

GENERALIZATION OF THE PEIERLS–BOGOLIUBOV INEQUALITY BY MEANS OF A QUANTUM-MECHANICAL VARIATIONAL PRINCIPLE

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The Peierls–Bogoliubov inequality was generalized and a set of inequalities was derived instead, so that every subsequent inequality in this set approximates the quantity in question with better precision than the preceding one. These inequalities lead to a sequence of improving upper bounds to the free energy of a quantum system if this system allows representation in terms of coherent states.

1. INTRODUCTION

It is well known that the following inequality

$$\langle \Psi | e^{-t\hat{H}} | \Psi \rangle \geq e^{-t\langle \Psi | \hat{H} | \Psi \rangle} \quad (1)$$

holds for any normalized quantum state $|\Psi\rangle$, self-adjoint Hamiltonian of a quantum system \hat{H} , and nonnegative parameter t . As a rule, this inequality is referred to in the theoretical physics as the Peierls–Bogoliubov inequality. It has been widely used as an intermediate step in numerous schemes of mathematical reasoning and in proofs of various theorems. For instance, it plays an important role in the proof of the left-hand side of the Lieb–Berezin inequality [1–3],

$$\int \exp(-tQ(\alpha, \bar{\alpha})) d\mu(\alpha) \leq \text{Sp}(\exp(-t\hat{H})) \leq \int \exp(-tP(\alpha, \bar{\alpha})) d\mu(\alpha) \quad (2)$$

which, in its turn, provides two-side bounds to the free energy of a quantum system in case the Hamiltonian of the system allows representation in terms of the set of coherent states $|\alpha\rangle$. Here $Q(\alpha, \bar{\alpha})$ and $P(\alpha, \bar{\alpha})$ are the so-called Wick and anti-Wick symbols of the Hamiltonian \hat{H} , such that

$$\hat{H} = \int P(\alpha, \bar{\alpha}) |\alpha\rangle\langle\alpha| d\mu(\alpha), \quad Q(\alpha, \bar{\alpha}) = \langle\alpha|\hat{H}|\alpha\rangle = \int e^{-|\alpha-\beta|^2} P(\beta, \bar{\beta}) d\mu(\beta),$$

$$\langle\alpha|\alpha\rangle = 1, \quad \langle\alpha|\beta\rangle = \exp\left(-\frac{1}{2}|\alpha|^2 - \frac{1}{2}|\beta|^2 + \bar{\alpha}\beta\right),$$

$$d\mu(\alpha) = \frac{1}{\pi} d\text{Re}(\alpha) d\text{Im}(\alpha),$$

and the integration in (2) is carried out over the whole complex plane α . The left-hand side of the inequality (2) is a direct consequence of the Peierls–Bogoliubov inequality:

$$\text{Sp} \left(e^{-t\hat{H}} \right) = \int \langle \alpha | e^{-t\hat{H}} | \alpha \rangle d\mu(\alpha) \geq \int e^{-t\langle \alpha | \hat{H} | \alpha \rangle} d\mu(\alpha) = \int e^{-tQ(\alpha, \bar{\alpha})} d\mu(\alpha).$$

At the same time the inequality (1) is of considerable value itself because it can be used to derive an upper bound to the ground state energy of a quantum system:

$$E_g \leq - \lim_{t \rightarrow +\infty} \frac{1}{t} \ln \langle \Psi | e^{-t\hat{H}} | \Psi \rangle \leq \langle \Psi | \hat{H} | \Psi \rangle. \quad (3)$$

Thus it is worthy to find a regular algorithm allowing to strengthen the inequality (1) so as to improve existing upper bounds obtained by the conventional variational method.

2. VARIATIONAL SCHEME

Assume that the Hamiltonian \hat{H} is of the form

$$\hat{H} = \sum_{n=1}^{\infty} E_n |E_n\rangle \langle E_n| + \int_{E'_1}^{E_{\max}} dE E |E\rangle \langle E|,$$

where $E'_1 \leq E_{\max} \leq +\infty$ and $\langle E | E_n \rangle = 0$. Energy levels may be degenerate in general case. Consider the Laplace transformation

$$f(s) = \int_0^{+\infty} dt e^{-st} \langle \Psi | e^{-t\hat{H}} | \Psi \rangle = \left\langle \Psi \left| \frac{1}{s + \hat{H}} \right| \Psi \right\rangle, \quad (4)$$

where $\text{Re}(s) > -\min(E_1, E'_1)$. An identity transformation made of two subsequent steps

$$\left\langle \Psi \left| \frac{1}{s + \hat{H}} \right| \Psi \right\rangle = \frac{1}{s + a_1} - \left\langle \Psi \left| \frac{\hat{H} - a_1}{(\hat{H} + s)(s + a_1)} \right| \Psi \right\rangle$$

and

$$\left\langle \Psi \left| \frac{1}{s + \hat{H}} \right| \Psi \right\rangle = \frac{1}{s + a_1} - \left\langle \Psi \left| \left[\frac{\hat{H} - a_1}{(s + a_1)^2} + \frac{(\hat{H} - a_1)^2}{(\hat{H} + s)(s + a_1)^2} \right] \right| \Psi \right\rangle \quad (5)$$

can be applied n times to the right-hand side of Eq.(4) leading to the identity

$$f(s) \equiv W_n(s, a_1, \dots, a_n) + R_n(s, a_1, \dots, a_n),$$

$$W_n(s, a_1, \dots, a_n) = \left\langle \Psi \left| \sum_{k=1}^n \left[\frac{1}{s + a_k} - \frac{\hat{H} - a_k}{(s + a_k)^2} \right] \prod_{j=1}^{k-1} \frac{(\hat{H} - a_j)^2}{(s + a_j)^2} \right| \Psi \right\rangle,$$

$$R_n(s, a_1, \dots, a_n) = \left\langle \Psi \left| \frac{1}{s + \hat{H}} \prod_{j=1}^n \frac{(\hat{H} - a_j)^2}{(s + a_j)^2} \right| \Psi \right\rangle,$$

where a_1, \dots, a_n is a set of arbitrary variational parameters chosen in such a way that both, W_n and R_n exist. To my knowledge, similar identity transformation was introduced firstly in [4]. The inverse Laplace transformation $\mathcal{L}^{-1}f(s)$ results in the identity

$$F(t) = \langle \Psi | e^{-t\hat{H}} | \Psi \rangle \equiv \rho_n(t, a_1, \dots, a_n) + \Omega_n(t, a_1, \dots, a_n), \quad (6)$$

where

$$\rho_n(t, a_1, \dots, a_n) = \mathcal{L}^{-1}R_n(t, a_1, \dots, a_n), \quad \Omega_n(t, a_1, \dots, a_n) = \mathcal{L}^{-1}W_n(t, a_1, \dots, a_n).$$

In case of real parameters a_1, \dots, a_n the following statements regarding the properties of $\rho_n(t, a_1, \dots, a_n)$ can be proved [5].

- (1.) $\rho_n(t, a_1, \dots, a_n) \geq 0$.
- (2.) $\rho_n(t, a_1, \dots, a_n)$ always has $n!$ absolute minima as a function of real parameters a_1, \dots, a_n and the location of these minima does not depend on t . All these minima are equivalent up to the permutation of parameters.
- (3.) The absolute minimum of $\rho_n(t, a_1, \dots, a_n)$ is provided by the solution to a system of equations

$$\frac{\partial}{\partial a_k} \rho_n(t, a_1, \dots, a_n) = 0$$

which can be effectively reduced to a polynomial equation of the n th order

$$P_n(x) = 0, \quad \text{where} \quad P_n(x) = \sum_{i=0}^n A_i x^{n-i}. \quad (7)$$

Here, $A_0 \equiv 1$ and the other n coefficients are given by the solution to a system of n linear equations

$$\mathcal{M}\vec{A} + \vec{Y} = 0,$$

where $Y_i = M_{2n-i}$, $\mathcal{M}_{ij} = M_{2n-(i+j)}$, $i, j = 1, 2, \dots, n$, and $M_n = \langle \Psi | (\hat{H})^n | \Psi \rangle$ are the moments of the Hamiltonian \hat{H} . Roots $(a_1^{(n)}, a_2^{(n)}, \dots, a_n^{(n)})$ of the polynomial $P_n(x)$ provide the absolute minimum for $\rho_n(t, a_1, \dots, a_n)$.

(4.) All roots $(a_1^{(n)}, a_2^{(n)}, \dots, a_n^{(n)})$ are real, mutually disjoint, i.e., $a_i^{(n)} \neq a_j^{(n)}$ if $i \neq j$, ($i, j = 1, 2, \dots, n$), and independent of the parameter t .

(5.) For any order n of approximation an inequality holds:

$$\rho_{n+1}(t, a_1^{(n+1)}, \dots, a_{n+1}^{(n+1)}) \leq \rho_n(t, a_1^{(n)}, \dots, a_n^{(n)}).$$

Moreover, if to take the statement (1.) into account, the limit

$$\lim_{n \rightarrow \infty} \rho_n(t, a_1^{(n)}, \dots, a_n^{(n)}) = \rho(t)$$

exists for any $t \geq 0$.

(6.) If \hat{H} is a bounded operator or if it possesses a discrete spectrum only, or the state $|\Psi\rangle$ can be expanded in the eigenstates corresponding to the discrete spectrum of \hat{H} exclusively, then $\rho(t) = 0$ for any $t \geq 0$. The same strict equality also holds if $|\Psi\rangle$ can be expanded in a set of eigenstates with bounded energies.

(7.) The following sequence of the upper bounds to the ground state energy of the Hamiltonian \hat{H} takes place

$$E_g \leq \min(a_1^{(n+1)}, \dots, a_{n+1}^{(n+1)}) \leq \min(a_1^{(n)}, \dots, a_n^{(n)}) \leq a_1^{(1)}, \quad (8)$$

and the limit exists $\mathcal{E}_0 = \lim_{n \rightarrow \infty} \min(a_1^{(n)}, \dots, a_n^{(n)})$, so that if the function $|\Psi\rangle$ is expanded in the eigenstates of \hat{H} as

$$|\Psi\rangle = \sum_{i=1}^{\infty} C_i |\tilde{E}_i\rangle + \int_{\tilde{E}'_1}^{+\infty} dEC(E) |E\rangle,$$

then

$$E_g \leq \min(\tilde{E}_1, \tilde{E}'_1) \leq \mathcal{E}_0,$$

and $\mathcal{E}_0 = \min(\tilde{E}_1, \tilde{E}'_1)$ in case of the bounded \hat{H} . The same strict equality also holds if $|\Psi\rangle$ can be expanded in a set of eigenstates with bounded energies.

In case when $|\Psi\rangle$ is only expanded in a set of eigenstates belonging to the discrete spectrum of \hat{H} , i.e.,

$$|\Psi\rangle = \sum_{i=1}^{\infty} C_i |E_i\rangle, \quad (9)$$

then the set of roots $(a_1^{(n)}, \dots, a_n^{(n)})$ converges to the set of eigenvalues $\{E_i\}$ which are present in the expansion (9):

$$(a_1^{(n)}, \dots, a_n^{(n)}) \xrightarrow{n \rightarrow \infty} \{E_i\}.$$

The same situation takes place in case of \hat{H} possessing discrete eigenvalues only. In case when the expansion (9) includes only the finite number N of different eigenvalues E_i , the proposed approximation algorithm stops at the order $n = N$. At this point $a_1^{(N)} = E_1$, $a_2^{(N)} = E_2$, ..., $a_N^{(N)} = E_N$ and the inequality (10) becomes an equality. Of course, it is formally possible to apply the identity transformation (5) several times more, thus introducing p additional parameters a_{N+1} , a_{N+2} , ..., a_{N+p} . In this case the function $\rho(t, a_1, a_2, \dots, a_N, a_{N+1}, \dots, a_{N+p})$, which is symmetric in its arguments $\{a_i\}$ by construction, has infinitely degenerate equivalent absolute minima at points $(E_1, \dots, E_N, a_{N+1}, \dots, a_{N+p})$ and the corresponding points obtained by the permutation of arguments, where this function is equal to zero. In effect, these minima are provided by only N out of total $N + p$ parameters $\{a_i\}$, those which are equal to the eigenvalues E_1, \dots, E_N . Only these parameters will make sense and enter the right-hand side of the inequality (10) transforming it into equality. The values of the remainder p parameters are totally irrelevant and drop out of the final results automatically.

3. GENERALIZED PEIERLS–BOGOLIUBOV INEQUALITY

As a consequence of statements (1.)–(5.), the following inequality holds

$$\langle \Psi | e^{-t\hat{H}} | \Psi \rangle \geq \Omega_n(t, a_1^{(n)}, \dots, a_n^{(n)}) \geq e^{-t\langle \Psi | \hat{H} | \Psi \rangle}, \quad (10)$$

and the middle part of this inequality can be calculated explicitly at the point $(a_1^{(n)}, \dots, a_n^{(n)})$:

$$\Omega \left(t, a_1^{(n)}, \dots, a_n^{(n)} \right) = \sum_{k=1}^n \langle \Psi | \left[\prod_{\substack{j=1 \\ j \neq k}}^n \frac{(\hat{H} - a_j^{(n)})^2}{(a_j^{(n)} - a_k^{(n)})^2} \right] | \Psi \rangle e^{-a_k^{(n)} t}.$$

The case $n = 1$ with the only variational parameter $a_1^{(1)} = \langle \Psi | \hat{H} | \Psi \rangle$ corresponds to the original Peierls–Bogoliubov inequality (1) which can be written in the form

$$\langle \Psi | e^{-t\hat{H}} | \Psi \rangle \geq \Omega_1(t, a_1^{(1)}) = e^{-ta_1^{(1)}}. \quad (11)$$

It follows from Eqs. (6), (11) and the statements (1.) and (5.) that

$$\begin{aligned} \Omega_1(0, a_1^{(1)}) &= \Omega_1(0, a_1^{(2)}, a_2^{(2)}) = \dots = \Omega \left(0, a_1^{(n)}, \dots, a_n^{(n)} \right) = 1, \\ \rho_1(0, a_1^{(1)}) &= \rho_1(0, a_1^{(2)}, a_2^{(2)}) = \dots = \rho \left(0, a_1^{(n)}, \dots, a_n^{(n)} \right) = 0. \end{aligned}$$

Therefore, good approximation is guaranteed for small t in all orders n .

4. GENERALIZED LIEB–BEREZIN INEQUALITY

The Lieb–Berezin inequality can also be generalized straightforward if one considers the coherent states $|\alpha\rangle$ in Eq.(2) as the $|\Psi\rangle$ state and is able to calculate explicitly the corresponding moments of \hat{H} as functions of complex variables $\alpha, \bar{\alpha}$. This results in the inequality

$$\begin{aligned} & \text{Sp} \left(e^{-t\hat{H}} \right) \geq \\ & \geq \int d\mu(\alpha) \sum_{k=1}^n \langle \alpha | \left[\prod_{\substack{j=1 \\ j \neq k}}^n \frac{\left(\hat{H} - a_j^{(n)}(\alpha, \bar{\alpha}) \right)^2}{\left(a_j^{(n)}(\alpha, \bar{\alpha}) - a_k^{(n)}(\alpha, \bar{\alpha}) \right)^2} \right] | \alpha \rangle e^{-a_k^{(n)}(\alpha, \bar{\alpha})t} \geq \\ & \geq \int e^{-tQ(\alpha, \bar{\alpha})} d\mu(\alpha) \end{aligned}$$

which can be constructed explicitly up to $n = 4$. For $n > 4$ the polynomial equation (7) cannot be solved analytically in general case.

5. CONCLUSION

It follows from Eqs.(3), (8), (11) that nearly any upper bound to the ground state energy obtained by the conventional variational principle can be improved by means of the proposed method. This can be done in two steps. First of all, one should construct a trial state $|\Phi(\{\xi\})\rangle$ as a function of variational parameters $\{\xi\}$ and choose these parameters to minimize the average $\langle \Phi(\{\xi\}) | \hat{H} | \Phi(\{\xi\}) \rangle$ as usual. In terms of the outlined above scheme, this step provides one with the first-order bound $a_1^{(1)}$. Then the subsequent better bounds (8) can be derived as it was shown if one takes the state $|\Phi(\{\xi\})\rangle$ with the optimal set of parameters $\{\xi\}$, defined at the first step, as the $|\Psi\rangle$ state throughout all computations.

What is more, the roots $(a_1^{(n)}, \dots, a_n^{(n)})$ of Eq.(7) provide not only the upper bound to the ground state energy but may also be used as estimations for the excited energy levels at least in the case of Hamiltonians with purely discrete spectrum.

It is worth noticing in conclusion that the proposed method of approximation has nothing to do with any kind of perturbation approach because the whole set of roots $(a_1^{(n)}, \dots, a_n^{(n)})$ of Eq. (7) is to be recalculated once again at any subsequent order of approximation n .

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