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Monotonic converging variational approximations to the functional integrals in quantum statistical mechanics

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We show, by making use of the functional integral technique, that, for a large class of useful quantum statistical systems, the partition function is, with respect to the coupling constant, the Laplace transform of a positive measure. As a consequence, we derive an infinite set of monotonicly converging upper and lower bounds to it. In particular, the lowest approximation appears to be identical to the Gibbs–Bogolioubov variational bound, while the next approximations, for which we give explicit formulas for the first few ones, lead to improve the previous bound. The monotonic character of the variational successive approximations allows a new approach towards the thermodynamical limit.

I. INTRODUCTION AND HISTORICAL BACKGROUND

Our aim is to extend to quantum statistical mechanical systems a variational and perturbative method introduced in a previous paper,[1] leading to monotonic converging bounds for the eigenvalues of a semibounded N particle Hamiltonian H.

More precisely, we showed that each pole of the Padé approximation (PA) constructed on the resolvent of H was providing, for the discrete part of the spectrum of H, an upper bound to the corresponding exact eigenvalue, and that this upper bound can be used as a variational bound in the pivot $|\varphi\rangle$ (the test vector, for which the mean value of the resolvant is computed). These variational upper bounds were clear generalizations of the Rayleigh—Ritz variational principle, which include more moments than the first one: the nth moment being $\langle\varphi|H^n|\varphi\rangle$.

In particular, when the moments do not exist (for instance, in the case of ultraviolet divergence), but admit a regularization, while the PA cannot have variational properties in the regulator (because they do not remain bounded in the vicinity of their poles), it was shown that the arctan of the PA admits nice variational properties in the regulator, which allow one to reconstruct the spectrum through an extended Padé—Rayleigh—Ritz variational principle which includes the regulator as variational parameter.

However, in physics, one is not only interested in reconstructing the spectrum, but also in computing, either the evolution operator $\exp(itH)$ or its "Euclidean version" $\exp(-\beta H)$. $\exp(itH)$ represents the evolution operator of the system between time zero and time t, while $\exp(-\beta H)$ is related to the Gibbs density matrix of the system at equilibrium and temperature $kT=1/\beta$.

In the previous paper, all mathematical properties, were based on the fact that the resolvent appears as a Stieltjes function in the energy or in the coupling constant parameter. Stieltjes functions are special types of Laplace transform of positive measure. Similarly, from the spectral decomposition of H, $\exp(-\beta H)$ is, in β, the Laplace transform of a positive valued measure:

$$\exp(-\beta H)=\int_{E_0}^{\infty}\exp(-\beta E)\,dP_E, \qquad (\text{I. }1)$$

where dP_E is the projector onto the eigenvalue E of H and dP_E is a positive operator valued measure.

The positivity of the measure allows us to construct, for the trace of (I. 1), approximations based on the Gaussian integration method.[2] This approximation is also known under the name of generalized Padé approximants (GPA), because the weights of the Gaussian integration method are simply the residues of the ordinary PA associated with the positive measure, while the zeroes of the Gaussian method are the poles of the same PA.

More precisely it was shown[2,3] that the GPA were providing, for a finite number of particles N, monotonic decreasing sequences of converging upper bounds for the diagonal GPA, while the subdiagonal ones were giving monotonic increasing sequences of converging lower bounds to the partition function. The exact solution is constrained between these bounds.

Furthermore,[3] these GPA can have variational properties in the number of particles N. By making use of this remark, it is possible to obtain, for $N\to\infty$ (the thermodynamical limit), a monotonic sequence of decreasing or increasing converging bounds.

This method converges clearly for any temperature and any density. However, one would like to start from an exactly solvable Hamiltonian H_0, for which, for example, the thermodynamical quantities are exactly known, and perturb it, to see how these quantities are changed. It is therefore of interest to study the following:

Question: What are the positivity properties of $\exp(-\beta H)$ in the coupling constant λ

$$(\text{where } H=H_0+\lambda H_I)? \qquad (\text{I. }2)$$

We propose the following

$$Z(\lambda)=\operatorname{Tr}\exp[-\beta(H_0+\lambda H_I)]=\int\exp(-\lambda\tau)\,d\mu(\tau), \qquad (\text{I. }3)$$

where $d\mu(\tau)$ is a *positive measure* the support of which is contained in the convex hull of the eigenvalues of H_I (that is, between the inf and the sup of the spectrum of H_I).

Up to now, we are able to prove this statement in the three following cases:

A—H_0 and H_I are Hilbert space commuting operators.

B—H_0 and H_I are 2×2 matrices, and more generally when $\exp(-\beta H_0)$ has all its matrix elements positive in a basis where H_I is diagonal.

C—When

$$H_0=\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m_i}+V(\mathbf{r}_1,\ldots,\mathbf{r}_N),\quad \mathbf{p}_k=-i\nabla_k, \tag{I. 4}$$

$$H_I=V'(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N).$$

Case A corresponds to classical statistical mechanics. Case C corresponds to an N-body quantum mechanical system of N spinless particles with the most general bounded from below *local* interaction. We could not find any counterexample to the general statement (I. 3). Whether (I. 3) stands in general or is subject to restrictions is an open question. A consequence of the theorem of case C is that it is possible to construct, for a system, with a finite number of particles N, a monotonic sequence of converging upper and lower bounds, to the free energy per particle of the system:

$$F_N(\rho,\beta,\lambda)=-(1/\beta N)\log[Z_N(\rho,\beta,\lambda)], \tag{I. 5}$$

where ρ is the density of the system. In particular, it is interesting to investigate the behavior $N\to\infty$ of these bounds: the thermodynamical limit.

The lowest approximation, which is constructed from the GPA $[0/1]$ to the partition function gives rise to the bound

$$F_N(\lambda)<[0/1]_N(\lambda)=F_N(0)+(1/N)\operatorname{Tr}(\rho_0\lambda H_I), \tag{I. 6}$$

where ρ_0 is the density matrix for the Hamiltonian H_0:

$$\rho_0=\exp(-\beta H_0)/\operatorname{Tr}\exp(-\beta H_0)\quad\text{and}$$

$$\rho=\exp(-\beta H)/\operatorname{Tr}\exp(-\beta H). \tag{I. 7}$$

(I. 6) is generally derived from the Gibbs—Bogolioubov variational bound:

$$\operatorname{Tr}(\rho_0\log\rho_0)>\operatorname{Tr}(\rho_0\log\rho). \tag{I. 8}$$

Due to the extensive properties of the terms in Eq. (I. 6), the $N\to\infty$ limit is straightforward and meaningful. The next approximations $[1/1]$ and $[1/2]$ do not enjoy the same extensivity property as the lowest approximation $[0/1]$. In particular, in the thermodynamical limit, all our bounds have the same limit as the lowest approximation $[0/1]$ or $[0/0]$ depending if one takes the $[P-1/P]$ or the $[P/P]$ approximation.

Therefore, if one wants to work directly with $N=\infty$ on the bounds, the information coming from the knowledge of more than the first two terms in the perturbation expansion in λ of the partition function seems to be lost.

However, it is easy to circumvent this difficulty by changing the traditions: One works with finite N (number of particles) which provides a natural cutoff for the perturbation terms of the expansion in λ of the partition function. Then, it is not difficult to show following the method described in Ref. 3 that the bounds are variational in N.

Then one obtains, for the true free energy per particle, in the thermodynamical limit, a succession of embedded variational converging bounds, the variational parameter being the number of particles itself.

Finally, we want to point out that, as will be shown in the sequel, our method for treating the operator $\exp[-\beta(H_0+\lambda H_I)]$ is based actually on Wiener's functional approach.

The reader will find:

– In Sec. II, the present status of the Laplace transform theorems.

– In Sec. III, the derivation of monotonic sequences of lower and upper bounds to the free energy of a quantum system of N particles.

– In Sec. IV, the analysis of the thermodynamical limit of the previous bounds, as well as the extension of the method to the case of singular interactions.

– In Sec. V, the conclusion and a general outlook for the Euclidean field theory.

II. THE LAPLACE TRANSFORM THEOREMS

We shall discuss under which conditions the following conjecture holds:

Conjecture ($\mathcal{C}$): Let A and B be two bounded from below selfadjoint operators, and $|\varphi\rangle$ be an eigenvector of B. Then

$$\langle\varphi|\exp[-(A+\lambda B)]|\varphi\rangle=\int\exp(-\lambda\tau)\,d\mu(\tau). \tag{II. 1}$$

$d\mu(\tau)$ is a positive measure with support contained in the convex hull of the spectrum of B.

We shall prove the following theorems:

Theorem 1: ($\mathcal{C}$) holds when A and B commute.

Theorem 2: ($\mathcal{C}$) holds when, for all real positive number ρ, $\exp(-\rho A)$ has nonnegative matrix elements in a basis where B is diagonal.

Corollary to Theorem 2: ($\mathcal{C}$) holds when:

(a) A, B are any two dimensional matrices.

(b) A is a tridiagonal matrix $[A_{ij}=0$ if $j\neq(i;i-1$ or $i+1)]$ in a basis where B is diagonal (A bounded).

(c) Off-diagonal matrix elements of A are negative in a basis where B is diagonal (A bounded).

Proof: —Theorem 1 is a trivial consequence of the spectral decomposition of B.

—Theorem 2 makes use of the Trotter's formula[4] for bounded from below auto-adjoint operators. We have

$$\langle\varphi|\exp[-(A+\lambda B)|\varphi\rangle=\lim\langle\varphi|\{\exp(-A/n)\times\exp(-\lambda B/n)\}^n|\varphi\rangle. \tag{II. 2}$$

Consider

$$\langle\varphi|\{\exp(-A/n)\exp(-\lambda B/n)\}^n|\varphi\rangle=X_n \tag{II. 3}$$

and

$$X_n=\int d\varphi_1\cdots d\varphi_{n-1}\exp\{-\lambda/n[b(\varphi_1)+\cdots+b(\varphi_{n-1})+b(\varphi)]\}$$

$$\times\langle\varphi\,|\exp(-A/n)|\,\varphi_1\rangle\langle\varphi_1|\exp(-A/n)|\,\varphi_2\rangle\cdots$$
$$\times\langle\varphi_{n-1}|\exp(-A/n)|\,\varphi\rangle, \tag{II.4}$$

where we have introduced $(2n-1)$ times the closure relation for the spectral decomposition of B:

$$B=\int\,|\varphi\rangle\, b(\varphi)\langle\varphi|\, d\varphi, \tag{II.5}$$

$$I=\int\,|\varphi\rangle\, d\varphi\langle\varphi|. \tag{II.6}$$

Therefore we have

$$X_n=\int \exp(-\lambda\tau)\, d\mu_n(\tau) \tag{II.7}$$

with

$$d\mu_n(\tau)=\int d\varphi_1\cdots d\varphi_{n-1}\,\delta\left(\tau-\frac{1}{n}\sum_{i=1}^{n} b(\varphi_i)\right)$$
$$\langle\varphi|\exp(-A/n)|\,\varphi_1\rangle$$
$$\times\langle\varphi_1|\exp(-A/n)|\,\varphi_2\rangle\cdots\langle\varphi_{n-1}|\exp(-A/n)|\,\varphi\rangle, \tag{II.8}$$

where we have set

$$\varphi_n=\varphi. \tag{II.9}$$

Since all matrix elements occurring in (II.8) are positive $d\mu_n(\tau)$ is a positive measure. Furthermore, the support of $d\mu_n(\tau)$ is clearly contained in the convex hull of the spectrum of B. The limit $n\to\infty$ of (II.8) is a positive measure [5] (see the Appendix for the proof). Theorem 2 is then proved.

For the corollary first prove (c). Consider $\exp(-\rho A/n)$ for n integer big enough such that $(\exp(-\rho A/n))_{ij}\sim\delta_{ij}-\rho A_{ij}/n$ is positive for all i and j. This is possible, if for $i\neq j$, A_{ij} is strictly negative and bounded. The positivity of $(\exp(-\rho A))_{ij}$ is then obtained by using $\exp(-\rho A)=(\exp(-\rho A/n))^n$. The case where some A_{ij} are zero can be dealt with by continuity. Conditions of Theorem 2 are fulfilled without any hypothesis on the diagonal elements of A, and therefore (c) is obtained.

The nondiagonal elements of a tridiagonal matrix can always be given real negative values by multiplying the basis vectors by a suitable phase factor. Then (b) becomes a particular case of (c). It is clear, on the other hand, that 2×2 matrices are all tridiagonal, which proves (a).

Remark on the 2×2 *matrix case*: In this case the direct computation of the measure is possible. The measure appears as the sum of δ functions the argument of which are the eigenvalues of B, plus an entire and positive Bessel function spread out between these eigenvalues. It would be interesting to investigate in the general case of $d\times d$ matrices the nature of the measure.

Finally we want to point out that conjecture $(\mathcal{C})$ does *not* extend to case where the mean value of $\exp(-(A+\lambda B))$ is taken in a general vector, instead of $|\varphi\rangle$ eigenvector of B: Explicit counterexamples can be worked out.

Conjecture $(\mathcal{C})$ holds in quantum statistical mechanics when we consider spinless particles. More precisely we have the fundamental theorem:

Theorem 3: Let T, V, $T+V=H_0$, V', and $H_0+\lambda V'$ be self-adjoint Hilbert space operators, bounded from below such that

$$T=\sum_{i=1}^{N}\mathbf{p}_i^{\,2};\ \mathbf{p}_K=-i\nabla_k \tag{II.10}$$

$$V=V(\mathbf{r}_1,\ldots,\mathbf{r}_N) \tag{II.11}$$

$$V'=V'(\mathbf{r}_1,\ldots,\mathbf{r}_N) \tag{II.12}$$

where V includes eventually the wall potential which describes the finite volume in which particles are confined. Then, if we represent by $\mathbf{r}$ the collection $\{\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N\}$, we can write

$$\mathcal{U}(\beta,\lambda)=\langle\mathbf{r}|\exp[-\beta(T+V+\lambda V')]|\,\mathbf{r}\rangle=\int\exp(-\lambda\tau)\,d\mu(\tau). \tag{II.13}$$

the support of the positive measure $d\mu(\tau)$ extends from the inf to the sup of the spectrum of V'. The proof goes along the same lines as that for Theorem 2, using the positivity of

$$\langle\mathbf{r}|\exp(-\beta/n\,T)|\,\mathbf{r}'\rangle=\left(\frac{\beta}{4\pi n}\right)^{3N/2}\ \exp\left(-\frac{n}{4\beta}\sum_{i=1}^{n}(\mathbf{r}_i-\mathbf{r}_i')^2\right). \tag{II.14}$$

We insert the closure relation for the position operator in Trotter's formula and set

$$\mathcal{U}(\beta,\lambda)=\langle\mathbf{r}|\exp[-\beta(T+V+\lambda V')]|\,\mathbf{r}\rangle$$
$$=\lim_{n\to\infty}\langle\mathbf{r}|(\exp(-\beta T/n)\exp(-\beta V/n)$$
$$\times\ \exp(-\beta\lambda V'/n))^n|\,\mathbf{r}\rangle \tag{II.15}$$
$$=\lim_{n\to\infty}\left(\frac{\beta}{4\pi n}\right)^{3Nn/2}\int d\mathbf{r}^{(1)}\cdots d\mathbf{r}^{(n-1)}$$
$$\times\exp\left[-\frac{\beta}{n}\left(\sum_{i=1}^{n}V(\mathbf{r}^{(i)})+V'(\mathbf{r}^{(i)})\right)\right.$$
$$\left.-\frac{n}{4\beta}\sum_{j=1}^{N}\sum_{i=0}^{n-1}(\mathbf{r}_j^{(i)}-\mathbf{r}_j^{(i+1)})^2\right], \tag{II.16}$$

where $\mathbf{r}^{(i)}$ stands symbolically for the set $\{\mathbf{r}_1^{(i)},\mathbf{r}_2^{(i)},\ldots,\mathbf{r}_N^{(i)}\}$ and $\mathbf{r}^{(n)}=\mathbf{r}=\mathbf{r}^{(0)}$.

$\mathcal{U}(\beta,\lambda)$ can be rewritten as

$$\mathcal{U}(\beta,\lambda)=\lim_{n\to\infty}\int\exp(-\lambda\tau)\,d\mu_n(\tau) \tag{II.17}$$

$$d\mu_n(\tau)=\left(\frac{\beta}{4\pi n}\right)^{3Nn/2}\int d\mathbf{r}^{(1)}\cdots d\mathbf{r}^{(n-1)}\,\delta\left(\tau-\frac{\beta}{n}\sum_{i=1}^{n}V'(\mathbf{r}^{(i)})\right)$$
$$\times\exp\left(-\frac{n}{4\beta}\sum_{i=0}^{n-1}\sum_{j=1}^{N}(\mathbf{r}_j^{(i)}-\mathbf{r}_j^{(i+1)})^2-\frac{\beta}{n}\sum_{i=1}^{n}V(\mathbf{r}^{(i)})\right). \tag{II.18}$$

Clearly $\mathcal{U}(\beta,\lambda)$ is the limit of the Laplace transform of positive measures $d\mu_n$. Trotter's theorem tells us that the limit in (II.17) exists and $d\mu_n(\tau)$ itself has a limit which is a positive measure $d\mu(\tau)$ (see the Appendix for the proof) and

$$\mathcal{U}(\beta,\lambda)=\int\exp(-\lambda\tau)\,d\mu(\tau). \tag{II.19}$$

Of course, the support of $d\mu(\tau)$ is obtained as the convex hull of the spectrum of V', which means the interval going from inf spectrum of V' to sup spectrum of V'.

It is clear that this proof of Theorem 3 could have been derived using the Wiener functional integration instead of Trotter's formula.[4] It is evident that, in all these theorems from 1 to 4, one can replace everywhere the mean value by the traces.

Extend our results at least for the trace to more general situations, such as the finite dimensional case, which can be thought to describe a discrete fermion field, could be of a great interest for the theory of functional integration itself.

III. UPPER AND LOWER BOUNDS TO THE FREE ENERGY OF A QUANTUM SYSTEM OF N PARTICLES

We are now faced with the problem of approximating [cf. (I.2) and (I.3)]:

$$Z(\lambda)=\int_a^{+\infty}\exp(-\lambda\tau)\,d\mu(\tau),\quad d\mu(\tau)>0. \tag{III.1}$$

In general, a, the lower bound of the spectrum of the perturbation, will depend on the number of body N. We shall give to ourselves the "perturbative" expansion of $Z(\lambda)$

$$Z(\lambda)=\sum_{n=0}^{\infty}\frac{(-\lambda)^n}{n!}\,\mu_n, \tag{III.2}$$

where the moments are

$$\mu_n=\int_a^{+\infty}\tau^n\,d\mu(\tau). \tag{III.3}$$

It is always possible when a is finite (finite number of bodies) to transform (III.1) into an analogous problem with $a=0$ by setting $\tau=a+\xi$. In (III.1) we get

$$Z(\lambda)=\exp(-\lambda a)\int_0^{+\infty}\exp(-\lambda\xi)\,d\mu(a+\xi). \tag{III.4}$$

The moments $\bar{\mu}_n$ of

$$\bar{Z}(\lambda)=\int_0^{\infty}\exp(-\lambda\xi)\,d\mu(a+\xi) \tag{III.5}$$

being simply related to the moments $\bar{\mu}_n$:

$$\mu_n=\sum_{p=0}^{n}C_n^p a^{n-p}\bar{\mu}_p \tag{III.6}$$

The interesting fact is that it is possible knowing a *finite* number of μ_n (or $\bar{\mu}_n$) to get lower and upper bounds to $Z(\lambda)$. In fact much better can be achieved: Monotonic sequences of lower or upper bounds can be constructed which constrain the solution $Z(\lambda)$.[2] We have the following set of inequalities:

$$Z^{[0/1]}(\lambda)<Z^{[1/2]}(\lambda)<\cdots<Z^{[P-1/P]}(\lambda)<\cdots<Z(\lambda),$$

and

$$Z(\lambda)<\cdots<Z^{[P/P]}(\lambda)<\cdots<Z^{[2/2]}(\lambda)<Z^{[1/1]}(\lambda)<Z^{[0/0]}(\lambda), \tag{III.7}$$

where

$$Z^{[P-1/P]}(\lambda)=\sum_{i=1}^{P}w_i^{(P)}\exp(-\lambda\xi_i^{(P)}), \tag{III.8}$$

$$Z^{[P/P]}(\lambda)=\sum_{i=0}^{P}\tilde{w}_i^{(P)}\exp(-\lambda\tilde{\xi}_i^{(P)})\quad(\tilde{\xi}_0^P=0). \tag{III.9}$$

These formulas are just the traditional Gaussian integration approximations. It is, however, simpler to interpret (III.8) and (III.9) as generalized Padé approximations.[2,6]

In fact, to build up the ξ's and w's, one has to introduce the Stieltjes function associated with the Laplace transform (III.5):

$$R(\lambda)=\int_0^{\infty}\frac{d\mu(a+\xi)}{1+\lambda\xi}, \tag{III.10}$$

for which we can construct the PA to $R(\lambda)$ in terms of a finite number of moments μ_n. They read

$$R^{[P-1/P]}(\lambda)=\sum_{i=1}^{P}\frac{w_i^{(P)}}{1+\xi_i^{(P)}\lambda},\quad R^{[P/P]}(\lambda)=\sum_{i=0}^{P}\frac{\tilde{w}_i^{(P)}}{1+\tilde{\xi}_i^{(P)}\lambda}, \tag{III.11}$$

$$\tilde{\xi}_0^{(P)}=0.$$

The ξ's are simply connected to the poles of the PA to $R(\lambda)$ and w's to their residues. On the other hand the denominators of PA are set of orthogonal polynomials with respect to the measure[6] $d\mu$. This allows us to understand how the Gaussian integration is a particularly simple generalized Padé approximation. For more details on generalized PA see Ref. 6, on the Gaussian integration see Ref. 2, and on the orthogonal polynomials, Ref. 7.

If we consider the partition function for a quantum system of N particles interacting via local N-body potentials, then

$$H_N=\sum_{i=1}^{i=N}\mathbf{p}_i^2+V(\mathbf{r}_1,\ldots,\mathbf{r}_N)+\lambda V'(\mathbf{r}_1,\ldots,\mathbf{r}_N) \tag{III.12}$$

$$=H_0+\lambda H_I. \tag{III.12$'$}$$

Using Theorem 3 and the inequalities (III.7), we get, introducing the free energy per particle,

$$F_N(\lambda)=-(1/\beta N)\log[Z(\lambda,N)], \tag{III.13}$$

as well as the free energy per particle given by the $[P/Q]$th approximation,

$$F_N^{[P/Q]}(\lambda)=-(1/\beta N)\log[Z^{[P/Q]}(\lambda,N)], \tag{III.14}$$

the following inequalities:

$$F_N^{[0/0]}(\lambda)<F^{[1/1]}(\lambda)<\cdots<F^{[P/P]}(\lambda)<\cdots<F_N(\lambda)<\cdots<F_N^{[P-1/P]}(\lambda)<\cdots<F_N^{[0/1]}(\lambda). \tag{III.15}$$

In this set of inequalities we recall that $F_N(\lambda)$ is the true free energy per particle (N finite) and $F_N^{[P/Q]}(\lambda)$ is $[P/Q]$ generalized Padé approximation to it:

$$F_N^{[P-1/P]}(\lambda)=-(1/\beta N)\log\exp[-\lambda a(N)]\sum_{i=1}^{P}w_i^{(P)}\times\exp(-\lambda\xi_i^{(P)}) \tag{III.16}$$

and an analogous formula for $F_N^{[P/P]}(\lambda)$.

Before going into the explicit formulas for the approximation let us remark that the $[P\text{-}1/P]$ approximation does not depend explicitly on the lower bound a of the integral in (III.1), this property is due to the well-known homographical transformation properties of the $[P\text{-}1/P]$ PA under a translation on the variable of integration, property which is not true for the $[P/P]$ approximation. As a consequence, for the $[P\text{-}1/P]$ GPA one does not need to make the a translation as in (III.6).

In general we shall give our approximations, in terms of the "moments":

$$\mu_k = (-)^k \left. \frac{d^k}{d\lambda^k} Z_N(\lambda) \right|_{\lambda=0}, \tag{III.17}$$

where $Z_N(\lambda)$ is the true partition function for N particles. However, it appears to be more convenient to introduce the cumulants defined by

$$C_k = (-1)^k \left. \frac{d^k}{d\lambda^k} \log[Z_N(\lambda)] \right|_{\lambda=0}, \quad k > 1. \tag{III.18}$$

The first three cumulants read

$$C_1 = \frac{\mu_1}{\mu_0}, \quad C_2 = \frac{\mu_2}{\mu_0} - \frac{\mu_1}{\mu_0}^2 > 0,$$
$$C_3 = \frac{\mu_3}{\mu_0} - 3\frac{\mu_1}{\mu_0}\frac{\mu_2}{\mu_0} + 2\frac{\mu_1}{\mu_0}^3 \tag{III.19}$$

This allows one to have a simple understanding of the lowest approximations, which make use only of the first three moments or cumulants.

With these remarks in mind, one can now consider:

— The $[0/0]$ approximation which reads

$$F_N^{[0/0]}(\lambda) = -\frac{1}{\beta N} \log(\exp(-\lambda a)\mu_0) \tag{III.20}$$

$$= F_N(0) + \frac{\lambda}{\beta}\frac{a(N)}{N} < F_N(\lambda), \tag{III.21}$$

which provides a lower bound to the exact free energy.

— The $[0/1]$ approximation which reads

$$F_N^{[0/1]}(\lambda) = -\frac{1}{\beta N} \log\left[\mu_0 \exp\left(-\lambda \frac{\mu_1}{\mu_0}\right)\right] \tag{III.22}$$

$$= F_N(0) + \frac{\lambda}{N} \operatorname{Tr}(\rho_0 H_I) > F_N(\lambda), \tag{III.23}$$

which provides an upper bound to the exact free energy, where we have introduced the unperturbed density matrix

$$\rho_0 = \exp(-\beta H_0)/\operatorname{Tr} \exp(-\beta H_0). \tag{III.24}$$

If we introduce also the exact density matrix

$$\rho = \exp[-\beta(H_0 + \lambda H_I)]/\operatorname{Tr} \exp[-\beta(H_0 + \lambda H_I)] \tag{III.25}$$

We can derive (III.23) from the Gibbs—Bogolioubov inequality:

$$\operatorname{Tr}\rho_0 \log\rho_0 > \operatorname{Tr}\rho_0 \log\rho. \tag{III.26}$$

One recognizes in (III.23) the traditional Gibbs—Bogolioubov inequality of quantum statistical mechanics for the free energy, which appears to be nothing but the $[0/1]$ GPA in our scheme.

— The $[1/1]$ approximation reads

$$F_N^{[1/1]}(\lambda) = F_N^{[0/0]}(\lambda)$$
$$- \frac{1}{\beta N} \log\left(\frac{C_2 + (C_1 - a)^2 \exp\{-\lambda[C_2 + (C_1 - a)^2]/C_1 - a\}}{C_2 + (C_1 - a)^2}\right). \tag{III.27}$$

This approximant clearly provides a better lower bound to $F_N(\lambda)$ than the previous $F_N^{[0/0]}(\lambda)$.

And the $[1/2]$ approximation reads

$$F_N^{[1/2]}(\lambda) = F_N^{[0/1]} + \frac{\lambda}{\beta N}\frac{C_3}{2C_2} - \frac{1}{\beta N} \log \cosh\left[\left(\frac{C_3}{2C_2}\right)^2 + C_2\right]^{1/2}$$
$$- \frac{1}{\beta N} \log\left\{1 + \frac{(C_3/2C_2)}{[(C_3/2C_2)^2 + C_2]^{1/2}} \times \tanh\left[\left(\frac{C_3}{2C_2}\right)^2 + C_2\right]^{1/2}\right\}. \tag{III.28}$$

$F_N^{[1/2]}(\lambda)$ provides a better upper bound to $F_N(\lambda)$ than $F_N^{[0/1]}(\lambda)$ (which is the Gibbs—Bogolioubov bound).

To understand clearly the content of these new bounds, it is necessary to consider the thermodynamical limit; this is the object of the next paragraph.

IV. UPPER AND LOWER BOUNDS FOR THE FREE ENERGY OF A QUANTUM SYSTEM OF N PARTICLES IN THE THERMODYNAMICAL LIMIT

Before we take the limit $N \to \infty$ (number of particles going to infinity) on the set of bounds (III.15), we want to point out that, for fixed N, if we let the order of approximations $P \to \infty$, the two bounds

$$F_N^{[P/P]}(\lambda) < F_N(\lambda) < F_N^{[P-1/P]}(\lambda) \tag{IV.1}$$

tend to each other and therefore to the true $F_N(\lambda)$, when the moment problem is determinate. For a finite number of particles and a bounded perturbation the moment problem is always determined because then, by Theorem 3, $Z_N(\lambda)$, the partition function, is an entire function of λ, the support of the measure being bounded. The radius of convergence of the Taylor expansion of $Z_N(\lambda)$ in λ being infinite, we have for the moments the inequality

$$|\mu_n| < \epsilon^n n!, \quad \epsilon > 0, \tag{IV.1'}$$

and therefore the Carleman[6] condition is fulfilled and the moment problem determined.

The limit we have to take is

$$\lim_{N\to\infty} \lim_{P\to\infty} F_N^{[P/P]}(\lambda) = F(\lambda). \tag{IV.2}$$

It is not possible to invert these two limits even with the use of PA instead of the perturbation series. However, we shall see that we can *connect* N and P *by a variational principle*, in such a way that P becomes a well-defined function of N, such that

$$P \to \infty, \quad N(P) \to \infty \tag{IV.3}$$

and

$$F(\lambda) = \lim_{P\to\infty} F_{N(P)}^{[P/P]}(\lambda). \tag{IV.4}$$

Before explaining this technique, let us see what are the limits for fixed P of the approximations:

$$\lim_{N\to\infty} F_N^{[P/P]}(\lambda) \quad \text{or} \quad \lim_{N\to\infty} F_N^{[P-1/P]}(\lambda).$$

— The thermodynamical limit of the $[0/0]$ approximation: From (III.21) taking the limit $N \to \infty$, we get

$$F(0) + (\lambda/\beta)a < F(\lambda), \tag{IV.5}$$

where a is the limit $a(N)/N$ which exists for physical situation.[8] We therefore obtain our lower bound for the true free energy, which is linear in the coupling λ.

— The thermodynamical limit of the [0/1] approximation: From (III. 23) we get, in the limit $N \to \infty$,

$$F(0) + \lambda F'(0) > F(\lambda). \tag{IV. 6}$$

This bound is equivalent to the Gibbs—Bogolioubov bound and gives rise to the concavity property of $F(\lambda)$ in λ. One can see making use of the extensitivity property of the cumulants that the other PA will give in the limit $N \to \infty$ either the bound (IV. 5) for the $[P/P]$ or the bound (IV. 6) for the $[P-1/P]$. This is not surprising, because it is due to the nonuniform convergence of the approximations in the limit $N \to \infty$. To set useful sets of converging bounds, we must now use the *variational* properties of our bounds in the number of particles N.

Those variational properties are deduced from the following theorem [9]:

Theorem 5: Let

$$A^{(1)}(N) < A^{(2)}(N) < \cdots < A^{(P)}(N) < \cdots < A(N) \tag{IV. 7}$$

be a monotonic sequence of converging lower bounds to $A(N)$ for any $N > 0$.

Suppose, for $N > N_0$, $A(N)$ reaches its sup for $N = \infty$,

$A(\infty) = A$.

Then, for $N > N_0$, $\bar{A}^{(P)}(N)$ has a sup in $N : \bar{A}^{(p)}$ which

$$\bar{A}^{(1)} < \bar{A}^{(2)} < \cdots < \bar{A}^{(P)} < \cdots < A \tag{IV. 8}$$

and

$$\lim_{P\to\infty} \bar{A}^{(P)} = A. \tag{IV. 9}$$

Therefore, we are able due to the monotonicity of the set of approximations to extract a variational subsequence which converges towards the exact ($N \to \infty$) limit.

A corresponding theorem can be derived also, obviously, for monotonic sequences of converging upper bounds provided $A(N)$, this time, reaches its inf for $N = \infty$, when $N > N_0$.

For a certain number [8,3] of physical problems the free energy appears to be a monotonic function of the number of particles. For such systems we can directly apply the previous technique and look for extremal values of the approximated free energy per particle $F_N^{[P-1/P]}(\lambda)$ in N, this will give an upper bound to the true $F(\lambda)$ for the case where $F_N(\lambda)$ reaches its inf at $N = \infty$. For the case, where $F_N(\lambda)$ reaches its sup at $N = \infty$, we shall use the extremal value of $F_N^{[P/P]}(\lambda)$ in N to get a lower bound to $F(\lambda)$. The interest of this method is that it is a *convergent* algorithm for *any temperature*, *density or coupling*. The price to pay to have these nice convergence properties in the coupling constant, temperature, and density is to work in a framework of a finite number of particles. In fact, if one uses periodical boundary conditions for the statistical system (such as to consider the system on a torus) it is very likely that $F_N(\lambda)$ as a function of N is extremely flat round $N = \infty$ (all derivatives in N equal to zero) and therefore extremely good numerical results can be achieved even with low approximations, that is, with low values of N.

It will be the object of forthcoming papers to illustrate by physical example the usefulness of such methods.

Extension of the method to singular interactions

In the previous section, we have treated the case where the perturbation series of the partition function for a finite number of particles N was existing and the moment problem determinate, that is, for bounded perturbations. In practice one has often to face the problem of an unbounded perturbation operator associated with hard cores or arbitrary singular interactions. In such cases the moment problem could become undeterminate or the perturbation series itself may not exist any more.

We shall show how the method we propose adapts itself to such a case.

Let us consider an N-body local interaction via a two body singular potential; for instance,

$$V_I(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = \sum_{i<j} V_{(2)}(|\mathbf{r}_i - \mathbf{r}_j|), \tag{IV. 10}$$

where $V_2(r)$ is an arbitrarily singular potential in the origin bounded from below (which corresponds to the physically interesting case).

Let us regularize $V_2(r)$ in the following way:

$$V_{(2)}^{(\epsilon)}(r) = \begin{cases} V_2(\epsilon), & r \leq \epsilon, \\ V_2(r), & r \geq \epsilon. \end{cases} \tag{IV. 11}$$

It is easy to see that for $0 < \epsilon_1 < \epsilon_2 < \epsilon_0$

$$V_{(2)}^{(\epsilon_1)} > V_{(2)}^{(\epsilon_2)}. \tag{IV. 12}$$

The inequality being taken in the sense of operators. Then defining the regularized N-body perturbation interaction by

$$V_I^{(\epsilon)}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = \sum_{i<j} V_2^{(\epsilon)}(|\mathbf{r}_i - \mathbf{r}_j|), \tag{IV. 13}$$

we see that in the sense of operators

$$V_I^{(\epsilon_1)} > V_I^{(\epsilon_2)} \quad 0 < \epsilon_1 < \epsilon_2 < \epsilon_0. \tag{IV. 14}$$

We have then [10]

$$\begin{aligned} Z_N(\lambda, \epsilon_1) &= \mathrm{Tr} \exp[-\beta(H_0 + \lambda V_I^{(\epsilon_1)})] \\ &< Z_N(\lambda, \epsilon_2) = \mathrm{Tr} \exp[-\beta(H_0 + \lambda V_I^{(\epsilon_2)})], \\ &\quad 0 < \epsilon_1 < \epsilon_2 < \epsilon_0. \end{aligned} \tag{IV. 15}$$

That is, the partition function appears as an *increasing* function of the ultraviolet cutoff ϵ, for ϵ sufficiently small.

We can now treat the "ultraviolet" cutoff ϵ on the same footing as the number of particles N in the previous section.

The regularized free energy per particle $F_N(\lambda, \epsilon)$ depends now on two cutoffs, N the number of particles and ϵ the ultraviolet cutoff. The true free energy is the limit

$$\lim_{N\to\infty} \lim_{\epsilon\to 0} F_N(\lambda, \epsilon) = F(\lambda). \tag{IV. 16}$$

However, $F(\lambda)$ is *also* by the previous argument

$$F_N = \lim_{N\to\infty} \sup_{\epsilon\to 0} F_N(\lambda, \epsilon). \qquad \text{(IV. 17)}$$

Let us suppose $F_N(\lambda, \epsilon)$ reaches its sup for $N=\infty$; then

$$F(\lambda) = \sup_N \sup_\epsilon F_N(\lambda, \epsilon), \quad N > N_0, \ \epsilon < \epsilon_0, \qquad \text{(IV. 18)}$$

and, by Theorem 5, we are able to extract from the sequence of $[P/P]$ generalized Padé approximations built on the knowledge of only a finite number of regularized terms of the perturbative expansion in λ of the partition function, a variational set of monotonously converging lower bounds to $F(\lambda)$.

It is not very difficult to treat the case where $F_N(\lambda, \epsilon)$ reaches its inf for $N=\infty$, in an analogous way, by multiplying the partition function by a suitable ϵ dependent factor.

Conclusion

In this paper, we have shown how the positivity properties of the partition function in the coupling constant lead to a new method for approximating it. This method enjoys the remarkable properties of converging for all temperatures, all densities, and all values of the coupling, still being built up from the standard perturbation series in the coupling, or its regularized version when the interaction is singular and the perturbation expansion does not exist. Furthermore, the approximation is achieved through monotonous sequences of increasing and decreasing bounds to the partition function.

To reach the thermodynamical limit, it is necessary to consider the variational properties that these monotonic bounds exhibit in the number of particles N (and in the cutoff ϵ when the interaction is singular). We then extract from the previous bounds monotonic sequences of converging upper (or lower) bounds to the free energy in the thermodynamical limit, which converge for any temperature, density, and value of the coupling.

Outlook

If one considers now the case of the Euclidean field theory, one deals with a double regularization: one for the volume divergences and the other for the ultraviolet ones. As we have shown for the statistical mechanical systems, it may be possible to construct PA which will give rise to variational properties both in the volume and the UV divergencies. This has been done explicitly for the UV divergencies coming from the theory of singular potentials in Ref. 9.

However, due to the lack of any existence theorem, it is not possible, for the moment, to use this technique in a rigourous way to achieve renormalization. We can, however, describe, shortly, what would be the procedure. In this approach, one first compute, PA for physical quantities at a given order P, in terms of the cutoff

$$G^{(P)}(\lambda, C),$$

where (P) is the order of PA, λ are the bare parameters, C the cutoffs. Then the cutoffs are fixed by requiring

$$\frac{\partial G^{(P)}(\lambda, C)}{\partial C} = 0. \qquad \text{(IV. 19)}$$

This fixes the "best" cutoff for the given order of approximations (P). Then the bare parameters λ, and the cutoffs C are eliminated with the help of the set of equations (IV. 19) among sufficient physical quantities G. This scheme would lead to have a renormalization procedure *simultaneous* with the summations of the perturbation series, in contradistinction with the ordinary process in which one renormalizes first and then is faced with the problem of summing up a divergent series. Furthermore, the difference between renormalizable and nonrenormalizable theories disappears in this scheme. Such scheme has been numerically tested for the four fermions interaction with zero mass.[11]

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APPENDIX

We want to prove the following:

Theorem: Let $d\mu_1, d\mu_2, \ldots, d\mu_n$ be positive measures having Laplace transforms $Z_1(\lambda), Z_2(\lambda), \ldots, Z_n(\lambda)$ Suppose that, for any positive or null λ, $Z_n(\lambda) \to Z(\lambda)$. (simple convergence) and that the support of all the measures $d\mu_n$ are contained in $(0, \infty)$. Then $Z(\lambda)$ is the Laplace transform of a positive measure $d\mu$ which is the limit of the $d\mu_n$ and the support of $d\mu$ is contained in $(0, \infty)$.

Proof: We first prove that $Z(\lambda)$ is the Laplace transform of a positive measure $d\mu$: $Z_n(\lambda)$ is holomorphic in $\mathrm{Re}\lambda > 0$. Furthermore, $Z_n(\lambda)$ is uniformly bounded in $\mathrm{Re}\lambda > 0$ because

$$|Z_n(\lambda)| < \int_0^\infty \exp(-\tau \mathrm{Re}\lambda)\, d\mu_n < \int_0^\infty d\mu_n = Z_n(0). \qquad \text{(A1)}$$

But for $n > n_0$

$$Z(0) - \epsilon < Z_n(0) < Z(0) + \epsilon. \qquad \text{(A2)}$$

Then for $n > n_0$

$$|Z_n(\lambda)| < C = Z(0) + \epsilon, \quad \mathrm{Re}\lambda > 0. \qquad \text{(A3)}$$

By Vitali's theorem, it follows due to the simple convergence for $\lambda > 0$ of the $Z_n(\lambda)$ towards $Z(\lambda)$ that:

$Z_n(\lambda) \to Z(\lambda)$ uniformly on arbitrary compacts in $\mathrm{Re}\lambda > 0$ and that $Z(\lambda)$ is holomorphic in $\mathrm{Re}\lambda > 0$.

As a consequence

$$\frac{d^P Z(\lambda)}{d\lambda^P} - \frac{d^P Z_n(\lambda)}{d\lambda^P} = \frac{p!}{2i\pi} \oint_C \frac{[Z(u) - Z_n(u)]}{(u-\lambda)^{P+1}}\, du. \qquad \text{(A4)}$$

Taking as circuit of integration a circle of radius R around λ, we have

$$\left| \frac{d^P Z(\lambda)}{d\lambda^P} - \frac{d^P Z_n(\lambda)}{d\lambda^P} \right| < \frac{p!}{R^P} \sup_C |Z(u) - Z_n(u)|, \qquad \text{(A5)}$$

which in $\mathrm{Re}\lambda > 0$ tends to zero for $n \to \infty$.

Therefore, the derivatives of $Z_n(\lambda)$ tend to the derivatives of $Z(\lambda)$ in $\mathrm{Re}\lambda > 0$.

Now, by using the Bernstein theorem[12] which states that the necessary and sufficient condition for a function to be the Laplace transform of a positive measure with support contained in $(0,\infty)$ is to be C_∞ on the interval $[0,\infty]$ with derivatives having alternating signs, it results that $Z(\lambda)$ is actually the Laplace transform of a positive measure $d\mu$.

We now proceed to prove that the $d\mu_n$ tend towards $d\mu$. It is clear that if the $d\mu_n$ converge, it is towards $d\mu$ because the inverse Laplace transform is unique up to trivial measure zero changes.

Let us introduce the Fourier transforms of the positive distributions $\exp(-\lambda\tau)\,d\mu_n(\tau)$ (λ real positive fixed):

$$Z_n(\lambda + i\rho) = \int_{-\infty}^{\infty} \exp(-i\rho\tau)\exp(-\lambda\tau)\,d\mu_n(\tau), \quad \rho > 0 \tag{A6}$$

(the support of $d\mu_n$ is $0,\infty$).

The *uniform* convergence of $Z_n(\lambda+i\rho)$ on arbitrary compacts in ρ, together with the bound (A3) implies the convergence of this sequence viewed as tempered distributions (convergence in the sense of S'). By Fourier transformation this gives the convergence of the $\exp(-\lambda\tau)\,d\mu_n(\tau)$ towards a limit distribution positive, therefore a positive measure. This convergence, proved for the test functions in S, can be extended to the continuous test functions, by using once again bound (A3).

We have used in the text a slightly generalized version of this theorem. In fact the support of $d\mu_n$ and $d\mu$ are all contained in an interval (b,∞), where b can be negative and finite. The convergence of $d\mu_n$ to $d\mu$ is obtained by an obvious change of variable to bring back the support to $(0,\infty)$.

Notes added in proof: M. Froissart has found an explicit example showing that the conjecture of paragraph II does not hold for the most general 3×3 matrix. However the conjecture seems to remain valid for the trace.

Theorem 3 obviously extends to nondiagonal elements in the position representation. This allows us to prove (I.3) in the boson case. Thanks to R. Balian for this remark.

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