point is gained by considering the expectation value \((iz)\)

\[ -\langle iz \rangle = y_0 - \langle i\chi \rangle_{y_0} \]

\[ = y_0 + \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \, x e^{-S(x,y_0)} \sin S_f(x, y_0). \]  

The approximation \(-\langle iz \rangle \approx y_0\), given by the saddle-point approximation, becomes more accurate if the second term is negligible. The saddle-point solution is identified with the mean-field approximation where the action is rewritten in terms of average quantities

\[ S_{\text{mf}} = -\langle i\chi \rangle_{\text{mf}}^2 - \lambda e^{\langle i\chi \rangle_{\text{mf}}}, \]

so that \( \Xi_{\text{mf}} \sim e^{-S_{\text{mf}}} \) and the quantity \( \langle i\chi \rangle_{\text{mf}} \) ought to minimize \( \Xi_{\text{mf}} \), which yields

\[ -\langle i\chi \rangle_{\text{mf}} = \lambda e^{\langle i\chi \rangle_{\text{mf}}}, \]

and recovers the relation in equation (16).

2.2. Gaussian fluctuations

Within a Gaussian approximation a partition function is approximated by expanding \( S \) around the saddle-point up to a harmonic term

\[ S(z) \approx S(z_0) + \frac{1}{2} S''(z_0)(z - z_0)^2. \]  

This generates a Gaussian functional form of the Boltzmann factor,

\[ e^{-S(z)} = e^{-S(z_0)} e^{-(z - z_0)^2/2\Gamma}. \]  

with variance

\[ \Gamma = \frac{1}{S''(z_0)} = \frac{\varepsilon}{1 + \varepsilon \lambda e^{-y_0}}. \]

For the contour intercepting the saddle-point \( y_0 \), the approximation in equation (20) becomes

\[ S(z) \approx S_{\text{R}}(z_0) + \frac{x^2}{2\Gamma}, \]

and the integrand becomes \( e^{-x^2/2\Gamma} \), without oscillations, and the approximate partition function is
\[ \Xi_G = e^{-S(z_0)} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi \varepsilon}} e^{-x^2/2\varepsilon} = e^{-S(z_0)} \left[ \frac{\Gamma}{\sqrt{\varepsilon}} \right]. \]  

(24)

The corresponding grand potential is

\[ \beta \Omega_G = S(z_0) - \log \left[ \frac{\Gamma}{\sqrt{\varepsilon}} \right]. \]  

(25)

Within this approximation \( -\langle iz \rangle = y_0 \), as for the mean-field. (The second term in equation (17) is zero since for the Gaussian approximation the imaginary part is suppressed.) The fluctuations, on the other hand, are given by a variance, \( \langle \xi^2 \rangle = \Gamma \).

A more accurate approximation is possible if one takes an alternative definition for \( \langle iz \rangle \)

\[ -\langle iz \rangle = \varepsilon \lambda \frac{\partial \beta \Omega_G}{\partial \lambda}, \]  

(26)

which yields

\[ -\langle iz \rangle = y_0 - \frac{\varepsilon \lambda}{2} \frac{\partial \log \Gamma}{\partial \lambda} = y_0 - \frac{1}{2} \lambda e^{-y_0} \Gamma^2, \]  

(27)

where the second term approximates the integral term in equation (17) and reduces the value of the mean-field.

### 2.3. Higher-order fluctuations

One wonders how higher-order fluctuations, beyond the harmonic term, contribute to the approximation. Accordingly, we write

\[ S_3(z) = S(z_0) + \frac{(z - z_0)^2}{2\Gamma} + \frac{S''(z_0)}{6} (z - z_0)^3, \]  

(28)

where \( S''(z_0) = i \lambda e^{-y_0} \). For the contour along the real axis and displaced by \( y_0 \) we get

\[ S_3(z) = S_R(z_0) + \frac{x^2}{2\Gamma} + i \left( \frac{\lambda e^{-y_0}}{6} \right) x^3, \]  

(29)

and the resulting Boltzmann factor now has a phase and associated with it oscillations due to the imaginary term. The resulting partition function is

\[ \Xi_3 = e^{-S(z_0)} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi \varepsilon}} e^{-x^2/2\varepsilon} e^{-i\lambda e^{-y_0}x^3/6}. \]  

(30)

If we simplify the expression, using \( e^a \approx 1 + a \), we get

\[ \Xi_3 \approx e^{-S(z_0)} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi \varepsilon}} e^{-x^2/2\varepsilon} \left( 1 - \frac{i}{6} \lambda e^{-y_0} x^3 \right). \]  

(31)
The expectation value $\langle iz \rangle$ becomes

$$\langle iz \rangle = y_0 = \frac{1}{6} \lambda e^{-\lambda z} \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}\varepsilon} x^4 e^{-x^2/2\varepsilon}$$

$$= y_0 = \frac{1}{2} \lambda e^{-\lambda z} \Gamma^2.$$ (32)

The result is exactly the same as that in equation (27).

However, using a complete expression $\Xi_3$ we find a worsening of the results. In figure 3 we plot various fluctuation distributions around the saddle-point. It is clear from the figure that the inclusion of the next term beyond the harmonic term gives rise to unphysical oscillations that deviate from the exact curve.

### 2.4. Non-perturbative approach

In an alternative procedure, a Gaussian approximation is improved non-perturbatively, that is, an action is still expanded up to a harmonic term,

$$S_z(z) \approx \frac{(z - z_0)^2}{2\Gamma}.$$ (33)

but the parameters $z_0$ and $\Gamma$ play the role of a fitting parameter. The standard construction to obtain these parameters is based on a variational procedure based on the GBF inequality

$$\Xi = \Xi_z \langle e^{-\Delta S} \rangle \geq \Xi_\varepsilon e^{-\langle \Delta S \rangle},$$ (34)

where

$$\langle \ldots \rangle_\varepsilon = \frac{\int dx \, e^{-S_z(x)} \langle \ldots \rangle}{\int dx \, e^{-S_z(x)}},$$ (35)

and

$$\Xi_\varepsilon = \int dx \, e^{-S_z(x)},$$ (36)

and $\Delta S = S - S_z$. Thus, the variational procedure provides an upper bound for a free energy and the sought parameters are obtained from minimization. The inequality in equation (34) is obtained from a more basic inequality, $e^a \geq 1 + a$, where $a$ is a real number. If $\Delta S$ were real, we could write

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**Figure 3.** A Boltzmann factor, $\text{Re}[e^{-\xi}]$, plotted along the real axis displaced by $y_0$ along the imaginary direction. The system parameters are $\lambda = 1$ and $\varepsilon = 10$. 

...
\[
\langle e^{-\Delta S} \rangle = e^{-\langle \Delta S \rangle} \langle e^{-(\Delta S - \langle \Delta S \rangle)} \rangle \geq e^{-\langle \Delta S \rangle},
\]

however, the problem is that \( \Delta S \) of the toy model is complex and the above inequality does not hold. One consequence is that the minimization principle is replaced by the stationarity principle \([12–14]\), where the true value is not approached from above but in oscillatory fashion, either from above and below, violating the GBF inequality.

To get around this difficulty we propose a different approach, wherein self-consistency is enforced by making sure that some known identities are satisfied. To derive these identities for the present toy model, we recall two alternative formulations of the partition function,

\[
\Xi = \sum_{N=0}^{\infty} \frac{\lambda^N}{N!} e^{-\xi(N-\varrho)^2}
= \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}\epsilon} e^{-S(x) - i\varrho x},
\]

where we have introduced a source term, \( S \rightarrow S + i\varrho x \), which in a final expression is taken to zero. From the original formulation of the partition function we know

\[
\lambda \frac{\partial \log \Xi}{\partial \lambda} = \frac{1}{\epsilon} \frac{\partial \log \Xi}{\partial \varrho} + \varrho.
\]  

When applied to the field theoretical formulation this relation yields (in the limit \( \varrho \rightarrow 0 \))

\[
\epsilon \lambda \langle e^{iz} \rangle = -\langle iz \rangle.
\]  

One can generate an arbitrary number of additional identities by repeated application of derivatives \( \frac{\partial}{\partial \varrho} \) and \( \frac{\partial}{\partial x} \) to both sides of equation (38). The first three identities are

\[
-\langle iz \rangle = \epsilon \lambda \langle e^{iz} \rangle \\
-\epsilon \lambda \left( \langle \delta e^{iz} \rangle (i\delta z) \right) = \epsilon - \langle \delta z^2 \rangle \\
-\epsilon \lambda \left( \langle \delta e^{iz} \rangle (i\delta z) \right) = \epsilon^2 \lambda \langle e^{iz} \rangle + \epsilon^2 \lambda^2 \left( \langle \delta e^{iz} \rangle \right)^2
\]  

where \( \delta z = z - \langle z \rangle \) and \( \delta e^{isz} = e^{iz} - \langle e^{iz} \rangle \). The second and third equation provide a relation between different second-order fluctuations. By continually applying the derivatives, one obtains equations for the third- and higher-order fluctuations. We are not interested in these higher-order relations.

Within the mean-field approximation the first identity yields

\[
y_0 = \epsilon \lambda e^{-\gamma_0},
\]

where the distribution over the auxiliary phase-space is a delta function at the saddle-point. The absence of fluctuations trivially satisfies the second and third equations as \( 0 = 0 \). Moving on to a Gaussian distribution, we start by listing relevant expectation values
The expectation values $-\langle iz \rangle$ and $\langle \delta z^2 \rangle$ as a function of the coupling constant $\varepsilon$ for $\lambda = 2$. These expectation values give an average number of particle and their fluctuations: $-\langle iz \rangle = \varepsilon \langle N \rangle$ and $\varepsilon - \langle \delta z^2 \rangle = \varepsilon^2 \langle \delta N^2 \rangle$.

\[
\begin{align*}
\langle iz \rangle_g &= -y_0 \\
\langle e^{iz} \rangle_g &= \varepsilon^{-\frac{3}{2}}e^{-\frac{\Gamma}{2}} \\
\langle \delta z^2 \rangle_g &= \Gamma \\
\left(\langle \delta iz \rangle\langle \delta e^{iz} \rangle\right)_g &= -\Gamma e^{-\frac{3}{2}}e^{-\frac{\Gamma}{2}} \\
\left(\langle \delta e^{iz} \rangle^2\right)_g &= e^{-\frac{3}{2}}e^{-\frac{\Gamma}{2}}(e^{-\Gamma} - 1),
\end{align*}
\]

and the three equalities in equation (40) become

\[
\begin{align*}
y_0 &= \varepsilon \lambda e^{-\frac{3}{2}}e^{-\frac{\Gamma}{2}}, \\
\Gamma \left(\varepsilon \lambda e^{-\frac{3}{2}}e^{-\frac{\Gamma}{2}}\right) &= \varepsilon - \Gamma \\
\left(1 - e^{-\Gamma}\right)\left(\varepsilon \lambda e^{-\frac{3}{2}}e^{-\frac{\Gamma}{2}}\right) &= \varepsilon - \Gamma
\end{align*}
\]

The perturbative approach of section 2.2 does not produce self-consistent relations. Self-consistency has to be enforced ‘by hand’ by choosing appropriate values for $y_0$ and $\Gamma$. For a two parameter model, one equation in equation (43) is superfluous. Closer examination reveals that the second equation is a linear version of the third.

Incidentally, the variational construction based on the GBF automatically satisfies the first two equations. By making this identification, we provide justification and a different interpretation of the GBF variational construction. Moreover, with other identities available, one can choose a different set of identities that yield a different self-consistent non-variational scheme.
In figure 4 we compare different schemes by plotting various expectation values. Self-consistent schemes are more accurate for a large coupling constant. Furthermore, the approach based on equations (1) and (3) (lines 1 and 3 in equation (43)) is more accurate than that based on equations (1) and (2) (that is equivalent to the GBF variational construction). The model and the test, however, are too simple to generalize the conclusion to all cases. In the subsequent section we consider a multiple species model, as a way to introduce complexity. However, we first discuss some aspects of the present simple model.

One possible question is: is a Gaussian distribution the best representation of a true distribution? Practical concerns demand that a distribution yields analytical results. A Gaussian distribution satisfies this requirement, and so it is a convenient tool. But the simplicity of the present model allows us to explore other distributions, such as a stretched Gaussian distribution:

$$e^{-|z-\gamma|^2/2\Gamma^2}$$

where $\gamma = 0.5$ corresponds to an exponential, $\gamma \to \infty$ to a square, and $\gamma = 1$ to a Gaussian distribution. Below we provide relevant expectation values for an exponential distribution (compare with equation (42) for the Gaussian case)

$$\langle iz \rangle_{\text{exp}} = -\gamma_0$$
$$\langle e^{iz} \rangle_{\text{exp}} = \frac{e^{-\gamma_0}}{1 + 2\Gamma}$$
$$\langle \delta z^2 \rangle_{\text{exp}} = 4\Gamma$$
$$\langle (\delta iz)(\delta e^{iz}) \rangle_{\text{exp}} = -\frac{4\Gamma e^{-\gamma_0}}{(1 + 2\Gamma)^2}$$
$$\langle (\delta e^{iz})^2 \rangle_{\text{exp}} = \frac{e^{-2\gamma_0}}{1 + 8\Gamma} - \frac{e^{-2\gamma_0}}{(1 + 2\Gamma)^2}.$$  

Plugging these expressions into corresponding equations in equation (40), we may obtain $\gamma_0$ and $\Gamma$. The results for the exponential and square distributions are shown in figure 5 (labeled as ‘var12a’ and ‘var12b’, respectively). The new curves are less accurate than those for a Gaussian distribution (‘var12’ or ‘var13’). On the other hand, their results are not inferior to a perturbative Gaussian approach. This seems to show that self-consistency is an important element of an approximation.

Another question is, is not a three parameter model more natural, as there are three available equations? Even if disregarding complexity, we found no improvement for a number of different three parameter models. This seems to imply that a three parameter model requires the identity involving fluctuations of a third-order
\[
\lambda \left\langle (i\hbar \partial_z)^2 \delta \psi_i \right\rangle = -\frac{1}{\varepsilon} \left\langle (i\hbar \partial_z)^3 \right\rangle \\
- \left\langle (i\hbar \partial_z) \delta \psi_i \right\rangle - \lambda \left\langle (i\hbar \partial_z)(\delta \psi)^2 \right\rangle = \frac{1}{\varepsilon} \left\langle (i\hbar \partial_z)^2 \delta \psi_i \right\rangle \\
2 \left\langle (\delta \psi_i)^3 \right\rangle + \lambda \left\langle (\delta \psi_i)^3 \right\rangle = -\frac{1}{\varepsilon} \left\langle (i\hbar \partial_z)(\delta \psi)^2 \right\rangle \\
\ldots
\]

(45)

This, however, would markedly complicate the calculations, and we stop here.

3. Multiple species

In this section we consider a partition function for multiple species

\[
\Xi = \sum_{\{N_i\}} \prod_{i=1}^{M} \left( \frac{\lambda N_i}{N_i!} \right) e^{-\frac{1}{2} \sum_{i,j} \varepsilon_{ij} N_i N_j} \\
= \sum_{\{N_i\}} \prod_{i=1}^{M} \left( \frac{\lambda N_i}{N_i!} \right) e^{-\frac{1}{2}(N^T \varepsilon N)},
\]

(46)

where \(M\) is the number of different species, and interactions between species are regulated by elements of the \(M \times M\) connectivity matrix, \(\varepsilon_{ij}\). The number of particles of each species spans the values \(N_i = 0, 1, 2, \ldots, \infty\).

Using a formal identity of a Gaussian integral

\[
e^{-\frac{1}{2}(N^T \varepsilon N)} = \int \frac{dx}{\sqrt{\det 2\pi \varepsilon}} e^{-\frac{1}{2}(x^T \varepsilon^{-1} x)} e^{N^T x},
\]

(47)

the partition function is rewritten as

\[
\Xi = \int \frac{dx}{\sqrt{\det 2\pi \varepsilon}} e^{-S(x)},
\]

(48)

where the action is

\[
S(x) = \frac{x^T \varepsilon^{-1} x}{2} - \sum_{i=1}^{M} \lambda_i e^{ib_i}.
\]

(49)

\(\varepsilon^{-1}\) is the inverse of \(\varepsilon\), \(x \equiv \{x_1, x_2, \ldots, x_M\}\) is a vector, and

\[
\int dx = \int_{-\infty}^{\infty} \prod_{i=1}^{M} dx_i.
\]

(50)

3.1. The saddle-point

As for the single species model, we generalize the real vector \(x\) to its complex counterpart, \(z = x + iy\). The saddle-point now corresponds to a vector \(z_0\) at which \(S\) is stationary

\[
\frac{\partial S(z)}{\partial z} \bigg|_{z = z_0} = 0,
\]

(51)
and, as for the case $M = 1$, a solution is strictly imaginary, $z_0 = i\eta_0$, where

$$y_i = \sum_{i=1}^{N} E_i \lambda_i e^{-\gamma_i}.$$  \hspace{1cm} (52)

To simplify the nomenclature, we use $y_i$ to indicate the saddle-point value, $y_i \equiv \eta_{0,i}$.

### 3.2. Gaussian fluctuations

By expanding the action up to a harmonic term, we capture fluctuations

$$S(z) \approx S(z_0) + \frac{1}{2} \sum_{i,j} \frac{\partial^2 S(z_0)}{\partial z_i \partial z_j} (z_i - z_{0,i})(z_j - z_{0,j}),$$  \hspace{1cm} (53)

and the partition function becomes

$$Z = \frac{e^{-S(z_0)}}{\sqrt{\det 2\pi E}} \int_c dz \ e^{-\frac{1}{2}(z-z_0)^T \Gamma^{-1} (z-z_0)} = e^{-S(z_0)} \sqrt{\det \Gamma E^{-1}},$$  \hspace{1cm} (54)

where

$$\Gamma^{-1}_{ij} = \frac{\partial^2 S(z_0)}{\partial z_i \partial z_j} = E^{-1}_{ij} + \lambda_i e^{iz_0} \delta_{ij}$$  \hspace{1cm} (55)

is a covariance matrix.

Introducing the source term into action, $S \rightarrow S + i \varphi \cdot z$, and using the definition $-\langle i z_i \rangle = \frac{\partial \ln Z}{\partial \varphi_i}$, we get

$$-\langle i z_i \rangle = \frac{\partial S(z_0)}{\partial \varphi_i} - \frac{\partial \ln \sqrt{\det \Gamma}}{\partial \varphi_i} = \gamma_i = \sum_{j=1}^{M} \frac{\partial \ln \sqrt{\det \Gamma}}{\partial y_j} \frac{\partial y_j}{\partial \varphi_i} = \gamma_i = \frac{1}{2} \sum_{j=1}^{M} \lambda_j e^{-\gamma_j} \Gamma_{ij} y_j,$$  \hspace{1cm} (56)

in the limit $\varphi \rightarrow 0$. Compare with equation (27) for $M = 1$.

### 3.3. Non-perturbative approach

We construct a non-perturbative approximation based on a Gaussian reference system

$$Z_0 = \int_c dz \ e^{-\frac{1}{2}(z-z_0)^T \Gamma^{-1} (z-z_0)},$$  \hspace{1cm} (57)

where $z_0$ and $\Gamma$ play the role of the variational parameters. As for the case $M = 1$, these parameters are obtained by enforcing self-consistency. To obtain relevant identities, we invoke two alternative formulations of the partition function:
\[ \Xi = \sum_{|\lambda|_1=1}^{M} \prod_{j=1}^{N} \left( \frac{\lambda_j}{\bar{N}_j!} \right) e^{-\frac{1}{2} N^{-\phi} \vec{E}(N^{-\phi})} \]
\[ = \int \frac{dz}{\sqrt{\text{det} 2\pi E}} \, e^{-z(z)^{\frac{1}{2}} \, \phi \, z}. \quad (58) \]

An analogous relation to that in equation (38) is
\[ \lambda_i \frac{\partial \log \Xi}{\partial \lambda_i} = \sum_{j=1}^{M} E^{-1}_{ij} \frac{\partial \log \Xi}{\partial \phi_j} + \phi_i. \quad (59) \]

Other identities follow by repeated application of \( \frac{\partial}{\partial \phi_j} \) or \( \frac{\partial}{\partial \lambda_i} \). The first three identities are
\[ \lambda_i \langle e^{\phi_j} \rangle = -\sum_{j=1}^{M} E^{-1}_{ij} \langle \psi_j \rangle \]
\[ -\lambda_i \langle i \hbar \delta_{ij} \phi e^{\phi_j} \rangle = \delta_{ij} - \sum_{k=1}^{M} E^{-1}_{ik} \langle \delta_{jk} \delta_{ij} \rangle \]
\[ \langle e^{\phi_j} \rangle \delta_{ij} + \lambda_i \langle \delta e^{\phi_j} \phi e^{\phi_j} \rangle = -\sum_{k=1}^{M} E^{-1}_{ik} \langle i \hbar \delta_{jk} \delta e^{\phi_j} \rangle \]
\[ ... \quad (60) \]

and the relevant expectation values for a Gaussian reference system are
\[ \langle \psi_j \rangle_g = -y_j \]
\[ \langle e^{\phi_j} \rangle_g = e^{-y_j} e^{-\Gamma_j/2} \]
\[ \langle \delta_{jk} \delta_{ij} \rangle_g = \Gamma_{ij} \]
\[ \langle i \hbar \delta_{jk} \phi e^{\phi_j} \rangle_g = -e^{-y_j} e^{-\Gamma_j/2} \Gamma_{ij} \]
\[ \langle e^{\phi_j} \delta e^{\phi_j} \rangle_g = \left( e^{-y_j} e^{-\gamma_j/2} \right) \left( e^{-y_j} - 1 \right). \quad (61) \]

Substituting these into the equations in equation (60) we get
\[ \sum_{j=1}^{M} E^{-1}_{ij} \psi_j = \lambda_i e^{-y_j} e^{-\Gamma_j/2} \]
\[ \sum_{k=1}^{M} E^{-1}_{ik} \Gamma_{kj} + \lambda_i e^{-y_j} e^{-\Gamma_j/2} \Gamma_{ij} = \delta_{ij} \]
\[ \sum_{k=1}^{M} E^{-1}_{ik} \Gamma_{kj} + \lambda_i e^{-y_j} e^{-\gamma_j/2} \left( 1 - e^{-\Gamma_j} \right) = \delta_{ij} \]
\[ ... \quad (62) \]

where the second equation is the linear version of the third equation.

We consider a two component system with the following simple interaction matrix
\[ \mathcal{E} = \epsilon \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}. \quad (63) \]

(Note that the matrix \( \mathcal{E} \) is singular, but the relevant equations can be set up in terms of a nonsingular matrix \( \mathcal{E}^{-1} \).) Particles of the same species repel and particles of different species attract each other. The average total number of particles is fixed, \( \langle N_1 + N_2 \rangle = N_T \).
Furthermore, we set \( \lambda_i = \lambda \). With these constraints \( y_i = 0 \), and it only remains to obtain the
matrix $\Gamma$. The variational construction based on equations (1) and (2) in equation (62) has an analytical solution for $\Gamma$,

$$\Gamma = \frac{\varepsilon}{1 + 2\varepsilon N} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix},$$

(64)

where the elements of the matrix $\Gamma$ are related to fluctuations in a particle number via

$$\langle \delta N_i \delta N_j \rangle = N \delta_{ij} - N^2 \Gamma_{ij}.$$  

(65)

The variational construction based on equations (1) and (3) does not admit an analytical solution and data points are obtained numerically.

Figure 6 plots different results for $\langle \delta N_i \delta N_j \rangle$. The upper curves represent correlation between the same and the lower curves between opposite species. Their conjoining at large $\varepsilon$ implies that different species form permanent pairs. The onset of pair formation is captured by both self-consistent schemes, but permanent pairs form only in the limit $\varepsilon \to \infty$, while the exact results indicate that pairing sets in much faster and is completed around $\varepsilon = 10$. The results for different variational schemes are not drastically different, but the gap between curves is smaller for the scheme based on equations (1) and (2).

3.4. Digression to the liquid-state theory

Given the present simple model, we make a digression into the liquid-state theories based on the Ornstein–Zernike equation [13]. The relevant quantity in the liquid-state formalism is the correlation function, $h_{ij}$, for the present system defined as

$$h_{ij} = \frac{\langle \delta N_i \delta N_j \rangle}{\langle N_i \rangle \langle N_j \rangle} - \delta_{ij}.$$  

(66)

The Kronecker delta function subtracts interactions of a particle with itself present in the first term. The Ornstein–Zernike equation relates $h_{ij}$ to the direct correlation function $c_{ij}$:

$$h_{ij} = c_{ij} + \sum_{k=1}^{M} \langle N_i \rangle h_{jk} c_{ki}.$$  

(67)

Figure 6. The particle number fluctuations as a function of $\varepsilon$. The total number of particles is kept fixed at $N_T = 2$. The upper curves represent the same-species and the lower curve the cross-species fluctuations.
Since \( c_{ij} \) is also unknown, a closure is required, which can be obtained from the exact relation

\[
h_{ij} = e^{-\varepsilon_c + h_{ij} - c_{ij}} - 1,
\]

which introduces the bridge function \( B_{ij} \) [15]. Within the hypernetted chain approximation (HNC) \( B_{ij} = 0 \). The present system is homogeneous, \( \langle N \rangle = N_f / 2 \), and no third closure is required for \( \langle N \rangle \). The two coupled equations to be solved are

\[
\begin{align*}
h_{ij} &= c_{ij} + N_f \frac{M}{M} \sum_{k=1}^{M} h_{jk} e_{ki}, \\
h_{ij} &= e^{-\varepsilon_c + h_{ij} - c_{ij}} - 1,
\end{align*}
\]

and the results are shown in figure 6. Although the gap between different curves closes only in the limit \( \varepsilon \to \infty \), precluding formation of permanent pairs, their absolute values are closer to the exact value than the Gaussian approximation.

4. One-component plasma

In this final section we consider a real system with a general partition function

\[
\Xi = \sum_{N=0}^{\infty} \frac{\lambda^N}{N!} \int \cdots \int \cd N e^{-\mathcal{H}_f},
\]

where the dimensionless Hamiltonian is

\[
\mathcal{H}_f = \frac{1}{2} \int \cd \int \cd \hat{\rho}(\mathbf{r}) \mathcal{E}(\mathbf{r}, \mathbf{r}') \hat{\rho}(\mathbf{r}') + \int \cd \hat{\rho}(\mathbf{r}) \beta U(\mathbf{r}),
\]

\[
\hat{\rho}(\mathbf{r}) = \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}'),
\]

is the density operator, \( U(\mathbf{r}) \) is an external potential, \( \mathcal{E}(\mathbf{r}, \mathbf{r}') \) denotes inter-particle interactions, which for Coulomb particles with charge \( q \) and inside a medium with dielectric constant \( \varepsilon \) are

\[
\mathcal{E}(\mathbf{r}, \mathbf{r}') = \frac{\beta q^2}{4\pi \varepsilon \lvert \mathbf{r} - \mathbf{r}' \rvert},
\]

and

\[
\lambda = \frac{e^{\beta U(\mathbf{r}, \mathbf{r}')/2}}{N^3}
\]

is the normalized fugacity that subtracts self-interactions in equation (71).

Using a formal identity analogous to that in equation (47),

\[
\int \frac{D\phi}{\sqrt{\det 2\pi \mathcal{E}}} e^{-\frac{1}{2} \int \cd \cd \phi(\mathbf{r}) \phi(\mathbf{r}) \mathcal{E}(\mathbf{r}, \mathbf{r}') \phi(\mathbf{r}') \phi(\mathbf{r}')} = e^{-\frac{1}{2} \int \cd \cd \hat{\rho}(\mathbf{r}) \mathcal{E}(\mathbf{r}, \mathbf{r}') \phi(\mathbf{r}')},
\]

but where the integral is a functional integral over a fluctuating field \( \phi(\mathbf{r}) \), and the determinant is the functional determinant, leads to a field-theoretical formulation of a partition function,

\[
\Xi = \int D\phi \ e^{-S[\phi]},
\]
where the action is
\[ S[\varphi] = \frac{1}{2} \int \! \! d\mathbf{r} \int \! \! d\mathbf{r}' \varphi(\mathbf{r}) \mathcal{E}^{-1}(\mathbf{r}, \mathbf{r}') \varphi(\mathbf{r}') - \int \! \! d\mathbf{r} \lambda e^{-\beta U(\mathbf{r})} e^{i\varphi(\mathbf{r})}, \] (77)
and
\[ \mathcal{E}^{-1}(\mathbf{r}, \mathbf{r}') = -\frac{e}{\beta q^2} \nabla^2 \delta(\mathbf{r} - \mathbf{r}') \] (78)
is the inverse of a Coulomb interaction \( \mathcal{E}(\mathbf{r}, \mathbf{r}') \).

4.1. The saddle-point approximation

As before, the auxiliary field is generalized to a complex function, \( \Phi = \phi + i\psi \). The saddle-point,
\[ \left. \frac{\delta S[\Phi]}{\delta \Phi(\mathbf{r})} \right|_{\Phi = \Phi_0} = 0, \] (79)
yields the following equation
\[ \int \! \! d\mathbf{r}' \mathcal{E}^{-1}(\mathbf{r}, \mathbf{r}') \Phi_0(\mathbf{r}') = i\lambda e^{-\beta U(\mathbf{r})} e^{i\Phi_0(\mathbf{r})}, \] (80)
where the solution is strictly imaginary, \( \Phi_0 = i\psi_0 \), and by using equation (78) we get
\[ \nabla^2 \psi_0(\mathbf{r}) = -\lambda \left( \frac{\beta q^2}{e} \right) e^{-\beta U(\mathbf{r})} e^{-\beta \psi_0(\mathbf{r})}, \] (81)
where \( \psi_0 \) is the reduced electrostatic potential related to a true electrostatic potential \( \Phi \) as \( \psi_0 = \beta q\Phi \). The resulting equation is the Poisson–Boltzmann equation for a one-component plasma in an external potential \( U(\mathbf{r}) \).

4.2. Non-perturbative approach

As for the toy model, we formulate a non-perturbative approach through enforcing self-consistency. We first generate the relevant identities between expectation values. By introducing a source term,
\[ S[\phi] \rightarrow S[\phi] + i \int \! \! d\mathbf{r} \varphi(\mathbf{r}) \phi(\mathbf{r}), \] (82)
the Hamiltonian becomes
\[ \mathcal{H}_N = \frac{1}{2} \int \! \! d\mathbf{r} \int \! \! d\mathbf{r}'[\hat{\rho}(\mathbf{r}) - \rho(\mathbf{r})] C(\mathbf{r}, \mathbf{r}')[\hat{\rho}(\mathbf{r}') - \rho(\mathbf{r}')] + \int \! \! d\mathbf{r} \hat{\rho}(\mathbf{r}) \beta U(\mathbf{r}). \] (83)

Identities analogous to equation (59) are generated from the relation
\[ \frac{1}{\beta} \frac{\delta \log \Xi}{\delta U(\mathbf{r})} = \left( \frac{e}{q^2 \beta} \right) \nabla^2 \left( \frac{\delta \log \Xi}{\delta \rho(\mathbf{r})} \right) - \rho(\mathbf{r}). \] (84)
The first three identities, after setting $U(r)$ and $\varrho(r)$ to zero, are

$$
\nabla^2 \langle i\tilde{\Phi}(r) \rangle = \lambda \left( \frac{\beta q^2}{\epsilon} \right) \langle e^{i\Phi(r)} \rangle \left( \frac{\epsilon}{q^2} \right) \nabla^2 \left\langle \delta \Phi(r) \delta \Phi(r') \right\rangle + \lambda \left\langle i\delta \Phi(r) \delta \Phi(r') \right\rangle

= -\delta \left( r - r' \right) \delta \left( r - r' \right) \langle e^{i\Phi(r)} \rangle + \lambda \left\langle \delta e^{i\Phi(r)} \delta e^{i\Phi(r')} \right\rangle

= \left( \frac{\epsilon}{q^2} \right) \nabla^2 \left\langle i\delta \Phi(r) \delta e^{i\Phi(r')} \right\rangle

\ldots

$$

(85)

where

$$
i\delta \Phi(r) = i\Phi(r) - \langle i\Phi(r) \rangle,
$$

and

$$
\delta e^{i\Phi(r)} = e^{i\Phi(r)} - \langle e^{i\Phi(r)} \rangle.
$$

(86)

(87)

For a Gaussian reference partition function

$$
\Xi_r = \int \mathcal{D} \Phi \ e^{-\frac{1}{2} \langle \Phi(r) - \Phi_0(r) \rangle^2 / \Gamma(r, r') \left( \Phi(r') - \Phi_0(r') \right)^2 / \beta}.
$$

(88)

The relevant expectation values are

$$
\langle i\Phi(r) \rangle_r = -\psi_0(r),
$$

$$
\langle e^{i\Phi(r)} \rangle_r = e^{-\psi_0(r)} e^{-\Gamma(r, r') / 2},
$$

$$
\left\langle \delta \Phi(r) \delta \Phi(r') \right\rangle_r = \Gamma(r, r'),
$$

$$
\left\langle i\delta \Phi(r) \delta e^{i\Phi(r')} \right\rangle_r = -e^{-\psi_0(r)} e^{-\Gamma(r, r') / 2} \Gamma(r, r'),
$$

$$
\left\langle \delta e^{i\Phi(r)} \delta e^{i\Phi(r')} \right\rangle_r = \left( e^{-\psi_0(r)} e^{-\Gamma(r, r') / 2} \right) \left( e^{-\psi_0(r') e^{-\Gamma(r, r') / 2}} \right) \left( e^{-\Gamma(r, r') - 1} \right).
$$

(89)

The three relations in equation (85) become

$$
\nabla^2 \psi_0(r) = -\frac{\beta q^2}{\epsilon} e^{-\psi_0(r)} e^{-\Gamma(r, r') / 2},
$$

$$
\nabla^2 \Gamma(r, r') = \lambda \frac{\beta q^2}{\epsilon} e^{-\psi_0(r)} e^{-\Gamma(r, r') / 2} \Gamma(r, r') - \left( \frac{\beta q^2}{\epsilon} \right) \delta (r - r'),
$$

$$
\nabla^2 \Gamma(r, r') = \lambda \frac{\beta q^2}{\epsilon} e^{-\psi_0(r)} e^{-\Gamma(r, r') / 2} \left( 1 - e^{-\Gamma(r, r')} \right) - \left( \frac{\beta q^2}{\epsilon} \right) \delta (r - r').
$$

(90)

5. Conclusion

Using a very simple model we review the basic steps for deriving the field-theoretical formulation of statistical mechanics. To avoid using the GBF inequality (inapplicable for complex actions) for constructing non-perturbative approximation, we explore alternative schemes. Within the scheme proposed in this work, we arrive at self-consistency by satisfying of a number of exact identities. The GBF variational construction automatically satisfies the first two relations in the hierarchy. On the other hand choosing a different set of identities within the hierarchy will lead to a different non-perturbative approximation.
Acknowledgments

This work was supported by the Agence Nationale de la Recherche via the project FSCF.

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