Dual free energies in Poisson-Boltzmann theory

R. Blossey\textsuperscript{1} and A.C. Maggs\textsuperscript{2}

\textsuperscript{1} University of Lille 1, Unité de Glycobiologie Structurale et Fonctionnelle, CNRS UMR8576, 59000 Lille, France
\textsuperscript{2} CNRS UMR7083, ESPCI Paris, PSL Research University, 10 rue Vauquelin, Paris, 75005, France

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Abstract – Poisson-Boltzmann theory is the underpinning to essentially all soft matter and biophysics problems involving point-like charges of low valencies, in the form of counter-ions or dissolved salts. Going beyond the mean-field approach typically requires the application of loop expansions around a mean-field solution for the electrostatic potential $\phi(r)$, or sophisticated variational approaches. Recently, Poisson-Boltzmann theory has been recast, via a suitably defined Legendre transform, as a theory involving the dielectric displacement field $D(r)$. In this paper we consider the path integral formulation of the dual theory. Exploiting the transformation between $\phi$ and $D$, we formulate a fluctuation-corrected dual theory in terms of the displacement field and provide a strategy to compute free energies beyond the leading order.

Introduction. – The description of electrolytes in soft-matter physics is commonly based on the Poisson-Boltzmann equation, which is a mean-field theory for the electrostatic potential $\phi(r)$ \cite{1}. Formally, this theory is derived from the partition function of a Coulomb system by performing a Hubbard-Stratonovich transformation to an (imaginary) fluctuating field $\phi(r)$, later identified with the electrostatic potential \cite{2,3}. This approach is valid in the so-called weak fluctuation regime, in which the saddle-point of the action yields the standard Poisson-Boltzmann equation, which can be systematically improved by a loop expansion \cite{3,4}. An alternative approach to go beyond mean-field theory is to invoke a variational approach \cite{5,6}.

A difficulty with these approaches is that the action of the path integral is complex, and hence not a convex functional. In particular, when the electrostatic degrees of freedom of a system are coupled to other degrees, the minimization of the functional becomes a complicated operation, as the extrema result from a combination of minima in the non-electrostatic degrees of freedom and maxima in the electrostatic degrees. This complicates many numerical studies of biophysical molecules in which the solvent is described by Poisson-Boltzmann theory, and also has repercussions for the validity limits of theories including fluctuation effects beyond Poisson-Boltzmann theory \cite{7}.

This technical problem is circumvented by a reformulation of the theory in terms of purely convex functionals, which is achieved by the means of a Legendre transform, with the complex field $\phi(r)$ being systematically replaced by the dielectric displacement field $D(r)$ \cite{8}. Expressed in terms of the field $D(r)$, the resulting theory yields a convex functional so that standard minimization techniques can be applied, and loop corrections or variational approaches be defined as for the original Poisson-Boltzmann theory. In fact, the one-loop correction in the dual theory has been shown to yield the same fluctuation spectrum as obtained within the usual formulation of Poisson-Boltzmann theory \cite{9}. This approach, however, working from mean-field theory, does not help in constructing a systematic improvement in the dual formulation of the theory.

In this paper we revisit the duality approach from a path integral perspective. We show that the dual theory can be reformulated by introducing transformations of the path integral using the Poisson summation formula which gives us access to both a saddle-point like limit, but equally allows us to explicitly calculate the corrections beyond the saddle-point which arise from the discrete nature of the charges. In the saddle-point limit, we derive a fluctuation-corrected functional expressed in terms of the dielectric displacement field.

The paper is organized as follows. In the second section, we recall the formulation of the duality transform. In section three we derive a prescription to formulate the path integral of the dual theory. In section four we discuss the solution of the first-order fluctuation-corrected theory by comparing it to the solution of the Poisson-Boltzmann equation. We conclude in section five.
Duality in field theory. — We first recall the notion of duality employed in the context of the Poisson-Boltzmann theory. The Legendre transform that carries the theory over into its dual theory has been defined in [8] on the level of the mean-field functional while we here are interested in the full path integral. For this more general theory it is a crucial feature for the correctness of the path integral representation that the duality transformation \( \phi \to D \) has been carried out solely via the introduction of delta functions. Only this approach guarantees the identity of the fluctuation spectra of the dual theory as discussed in detail by Fradkin and Tseytlin in a general field theory setting [10]. By contrast, theories derived from reparametrizations are called pseudo-dual theories [10] for which this property in general does not hold. This is the case for the reparametrizations of the Poisson-Boltzmann theory recently developed in [11][12] with the aim of defining convex functionals for the electrostatic potential. These theories fail to produce the correct fluctuation spectra as was shown explicitly in the calculation of the one-loop correction in [9].

We note, too, a renewed interest in dual lattice gauge theories, which have similar technical advantages of positivity and convexity which are an active research topic [13].

We start with the usual expression of the partition function for a set of charged particles interacting through the Coulomb interaction, described through a fluctuating potential field \( \phi \):

\[
Z = \int D[\phi] e^{-\beta \int d^3 r h(\phi)}
\]  

(1)

with

\[
h(\phi) = \varepsilon \left( \nabla \phi \right)^2 + g(i\phi) - i\varrho_f \phi,
\]

(2)

where \( g(i\phi) \) is the grand potential [14] (related to the fluid pressure) of the ions in solution, while \( \varrho_f \) is the density of fixed charges, which are typically confined to a small part of the system, for instance a charged wall. Introducing the electric field \( E \) via a delta function (and being free with non-essential normalisation factors)

\[
Z = \int D[\phi] D[E] e^{-\beta \int d^3 r h(\phi)} \delta(E + \nabla \phi)
\]  

(3)

yields after Fourier representation of the delta function with multiplier \( D \)

\[
Z = \int D[\phi] D[E] D[D] e^{-\beta \int d^3 r h(\phi, E, D)}
\]

(4)

with

\[
h(\phi, E, D) = \varepsilon \frac{E^2}{2} + g(i\phi) - i D \cdot (\nabla \phi + E) - i\varrho_f \phi
\]

(5)

from integration by parts and imposing the boundary conditions that

\[
\int \phi D \cdot dS = 0
\]

(6)

so that one has to require either \( \phi = 0 \) or \( D_n = 0 \) at infinity. Performing the integration over the electric field \( E \), one ends up with

\[
Z = \int D[D] e^{-\beta \int d^3 r h(\phi, D)}
\]

(7)

with

\[
h(\phi, D) = \frac{D^2}{2\varepsilon} + g(i\phi) + i\phi(\text{div} D - \varrho_f).
\]

(8)

In this expression, \( \text{div} D - \varrho_f \equiv s \) can be read as a Fourier transform variable such that we arrive at the formal expression

\[
Z = \int D[D] e^{-\beta \int d^3 r h(D)}
\]

(9)

with \( F \) the Fourier operator. The final task is to perform the integration over the field \( \phi \) to obtain

\[
Z = \int D[D] e^{-\beta \int d^3 r h(D)}
\]

(10)

If one neglects the fluctuations at the saddle-point, the Fourier transform can be replaced by a Legendre transform.

For definiteness we specialize in the following to the case of monovalent ions in the bulk (1:1 salt) so that the pressure contribution reads as

\[
g(i\phi) = -2k_B T c_0 \cos(\phi e \beta).
\]

(11)

By a rescaling of the potential we render the argument of the cosine dimensionless and introduce a discretization length scale \( \ell \), see Figure 1.

We now use a notation in which \( (\nabla \cdot) \) is a discrete difference operator on the lattice of Figure 1 which is the net flux out of each lattice site, where we associate the components of \( D \) to the links of the same lattice, in a way familiar in discretizations of Maxwell’s equations. This gives the discretized, and regularized partition function

\[
Z = \int D[D] D[\phi] e^{-\beta \sum \left( \frac{\ell^2}{\pi^2} D^2 + (\nabla \cdot D - \bar{\rho})^2 + 2n_0 \cos(\phi) \right)}
\]

(12)

in which \( n_0 \) is the number of ions of each species on a lattice of spacing \( \ell \) and \( \bar{\rho} = \rho_f \ell^3 \) is the scaled external charge. The expression can be reorganized into

\[
Z = \int D[D] e^{-\sum \frac{\ell^2}{\pi^2} D^2} \int D[\phi] e^{\sum (-i\phi + 2n_0 \cos(\phi))}
\]

(13)

with again \( s \equiv \nabla \cdot D - \bar{\rho} \). Here sums in the exponentials are over site for potentials and charges and over links for field components.
the potential we find of the discretized electrolyte. The smallest density correlations are screened so that \( \ell_D > \ell > c_0^{-1/3} \).

We now need to first calculate the integral over the Lagrange multiplier field \( \phi \),

\[
\int D[\phi] e^{\sum (-i\phi + 2n_0 \cos(\phi))} \quad (14)
\]

As the field \( \phi \) is purely local, we can drop the functional notation and thus have to deal with a simple integral for each site of the discretization

\[
z = \int d\phi e^{(-i\phi + 2n_0 \cos(\phi))} \quad (15)
\]

to which we now turn.

**Potential integral.** – In this section we show how to transform the potential formulation of the Poisson-Boltzmann free energy into an exactly equivalent dual version going beyond simple mean-field and saddle-point formulations. The key mathematical component in this formulation is the Poisson summation formula which expresses a sum over integer occupation numbers by an equivalent sum over Fourier coefficients. This gives a mathematically rigorous formulation in which the dominant contribution is the mean-field free energy already discussed but a framework in which higher order corrections are expressed as an exact series.

We expand the exponential function in eq. (15) as a Taylor series of the two complex exponentials using:

\[
\exp(n_0 e^{i\theta}) = \sum_{n=0}^{\infty} \frac{e^{i n \theta + n \mu}}{n!} \quad (16)
\]

where for convenience we define \( \mu = \log(n_0) \). Substituting eq. (16) in eq. (15) and performing the integral over the potential we find

\[
z = \sum_{n_1, n_2} \frac{1}{n_1! n_2!} e^{\mu(n_1 + n_2)} \delta(s + n_1 - n_2) \quad (17)
\]

where \( n_1 \) and \( n_2 \) represent the occupation numbers of positive and negative ions. This formulation is close to the “collective variable” representation familiar in the theory of fluids \([15]\).

By treating separately the cases \( s > 0 \) and \( s < 0 \) we solve the delta-function constraint and reduce the problem to a single summation, leading to

\[
z(s) = \sum_n \frac{1}{n! (n+|s|)!} e^{\mu(2n+|s|)} \quad (18)
\]

This is, at least in principle, a simple function of the variable \( s \), which can be tabulated, or interpolated to arbitrary precision for numerical work.

The standard way forwards in field theory treatments would be to use the Stirling formula to express the factorial functions as the exponential of an integral and then invoke a mean-field or saddle-point approximation by replacing the discrete sum by a continuous integral. Here we proceed in a manner that allows us to explicitly control and evaluate the errors in the approximations and avoids ambiguities in the choice of complex integration paths. This will give us an analytic approximation to the function \( z(s) \) which we will compare to an exact evaluation of eq. (15).

The Poisson summation formula tells us that if \( f(n) \) is a function defined on the integers and \( \tilde{f} \) is its continuous Fourier transform

\[
z = \sum_n f(n) = \sum_k \tilde{f}(2\pi k) = \sum_k z_k \quad (19)
\]

where \( z_k \) is the contribution to the \( k \)-th mode to the total partition sum \( z \).

Some care is needed for our physical problem eq. (18): we require the sum over positive integers, whereas the Poisson formula applies for a sum over positive and negative integers. This constraint can be imposed by the use of a smooth, multiplicative, weighting function

\[
w(n) = \begin{cases} 
0 & \text{if } n < -1 \\
\frac{e^{-1/n}}{e^{-1/n} + e^{1/(1+n)}} & \text{if } -1 < n < 0 \\
1 & \text{if } n > 0 
\end{cases} \quad (20)
\]

This cross-over function has an infinite number of derivatives and smoothly increases from zero to unity. This choice is non-unique, but the existence of a high number of derivatives gives a Fourier transform which decays rapidly with wave-number.\(^1\) We thus apply the Poisson formula to the function

\[
f(n) = w(n) \exp(-\log(n!)) - \log((ns + |s|)! + \mu(2n + |s|)) \quad (20)
\]

This expression is the basis of our reformulation. We now continue by approximately evaluating contributions to this

\(^1\)Note that the extension of the factorial function to the reals is also non-unique. The usual extension is the Euler Gamma function, but alternative extensions due to Hadamard also exist.
sum, and find an approximation to the higher coefficients \( z_k \) which incorporate the discrete nature of elementary charges into a continuum partition function integral.

The \( k = 0 \) contribution to the full partition sum eq. \([19]\) is then simply an integral over the summand of eq. \([18]\): It is the naive field theory integral over the occupation number, forgetting the discrete nature of the elementary charges.

\[
z_0 = \int_{-\infty}^{\infty} dn \, w(n) f(n).
\] (21)

It is simple to see that this integral is dominated, for \( n_0 \gg 1 \) by a simple saddle contribution, which we now evaluate. We perform the calculation with an improved approximation to the Stirling formula

\[
\ln(n!) \approx (n + 1/2) \ln(n + 1/2) - (n + 1/2) + O(1) = S(n)
\] (22)

which correctly includes the term \( \ln(n)/2 \) in its expansion.

**Large density approximation.** To proceed further with the saddle calculation we return to a formulation in terms of two, now continuous fields \( n_1 \) and \( n_2 \), with a delta-function constraint. We start by finding the value of \( n_1 \) and \( n_2 \) which dominate in a saddle-point evaluation of the function,

\[
z_0 = \int_n \exp \left( \mu(n_1 + n_2) - S(n_1) - S(n_2) \right) \delta(s + n_1 - n_2).
\] (23)

This saddle point is best studied by using a Lagrange multiplier \( \lambda \) which leads to the following saddle-point equation in \( n \),

\[
s = 2n_0 \sinh(\lambda)
\]

\[
n_1 + 1/2 = n_0 e^{-\lambda}
\]

\[
n_2 + 1/2 = n_0 e^{+\lambda}.
\] (24)

On eliminating \( \lambda \) we find the values of the occupation numbers which extremize the integrand:

\[
n_2 + 1/2 = \left( s + (s^2 + 4n_0^2)^{1/2} / 2 \right)
\]

\[
n_1 + 1/2 = \left( -s + (s^2 + 4n_0^2)^{1/2} / 2 \right).
\] (25)

When the variable \( s \) is small both \( n_1 \) and \( n_2 \) both converge to the background occupation number \( n_0 \), as expected. The value of the saddle point eq. \([23]\) is thus:

\[
\ln(z_0) \approx s \ln \left[ \frac{s}{2n_0} + \sqrt{1 + (s/2n_0)^2} \right] - \sqrt{s^2 + 4n_0^2} - \ln(n_0)
\] (26)

and we define \( f_0 = -\log z_0 \). When \( s \) is small we see that \( z_0 = O(e^{2n_0}) \gg 1 \).

We now evaluate the second derivative of action at the saddle to find

\[
\Delta(s) = \frac{1}{n_1 + 1/2} + \frac{1}{n_2 + 1/2} = \frac{1}{n_0^2} \sqrt{4n_0^2 + s^2}.
\] (27)

For small \( s \) we find \( \Delta(s) = 2/n_0 \). At saddle point we thus have a quadratic approximation to the action:

\[
f = f_0 + \frac{1}{2} \Delta(n - n_s)^2.
\] (28)

According to the sign of \( s \) we use the smaller of \( n_1 \) and \( n_2 \) as the primary variable mean-field occupation number \( n_s \). Performing the integral over the full occupation number \( n \) in eq. \([28]\) we find that the effective action is

\[
f(s) = f_0(s) + \frac{1}{2} \ln(\Delta(s)).
\] (29)

![Fig. 2: Comparison of the evaluation of the sum eq. \([17]\), (blue dot-dash) compared to the saddle point approximation eq. \([26]\), (red dash) and the quadratic approximation, eq. \([28]\), (yellow dotted). Three different values of \( n_0 \). For already modest values of \( n_0 = 3 \) (bottom) the quadratic approximation is already excellent with a good overlay of the exact and approximate curves. For \( n_0 < 1 \) (top) the mean field and quadratic approximations underestimate the true free energy. Curves shifted so that \( f(0) = 0 \).

We now calculate the higher Fourier contributions to the sum eq. \([19]\) which come from the discrete nature of the elementary charges. For \( n_0 > 1 \) the Fourier components are
also be estimated in the saddle point approximation. We take the quadratic approximation to the energy eq. [25] and regroup the positive and negative Fourier coefficients:

\[ \tilde{z}_k = (z_k + z_{-k}) = e^{-f_0} \int \cos(2\pi k n)e^{-\Delta(n-n_0)}/2 \, d\nu \]  

(30)

which gives

\[ \tilde{z}_k = e^{-f_0} \cos(2\pi k n_0)e^{-2k^2\pi^2/\Delta} \]  

(31)

If we consider that \( \Delta = O(2/n_0) \) then the amplitude of this contribution is

\[ \tilde{z}_k/z_0 = O(e^{-2k^2n_0}) \]  

(32)

If \( n_0 \gg 1 \) then this contribution is strongly suppressed in comparison with the \( k = 0 \) contributions to the partition function.

We now finally estimate the importance of the crossover function \( w(n) \) constraining the sums and integrals to be over positive occupations. Near \( n = 1 \) the function \( \ln(n!) = O(1) \). The Fourier transform of the weighting function can be estimated by a further saddle point calculation to be \( O(1) \times e^{-\sqrt{k}} \). \[16\]. We thus expect that the contribution to the partition sum coming from the constraint of the sum over positive occupation numbers is \( O(1) \).

Regrouping contributions we conclude that an approximation to the Fourier partition sum eq. \[19\] is given by

\[ z = e^{-f_0} (1 + 2 \cos(2n_0)e^{-2\pi^2/\Delta(s)}) + O(1) \]  

(33)

where \( f_0 \sim 2n_0 \) and we have kept just the first and largest non-trivial Fourier component for \( \tilde{z}_k \).

If the discretization is coarse so that \( n_0 > 1 \) we can drop the oscillating terms as well as the end-point corrections, to find the simplified expression

\[ f(s) = f_0(s) + \frac{1}{4} \ln \left( \frac{s^2 + 4n_0^2}{n_0^2} \right) \]  

(34)

This is compared to the exact sum eq. \[17\] in Fig. 2.

Thus the effective functional for the displacement field \( D \) is:

\[ A_{eff} = \sum \left[ \frac{e^2 \beta D^2}{2\varepsilon} + f(\text{div}D - \bar{\rho}) \right] \]  

(35)

if working on a scale \( \ell \) such that \( n_0 > 1 \). This is a functional, which is beyond mean field and includes fluctuations in the underlying field \( \phi \).

We also note that the integral over the displacement field \( D \) in eq. \[35\] can be studied by sampling the improved functional in simulations. In this case we have an improved description of the properties of the dielectric which goes beyond mean field and can include features of dielectric contrast \[17\] and image-charge interactions.

\textbf{Low density expansion.} When \( n_0 \) is small only a small number of terms in the sum eq. \[17\] contribute. We can find a simple approximation to \( z \) by taking just the very first term in the series:

\[ z = e^{\mu s}/\Gamma(1 + s); \quad f = -\log z \]  

(36)

The result of this approximation is plotted in Figure 3. It can be seen that the result works very well. However, this limit does not have equivalent of the Poisson formula, where we replace summation over the partition function by an integral. We have also checked that at intermediate values of \( n_0 \), the function \( z(s) \) can be replaced by a simple interpolation to very high accuracy.

\[ \text{Fig. 3: Comparison of the evaluation of the sum eq. \[17\], (blue dot-dash) compared to the approximation of taking the very first term in the summation, eq. \[36\] (red dots). The approximation of keeping two terms in the series is shown in yellow dash. Curves shifted so that } f(0) = 0. \text{ Three different values of } n_0. \text{ The approximation of a single term is already excellent for } n_0 \sim 0.2. \]

\textbf{Solution of the fluctuation-corrected saddle-point equation of the dual theory.} – As a final note we illustrate the effect of the logarithmic correction term
of eq. [29] in the dual functional. For this we consider the standard example of a single charged plate next to a solution of 1:1 salt in a 1-d geometry. Rather than performing a full integration, the profile of the dielectric displacement field can be obtained either by a direct minimization of the free energy functional

\[ F[D] = \int dr \left[ \frac{D^2(r)}{2\varepsilon} + f(D(r)) \right] \]

or, equivalently, by the computation of the resulting variational equation with respect to \( D \). Following the second approach, first without the logarithmic correction term, \( i.e. f(D) = f_0(D) \), yields the equation (setting \( \varepsilon = 1 \))

\[ D''(x) = (4n_0^2 + (D'(x))^2)^{1/2} D(x), \]

which is easily seen to be equivalent to the Poisson-Boltzmann equation

\[ \phi''(x) = 2n_0 \sinh(\phi(x)). \]

The equivalence is easily seen from differentiating the Poisson-Boltzmann equation with respect to \( x \), yielding \( \phi'''(x) = 2n_0 \cosh(\phi(x))\phi'(x) \), and using the inverted equation \( \phi(x) = \sinh^{-1} (\phi''(x)/(2n_0)) \) so that

\[ \phi'''(x) = 2n_0\phi'(x) \sqrt{1 + \frac{\phi''(x)^2}{4n_0^2}} \]

from which the equation for \( D(x) \) follows from the identity \( D = -\phi'(x) \). The inclusion of the correction term in the dual functional yields the fluctuation-corrected dual equation

\[ D(x) = \frac{D''(x)}{(4n_0^2 + D'(x)^2)^{1/2}} \left[ 1 + \frac{1}{2} \frac{4n_0^2 - D'(x)^2}{(4n_0^2 + D'(x)^2)^{3/2}} \right] \]

which shows that the correction term is on the order of \( n_0^{-1} \). Figure 3 compares solutions for the Poisson-Boltzmann equation and corrected dual equations for different values of \( n_0 \).

**Conclusions.** – In this Letter we have given an explicit formulation of the path integral of the duality-transformed Poisson-Boltzmann theory, for the illustrative case of a system containing a 1:1 salt solution. We calculate the arising path integral over the potential field variable \( \phi \) by making use of the Poisson summation formula. Having made explicit the number of charges \( n_0 \) in a discretized version of the theory, we can derive a new saddle-point approximation for the dual theory, which contains a functional of the dielectric displacement field in which the fluctuations of the potential field have been included. They give rise to a logarithmic correction in the free energy which is a local function of the dielectric displacement field. Furthermore, our formulation allows us to capture corrections due to the discrete nature of the charges, by including higher Fourier components of the Poisson formula.

Our new formulation of the dual Poisson-Boltzmann theory can be seen as similar in spirit to theories invoking a large system parameter, such as \( N \) in phase transitions of the \( N \)-vector model. In the limit of large \( n_0 \), our theory recovers the known PB theory, and fluctuation corrections will therefore be covered by previous results. For \( n_0 \approx O(1) \), this ceases to be true. We therefore expect that our novel formulation will be of use to treat fluctuation effects so far analytically inaccessible.

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Fig. 4: Comparison of the solutions to the saddle-point and one-loop corrected equations, eq. 10 (blue) and eq. 41 (brown), for three different values of \( n_0 \).

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\[^3\text{Here, we have gone back to the continuum with all scaling factors involved in the definition of } D \text{ removed.}\]
in that parameter range.

Two surprising results of the use of the Poisson summation formula is that the discreteness of the elementary charges comes out in exponentially small corrections the main functional integral for the field \( D \); there also seems to be a weak non-analyticity in the results at \( s = 0 \) due the presence of the term \( |s| \) in eq. \([18]\).

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