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Upper bounds for the free energy. A generalisation of the Bogolubov inequality and the Feynman inequality

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Abstract. A set of lower bounds is obtained for $\langle e^{-A}\rangle$ from which a corresponding set of upper bounds is derived for the free energy. If the expectation values are expressed in the operator formalism the Bogolubov inequality (for Hermitian operators) is obtained as the first upper bound. When the expectation value is written as a path integral the Feynman inequality (for real actions) results as the first upper bound. It is shown that the second upper bound is identical to the one derived by Zeile for the path integral formalism while in the operator formalism this second upper bound is the one given by Dörre *et al.*

1. Introduction

Inequalities provide an important tool to obtain an approximation for some physical quantities; e.g. they allow us to find an upper bound for the free energy. Such inequalities permit us to approximate the real system (often too complicated to be solved exactly) by a model system which can be solved exactly. Using these inequalities one can choose the model system in such a way that the physical quantity under study is approximated as closely as possible. The advantage of considering problems via such inequalities is that it is often possible to handle problems beyond the scope of perturbation theory (treatment of systems for arbitrary coupling strength).

The quantity of main interest in statistical mechanics is the free energy. The relation between the free energy F and the partition function Z is

$$Z = e^{-\beta F}. \tag{1}$$

In the operator formalism the partition function is given by

$$Z = \mathrm{Tr}\,(e^{-\beta H}). \tag{2}$$

Suppose that the system with Hamiltonian H can be approximated by a model Hamiltonian H_0. When H and H_0 are Hermitian Hamiltonians the Bogolubov inequality is valid (Bogolubov 1947)

$$F \leqslant F_0 + \langle (H - H_0)\rangle \tag{3}$$

with F_0 the free energy corresponding with the Hamiltonian H_0. This Hamiltonian

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defines an expectation value

$$\langle A\rangle = \frac{1}{Z_0}\,\mathrm{Tr}\,(\mathrm{e}^{-\beta H_0}A) \tag{4}$$

with

$$Z_0 = \mathrm{e}^{-\beta F_0} = \mathrm{Tr}\,(\mathrm{e}^{-\beta H_0}). \tag{5}$$

In Feynman's path integral formulation (Feynman and Hibbs 1965) of quantum mechanics the partition function is written as

$$Z = \int_R \mathrm{d}x \int Dx(t)\,\exp(S[x(t)])\,\delta(x(0)-x)\,\delta(x(\beta)-x) \tag{6}$$

where the integration over x extends over the interval R (which may be the whole real space). For convenience a system with only one variable is considered in equation (6); the generalisation to an arbitrary number of variables is trivial. In the path integral formulation the system is described by the action functional S. In the path integral formalism one has the inequality (Feynman 1955, Feynman and Hibbs 1965)

$$F \leqslant F_0 - \beta^{-1}\langle (S - S_0)\rangle \tag{7}$$

with the expectation value

$$\langle A[x]\rangle = \frac{1}{Z_0}\int_R \mathrm{d}x \int Dx(t)\,A[x(t)]\,\exp(S_0[x(t)])\,\delta(x(0)-x)\,\delta(x(\beta)-x) \tag{8}$$

and the partition function

$$Z_0 = \int_R \mathrm{d}x \int Dx(t)\,\exp(S_0[x(t)])\,\delta(x(0)-x)\,\delta(x(\beta)-x). \tag{9}$$

Inequality (7) results immediately for real actions S and S_0 if Jensen's theorem for a convex function is applied. As far as we know this inequality has not been proved for complex actions. Such actions appear for systems described by a Lagrangian containing terms with an odd power of the velocity (e.g. if a magnetic field is present). In such a case one is no longer sure† about the validity of equation (7). From this point of view Bogolubov's inequality is more general than Feynman's inequality. On the other hand in some sense the action is a more general concept than the Hamiltonian. For example it is possible that the action contains a memory effect (i.e. an interaction which is non-local in time). A well known example for a non-local interaction is the polaron problem (Feynman 1955).

The structure of the paper is as follows: first an alternative derivation of the Bogolubov inequality and the Feynman inequality is presented in § 2. In § 3 a set of upper bounds to the free energy is constructed. Bogolubov's and Feynman's inequality result as the first upper bound in this set. In § 4 it is shown that the second upper bound is identical with the one derived by Zeile (1978) for the path-integral formalism and by Dörre *et al* (1979) for the operator formalism. In appendix 1 it is demonstrated that the inverse Laplace transform of a certain class of functions is positive. This result is of essential importance in the derivation of the different inequalities. The proof is based on Widder's formula (Widder 1934).

† There exist intuitive arguments (see e.g. Feynman and Hibbs 1965, Peeters and Devreese 1982) that the Feynman inequality is also valid for certain complex actions (i.e. when the actions can be derived from Hermitian Hamiltonians).

2. An alternative proof of the Bogolubov inequality and the Feynman inequality

As an illustration of our method the well known inequalities of Bogolubov and of Feynman are derived in this section. Because an inequality between two expectation values will be proved it is not necessary to say in which representation one works.

Consider the function

$$F(t) = \langle e^{-tA} \rangle, \qquad t \in \mathbb{R} \tag{10}$$

and its Laplace transform

$$f(s) = \mathscr{L}(F(t)) = \langle 1/(s+A) \rangle \tag{11}$$

with $\mathscr{L}$ the Laplace transform operator and $s > \min[A]$ which in the operator formalism is understood as $\min[A]$ = smallest eigenvalue of A. A and the expectation value $\langle \cdot \rangle$ are interpreted in the following way: (i) in the operator formalism, A is a Hermitian operator; the expectation value is defined by equation (4), (ii) in the path-integral formalism A is a real functional $A[x]$, the expectation value is defined by equation (8).

In earlier work by one of us (Devreese 1978), one started from $\langle e^{-tA} \rangle \geq e^{-t\langle A \rangle}$ to prove a corresponding inequality for the Laplace transform; i.e. $\langle 1/(s+A) \rangle \geq 1/(s+\langle A \rangle)$. In the present paper the reverse way will be followed: starting from successive approximations for the Laplace transform a set of bounds will be obtained for the inverse Laplace transform $\langle e^{-tA} \rangle$.

Following Devreese (1978) (see also appendix B of Devreese *et al* 1975) we introduce a parameter a_1 in the following way

$$f(s) = 1/(s+a_1) - \langle (A-a_1) \rangle / [(s+a_1)^2] + R_1(s; a_1) \tag{12}$$

with

$$R_1(s; a_1) = [1/(s+a_1)^2] \langle (A-a_1)^2/(s+A) \rangle. \tag{13}$$

Equation (12) is derived by using twice the identity

$$1/(a+x) = 1/x - a/x(a+x) \tag{14}$$

with $x = s + a_1$ and $a = A - a_1$. In appendix 1 it is shown that the inverse Laplace transform of $R_1(s; a_1)$ is positive. The approximation in this section consists of neglecting this positive term. Consequently the closest approximation is obtained when R_1 is a minimum; this means

$$\partial R_1 / \partial a_1 = 0 \tag{15}$$

or

$$a_1 = \langle A \rangle. \tag{16}$$

This extremum is indeed a minimum because (see appendix 1)

$$\mathscr{L}^{-1}\, \partial^2 R_1 / \partial a_1^2 |_{a_1 = \langle A \rangle} > 0. \tag{17}$$

Combining equations (11), (12) and (16) one finds for the inverse Laplace transform

$$F(t) = \mathscr{L}^{-1} f(s), \tag{18}$$

in the case that $t = 1$, the inequality

$$\langle e^{-A} \rangle \geq e^{-\langle A \rangle}. \tag{19}$$

The Bogolubov inequality results by taking A equal to the Hermitian operator

$$A = \beta(H - H_0) \tag{20}$$

which means that equation (19) becomes

$$Z \geqslant Z_0 \exp[-\beta(H - H_0)]. \tag{21}$$

Taking the logarithm of this inequality results in the upper bound (3) for the free energy.

To obtain the Feynman inequality one takes A equal to the real functional

$$A = -S[x] + S_0[x]. \tag{22}$$

With (22) in the inequality (19) and taking the logarithm one gets the Feynman inequality (7).

3. Generalisation of the inequality of Bogolubov and the inequality of Feynman

Introducing more parameters into the theory and applying equation (14) successively one will find a better approximation, i.e. a lower upper bound to the free energy. The aim of this chapter is to derive a set of lower bounds to the expectation value $\langle e^{-A}\rangle$.

In the same way as in § 2 (see also Devreese *et al* 1975) we introduce a new parameter a_2 in the term (13)

$$R_1(s; a_1) = \frac{1}{(s+a_1)^2}\left(\left\langle\frac{(A-a_1)^2}{(s+a_2)}\right\rangle - \left\langle\frac{(A-a_1)^2(A-a_2)}{(s+a_2)^2}\right\rangle\right) + R_2(s; a_1, a_2) \tag{23}$$

with

$$R_2(s; a_1, a_2) = \left\langle\frac{(A-a_1)^2}{(s+a_1)^2}\frac{(A-a_2)^2}{(s+a_2)^2}\frac{1}{(s+A)}\right\rangle. \tag{24}$$

Proceeding in the same way one can introduce n parameters $(a_1, \ldots, a_n)$. Finally one finds for the Laplace transform (11) the expression

$$f(s) = I_n(s; a_1, \ldots, a_n) + R_n(s; a_1, \ldots, a_n) \tag{25}$$

with

$$I_n(s; a_1, \ldots, a_n) = \sum_{m=1}^{n}\left\langle\left[\frac{1}{s+a_m} - \frac{(A-a_m)}{(s+a_m)^2}\right]\prod_{i=1}^{m-1}\frac{(A-a_i)^2}{(s+a_i)^2}\right\rangle \tag{26}$$

and

$$R_n(s; a_1, \ldots, a_n) = \left\langle\frac{1}{s+A}\prod_{i=1}^{n}\frac{(A-a_i)^2}{(s+a_i)^2}\right\rangle. \tag{27}$$

The product $\Pi_{i=1}^{m-1}$ in equation (26) should be interpreted as equal to 1 for $m = 1$. With the techniques given in appendix 1 one can prove that

$$\mathscr{L}^{-1}R_n(s; a_1, \ldots, a_n) \geqslant 0. \tag{28}$$

The present approximation consists in neglecting this term. The best approximation is obtained if the parameters a_i are determined by

$$\partial R_n/\partial a_i = 0, \qquad i = 1, \ldots, n \tag{29}$$

which results in

$$\left\langle \prod_{j=1}^{i-1} (A-a_j)^2(A-a_i) \prod_{j=i+1}^{n} (A-a_j)^2 \right\rangle = 0, \qquad i=1,\ldots,n. \tag{30}$$

Again the definition that $\Pi_{i=1}^{m-1} g_i = 1$ for $m=1$ and $\Pi_{i=m+1}^{n} g_i = 1$ for $m=n$ has been adopted. The solution of this set of equations will be denoted by $a_i^{(n)}$, $i=1,\ldots,n$. From equation (30) it is clear that for the nth bound one needs to calculate moments up to M_{2n-1}. These moments are defined by

$$M_n = \langle A^n \rangle. \tag{31}$$

In what follows several properties of the solutions of (30) are proved.

(1) The solutions $a_i^{(n)}$ of the n-nonlinear algebraic equations (30) are given by the roots of a polynomial of degree n. To see this rewrite (30) in the following way (see appendix 2)

$$\mathcal{M}\boldsymbol{X} + \boldsymbol{Y} = 0 \tag{32}$$

with $\mathcal{M}$ an $(n \times n)$ matrix with elements

$$\mathcal{M}_{ij} = M_{2n-(i+j)}, \qquad i,j=1,\ldots,n \tag{33}$$

and the vectors

$$Y_i = M_{2n-i}, \qquad i=1,\ldots,n \tag{34}$$

$$X_m = (-)^m \sum_{n_1=1}^{n} a_{n_1}^{(n)} \sum_{n_2=n_1+1}^{n} a_{n_2}^{(n)} \cdots \sum_{n_m=n_{m-1}+1}^{n} a_{n_m}^{(n)}, \qquad m=1,\ldots,n \tag{35}$$

with the definition $\Sigma_{n_1=p}^{n} = 0$ if $p > n$.

Inverting (32) results in a solution for X_i from which one can obtain $a_i^{(n)}$. From equation (35) it is clear that the X_i can be considered as the coefficients of the polynomial (define $X_0 = 1$)

$$\begin{aligned} P_n(x) &= \sum_{i=0}^{n} X_i x^{n-i} \\ &= \prod_{i=1}^{n} (x - a_i^{(n)}). \end{aligned} \tag{36}$$

(2) All the roots $a_i^{(n)}$ of equation (36) are real. From (32) (see also equation (30)) we know that all X_i are real because $\mathcal{M}_{ij}$ and Y_i are real. Suppose that $a_{n_0}^{(n)}$ is a complex root; then also its complex conjugate must be a root of (36). Consider equation (30) for $m = n_0$

$$\left\langle \prod_{\substack{m=1\\ m\neq n_0}}^{n} (A-a_i^{(n)})^2 A \right\rangle = a_{n_0}^{(n)} \left\langle \prod_{\substack{m=1\\ m\neq n_0}}^{n} (A-a_i^{(n)})^2 \right\rangle. \tag{37}$$

The expectation values on the left and the right-hand side of the above equation are real because (1) A is either a real functional or a Hermitian operator (which has real eigenvalues) and (2) $a_i^{(n)}$ is real or if $a_i^{(n)}$ is complex also its complex conjugate $\bar{a}_i^{(n)}$ is present which makes $(A-a_i^{(n)})(A-\bar{a}_i^{(n)})$ real. This forces us to conclude that $a_{n_0}^{(n)}$ has to be real and thus that all $a_i^{(n)}$ must be real.

(3) Now it is proved that the extremal points $a_i^{(n)}$ provide indeed a minimum for $\mathscr{L}^{-1}R_n(s; a_1, \ldots, a_n)$. To show this one calculates the second derivative

$$\partial^2 R_n/\partial a_m^2 = \left\langle \frac{2}{(s+a_m)^2} \prod_{\substack{i=1 \\ i\neq m}}^{n} \frac{(A-a_i)^2}{(s+a_i)^2} \right\rangle, \qquad m=1, \ldots, n. \tag{38}$$

With the same methods as in the appendix (using Widder's inversion formula) one proves that

$$\mathscr{L}^{-1}\, \partial^2 R_n/\partial a_m^2 |_{\{a_i=a_i^{(n)}\}} \geq 0, \qquad m=1, \ldots, n; \tag{39}$$

also

$$\partial^2 R_n/\partial a_i\, \partial a_j = \frac{2}{a_i - a_j}\left[\frac{1}{s+a_i}\frac{\partial R_n}{\partial a_j} - \frac{1}{s+a_j}\frac{\partial R_n}{\partial a_i}\right], \qquad i, j=1, \ldots, n \tag{40}$$

for $i\neq j$. If the parameters a_m are taken at the extremal point $a_m^{(n)}$ one has

$$\partial^2 R_n/\partial a_i\, \partial a_j |_{\{a_m=a_m^{(n)}\}} = 0, \qquad i\neq j, i; j=1, \ldots, n. \tag{41}$$

Intuitively one expects that with increasing n the rest term $\mathscr{L}^{-1} R_n$ decreases. This can be proved. Consider

$$R_{n-1}(s; a_1, \ldots, a_{n-1})$$
$$= \left\langle \frac{1}{s+a_n} \prod_{i=1}^{n-1} \frac{(A-a_i)^2}{(s+a_i)^2}\right\rangle - \left\langle \frac{(A-a_n)}{(s+a_n)^2} \prod_{i=1}^{n-1} \frac{(A-a_i)^2}{(s+a_i)^2}\right\rangle + R_n(s; a_1, \ldots, a_n); \tag{42}$$

this equality is valid for arbitrary parameters a_i. Because of equation (30) the second term on the RHS of (42) is zero when we take $a_n = a_n^{(n)}$. In the same way as before one proves that

$$\mathscr{L}^{-1} \left\langle \frac{1}{s+a_n} \prod_{i=1}^{n-1} \frac{(A-a_i)^2}{(s+a_i)^2}\right\rangle \geq 0. \tag{43}$$

Combining this inequality with equation (42) leads to the inequality

$$\mathscr{L}^{-1}R_{n-1}(s; a_1, \ldots, a_{n-1}) \geq \mathscr{L}^{-1}R_n(s; a_1, \ldots, a_{n-1}, a_n^{(n)}). \tag{44}$$

For the $(n-1)$th bound the parameters are determined by

$$\partial R_{n-1}/\partial a_i = 0, \qquad i=1, \ldots, n-1 \tag{45}$$

which gives the values $a_i = a_i^{(n-1)}$, while for the nth bound the condition

$$\partial R_n/\partial a_i = 0, \qquad i=1, \ldots, n \tag{46}$$

determines the parameters $a_i = a_i^{(n)}$. This means that

$$\mathscr{L}^{-1}R_n(s; a_1^{(n-1)}, \ldots, a_{n-1}^{(n-1)}, a_n^{(n)}) \geq \mathscr{L}^{-1}R_n(s; a_1^{(n)}, \ldots, a_{n-1}^{(n)}, a_n^{(n)}) \tag{47}$$

and combining this inequality with inequality (44) leads to

$$\mathscr{L}^{-1}R_{n-1}(s; a_1^{(n-1)}, \ldots, a_{n-1}^{(n-1)}) \geq \mathscr{L}^{-1}R_n(s; a_1^{(n)}, \ldots, a_n^{(n)}). \tag{48}$$

$t>0$ in the foregoing calculations (t is the variable in the inverse Laplace transforms). From the equations (25), (28) and (48) the final result can be formulated as

$$\langle e^{-A}\rangle \geq \mathscr{L}^{-1}I_n(s; a_1^{(n)}, \ldots, a_n^{(n)})|_{t=1} \tag{49}$$

and

$$\mathscr{L}^{-1}I_n(s;a_1^{(n)},\ldots,a_n^{(n)})|_{t=1} \geqslant \mathscr{L}^{-1}I_{n-1}(s;a_1^{(n-1)},\ldots,a_{n-1}^{(n-1)})|_{t=1} \tag{50}$$

where I_n is given by equation (26).

4. Discussion

Zeile (1978) has given a similar set-up of upper bounds to the free energy within Feynman's path integral formulation. If A is a real functional he finds the inequality

$$\langle \mathrm{e}^{-A}\rangle \geqslant \sum_{i=1}^{n} b_i^{(n)}\,\mathrm{e}^{x_i^{(n)}} \tag{51}$$

which is analogous to equation (49); $b_i^{(n)}$ and $x_i^{(n)}$ in (51) are determined by a set of $2n$ nonlinear algebraic equations. Dörre *et al* (1979) have derived a similar inequality for $n=1,2$ in the operator formalism. Taking the inverse Laplace transform of equation (26) we find the same form as equation (51). But in our case one only has to determine n-parameters $a_i^{(n)}$ $(=x_i^{(n)})$ which are the roots of a polynomial equation of degree n (given by equation (36)). The $b_i^{(n)}$ are immediately expressed in terms of the $x_i^{(n)}$ when one performs the inverse Laplace transform of (26). In the work of Zeile and Dörre *et al* and in our approach the parameters $b_i^{(n)}$, $x_i^{(n)}$ are a function of the moments M_1 up to M_{2n-1}. This suggests that both approaches are equivalent.

For $n=1$ and $n=2$ we have proved that one gets the same upper bound to the free energy. The case $n=1$ was considered in § 2. For $n=2$ in which then the parameters $x_i^{(n)}$ are determined by the polynomial (see (36))

$$x^2+Bx-C=0 \tag{52}$$

with

$$B=(M_3-M_1M_2)/(M_2-M_1^2), \tag{53}$$

$$C=(M_1M_3-M_2^2)/(M_2-M_1^2). \tag{54}$$

The solutions are

$$a_1^{(2)}=x_1^{(2)}=K_1+K-\lambda, \tag{55}$$

$$a_2^{(2)}=x_2^{(2)}=K_1+K+\lambda, \tag{56}$$

with the cumulants $K_1=M_1$, $K_2=M_2-M_1^2$, $K_3=M_3-3M_2M_1+2M_1^3$ and the parameters $K=K_3/2K_1$, $\lambda=(K^2+K_2)^{1/2}$. Finally in the path integral formalism we found the same upper bound as Zeile

$$F\leqslant F_0-\beta^{-1}(K_1+K)-\beta^{-1}\ln(\cosh\lambda-K\beta^{-1}\sinh\lambda) \tag{57}$$

with the moments given by $M_n=\langle(S_0-S)^n\rangle$.

The advantage of our method to the one of Zeile (1978) is that without additional effort we find at the same time upper bounds in the operator formalism and in the path integral formalism. In the operator formalism the moments are defined by $M_n=\beta^n\langle(H-H_0)^n\rangle$ while in the path integral formalism they are given by $M_n=\langle(S_0-S)^n\rangle$.

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Appendix 1.

In this appendix it is shown that several functions needed in §§ 2 and 3 are positive. In §§ 2 and 3 these functions were written as the inverse Laplace transform of another function. Therefore it is natural to look for an inversion formula (inverse Laplace transform) which relies on real variables only (avoiding the Bromwhich contour integration in the complex s-space).

Such a real inversion technique is realised by Widder's inversion formula (Widder (1934); for a nice application of this formula to the problem of Landau damping in plasma physics see Bohn and Flynn (1978))

$$F(t) = \lim_{n\to\infty}\left[\frac{(-)^n}{n!}s^{n+1}f^{(n)}(s)\right]_{s=n/t} \tag{A1.1}$$

with $f^{(n)}(s)$ the nth derivative of the Laplace transform $f(s) = \mathscr{L}F(t)$.

This formula will be used to prove that $\mathscr{L}^{-1}R_n \geqslant 0$ and $\mathscr{L}^{-1}\,\partial^2 R_n/\partial a_i^2 \geqslant 0$ (see equations (27) and (38)). First a few formulae which are needed in the proof are given. Consider the function

$$F(s) = 1/(s+a); \tag{A1.2}$$

after differentiating n times one has

$$F^{(n)}(s) = \frac{(-)^n n!}{(s+a)^{n+1}}. \tag{A1.3}$$

The nth derivation of a product of functions is given by

$$\frac{d^n}{ds^n}F(s)G(s) = \sum_{m=0}^{n}\binom{n}{m}G^{(n-m)}(s)F^{(m)}(s) \tag{A1.4}$$

with the binomial coefficient

$$\binom{n}{m} = \frac{n!}{m!(n-m)!} \tag{A1.5}$$

Applying this formula to the function

$$G_m(s) = 1/(s+a)^m \tag{A1.6}$$

gives for the nth derivative

$$G_m^{(n)}(s) = \frac{(-)^n(n+m-1)!}{(s+a)^{n+m}}. \tag{A1.7}$$

With these formulae it becomes easy to prove the following theorem.

Theorem. Given the function

$$g(s) = \prod_{i=1}^{m}\frac{1}{(s+x_i)^{k_i}}, \qquad x_i \in \mathbb{R}, \qquad k_i,\, m \in \mathbb{N} \tag{A1.8}$$

the sign of the inverse Laplace transform $G(t)=\mathscr{L}^{-1}g(s)$ is given by

$$\operatorname{sgn} G(t)=\operatorname{sgn} t^M, \qquad t\in\mathbb{R} \tag{A1.9}$$

with

$$M=\sum_{i=1}^{m} k_i-1. \tag{A1.10}$$

Proof. Using equations (A1.4) and (A1.7) one finds for the nth derivative of $g(s)$

$$g^{(n)}(s)=(-)^n\sum_{n_1=0}^{n}\sum_{n_2=0}^{n_1}\cdots\sum_{n_{m-1}=0}^{n_{m-2}}\prod_{i=1}^{m}\binom{n_{i-1}}{n_i}\frac{(n_{i-1}-n_i+k_i-1)!}{(s+x_i)^{n_{i-1}-n_i+k_i}} \tag{A1.11}$$

with the definition $n_0\equiv n$ and $n_m\equiv 0$. Putting this expression in Widder's formula (A1.1) one has for the inverse Laplace transform

$$G(t)=t^M H(t), \qquad t\in\mathbb{R} \tag{A1.12}$$

with

$$H(t)=\lim_{n\to\infty}\frac{n}{n!}\sum_{n_1=0}^{n}\sum_{n_2=0}^{n_1}\cdots\sum_{n_{m-1}=0}^{n_{m-2}}\prod_{i=1}^{m}\binom{n_{i-1}}{n_i}\frac{(n_{i-1}-n_i+k_i-1)!}{n^{k_i}(1+x_it/n)^{n_{i-1}-n_i+k_i}}. \tag{A1.13}$$

In the limit $n\to\infty$ each term in the sum of equation (A1.13) becomes positive. Thus $H(t)$ is positive because it is a sum of positive terms. This proves the theorem.

As an application of this theorem one can prove that the inverse Laplace transform of (see equation (13))

$$R_1(s;a_1)=[1/(s+a_1)^2]\langle(A-a_1)^2/(s+A)\rangle \tag{A1.14}$$

is positive for positive t. The proof is as follows.

In the path integral formulation A becomes a real quantity, thus $a_1=\langle A\rangle$ is also real. So we can apply the foregoing theorem. In the operator formalism the expectation value in equation (A1.14) can be expressed in a basis of eigenvectors of A. The eigenvalues of A are real because A is a Hermitian operator. And thus one can apply the theorem again. This proves that

$$\mathscr{L}^{-1}R_1(s;a_1)|_{a_1=\langle A\rangle}>0, \qquad t\in\mathbb{R}^+. \tag{A1.15}$$

As a second example consider the second derivative of $R_1(s;a_1)$ with respect to a_1 for $a_1=\langle A\rangle$

$$\partial^2R_1/\partial a_1^2|_{a_1=\langle A\rangle}=2/(s+\langle A\rangle)^3. \tag{A1.16}$$

From the theorem (equation (A1.9)) it is clear that the inverse Laplace transform of (A1.16) is indeed positive for $t\in\mathbb{R}^+$. In the same way one can prove similar properties for $R_n(s;a_1,\ldots,a_n)$.

Appendix 2.

In this appendix equation (30) of § 3

$$\left\langle\prod_{j=1}^{i-1}(A-a_j)^2(A-a_i)\prod_{j=i+1}^{n}(A-a_j)^2\right\rangle=0, \qquad i=1,\ldots,n \tag{A2.1}$$

will be simplified considerably. To do so write equation (A2.1) as

$$\left\langle \prod_{j=1}^{n} (A-a_j) \prod_{\substack{m=1 \\ m\neq i}}^{n} (A-a_m)^2 \right\rangle = 0, \qquad i=1,\ldots,n \tag{A2.2}$$

and after introducing the matrix

$$S_{ij} = X_{j-1}|_{a_i=0}, \qquad i,j=1,\ldots,n \tag{A2.3}$$

with the definitions

$$X_m = (-)^m \sum_{n_1=1}^{n} a_{n_1} \sum_{n_2=n_1+1}^{n} a_{n_2} \ldots \sum_{n_m=n_{m-1}+1}^{n} a_{n_m}, \qquad m=1,\ldots,n$$

$$X_0 = 1 \tag{A2.4}$$

$$\sum_{n_i=p}^{n} = 0 \qquad \text{if } p>n,$$

one can write equation (A2.2) as

$$\left\langle \prod_{j=1}^{n} (A-a_j) \left(\sum_{m=1}^{n} S_{im} A^{m-1} \right) \right\rangle = 0, \qquad i=1,\ldots,n. \tag{A2.5}$$

Writing out the product in equation (A2.5) leads to

$$\left\langle \left(\sum_{j=0}^{n} X_j A^{n-j} \right) \left(\sum_{m=1}^{n} S_{im} A^{m-1} \right) \right\rangle = 0, \qquad i=1,\ldots,n \tag{A2.6}$$

and remembering that $M_m = \langle A^m \rangle$ gives

$$\sum_{m=1}^{n} S_{im} \sum_{j=0}^{n} X_j M_{n+m-j-1} = 0, \qquad i=1,\ldots,n \tag{A2.7}$$

which becomes

$$S(\mathcal{M}\boldsymbol{X} + \boldsymbol{Y}) = 0 \tag{A2.8}$$

if we introduce the $n\times n$ matrix

$$\mathcal{M}_{ij} = M_{2n-(i+j)}, \qquad i=1,\ldots,n \tag{A2.9}$$

and the vector

$$Y_i = M_{2n-i}, \qquad i=1,\ldots,n, \tag{A2.10}$$

Multiplying equation (A2.8) with the inverse of the matrix S leads to

$$\mathcal{M}\boldsymbol{X} + \boldsymbol{Y} = 0 \tag{A2.11}$$

the result of this appendix. S^{-1} exists indeed because

$$\det S = (-)^n \prod_{i<j=1}^{n} (a_i - a_j) \tag{A2.12}$$

is non-zero due to the fact that all a_i are different from each other.

To get a clearer idea what equation (A2.11) looks like, we will write it down explicitly for the particular case of $n=3$

$$\begin{pmatrix} M_4 & M_3 & M_2 \\ M_3 & M_2 & M_1 \\ M_2 & M_1 & 1 \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} + \begin{pmatrix} M_5 \\ M_4 \\ M_3 \end{pmatrix} = 0 \tag{A2.13}$$

where

$$X_1 = -(a_1 + a_2 + a_3), \qquad X_2 = a_1 a_2 + a_1 a_3 + a_2 a_3, \qquad X_3 = a_1 a_2 a_3. \tag{A2.14}$$

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