BOGOLYUBOV'S APPROXIMATION FOR BOSONS

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We analyze the approximating Hamiltonian method for Bose systems. Within the framework of this method, the pressure for the mean field model of an imperfect boson gas is calculated. The problem is considered by the systematic application of the Bogolyubov–Ginibre approximation.

1. Introduction

The approximating Hamiltonian method [1], having its roots in the work of Bogolyubov [2], gives possibility to provide an elegant way of proving the thermodynamical equivalence of some Hamiltonians. In the main, this method was applied for fermion models. In boson systems exhibiting the Bose condensation, we meet certain difficulties.

Pulé and Zagrebnov [3] considered the mean field boson gas by the approximating Hamiltonian technique and found the pressure of this model in the thermodynamic limit. The essential feature of their proof is the addition of sources, i.e. they used the Bogolyubov concept of quasiaverages. Here, we suggest an alternative way of applying the approximating Hamiltonian method for boson models.

Consider a system of identical bosons of mass m confined to a d-dimensional cubic box $\Lambda \subset \mathbb{R}^d$ of volume V centered around the origin. Let $E_0^\Lambda < E_1^\Lambda \leq E_2^\Lambda \leq \dots$ be the eigenvalues of the operator $h_\Lambda \doteq -\Delta/(2m)$ (we suppose $\hbar = 1$) on Λ with some linear boundary conditions, and let $\{\Phi_l^\Lambda\}$ with $l = 0, 1, 2, \dots$ be the corresponding eigenfunctions. Let $\mathcal{F}_\Lambda$ be the symmetric Fock space constructed from $L^2(\Lambda)$. Let $a_l \doteq a(\Phi_l^\Lambda)$ and $a_l^\dagger \doteq a^\dagger(\Phi_l^\Lambda)$ be the boson annihilation and creation operators on $\mathcal{F}_\Lambda$. Denote, by T_Λ, the Hamiltonian of the free Bose gas on $\mathcal{F}_\Lambda$ constructed from h_Λ in the usual manner, that is $T_\Lambda = \sum_{l=0}^\infty E_l^\Lambda N_l$, where $N_l = a_l^\dagger a_l$. Let $N_\Lambda = \sum_{l=0}^\infty N_l$ be the operator of the number of particles on $\mathcal{F}_\Lambda$.

The Hamiltonian we consider is

$$H_\Lambda = T_\Lambda + \frac{a}{2V} N_\Lambda^2, \tag{1}$$

where a is a positive coupling constant. Hamiltonian (1) is known as the mean field Bose gas model [4].

Let $\mu_0 \doteq \lim_{\Lambda\uparrow\mathbb{R}^d} E_0^\Lambda$. Denote, by $p_0(\mu)$ and $\rho_0(\mu)$, the grand-canonical pressure and the density, respectively, for the free Bose gas at chemical potential $\mu < \mu_0$, that is

$$p_0(\mu) = -\int \ln[1 - \exp(-\beta(\nu - \mu))] F(d\nu),$$

$$\rho_0(\mu) = \int \frac{1}{\exp(\beta(\nu - \mu)) - 1} F(d\nu),$$

F being the integrated density of states of h_Λ in the limit $\Lambda \uparrow \mathbb{R}^d$. Let $\rho_c \doteq \lim_{\mu\to\mu_0} \rho_0(\mu)$. The grand-canonical pressure of the mean field Bose gas model is

$$p_\Lambda(\mu) = \frac{1}{\beta V} \ln \operatorname{Tr} \exp[-\beta(H_\Lambda - \mu N_\Lambda)]. \tag{2}$$

We put $p(\mu) = \lim_{\Lambda\uparrow\mathbb{R}^d} p_\Lambda(\mu)$.

The main result of work [3] is the following:

Proposition 1. *Pressure (2) in the thermodynamic limit exists and is given by*

$$p(\mu) = \begin{cases} \dfrac{1}{2} a\rho^2(\mu) + p_0(\mu - a\rho(\mu)) & \text{if } \mu \leq \mu_c, \\ \dfrac{(\mu - \mu_0)^2}{2a} + p_0(\mu_0) & \text{if } \mu > \mu_c, \end{cases} \tag{3}$$

where $\mu_c = \mu_0 + a\rho_c$, and $\rho(\mu)$ is the unique solution of the equation $\rho = \rho_0(\mu - a\rho)$.

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This result was obtained by many authors for special boundary conditions (see [3] for references). The innovation of work [3] is in proving Proposition 1 by the approximating Hamiltonian method.

The main technical ingredient of the approximating Hamiltonian method is an estimate for the difference of the appropriate pressures of model and approximating Hamiltonians obtained by using the Bogolyubov convexity inequality [5]. But, in the case of model (1), the obvious intention to use this inequality for the "natural" approximating Hamiltonian

$$H_\Lambda^{\rm appr}(\rho) = T_\Lambda + a\rho N_\Lambda - \frac{a\rho^2}{2}V, \qquad (4)$$

where ρ is the self-consistency parameter, meets the failure. Really, by Bogolyubov's inequality,

$$0 \le p_\Lambda^{\rm appr}(\bar\rho_\Lambda,\mu) - p_\Lambda(\mu) \le$$

$$\le \frac{1}{V}\langle H_\Lambda - H_\Lambda^{\rm appr}(\bar\rho_\Lambda)\rangle_{H_\Lambda^{\rm appr}(\bar\rho_\Lambda)}, \qquad (5)$$

where

$$p_\Lambda^{\rm appr}(\rho,\mu) = \frac{1}{\beta V}\ln {\rm Tr}\exp[-\beta(H_\Lambda^{\rm appr}(\rho) - \mu N_\Lambda)],$$

$\langle \dots \rangle_\Gamma$ denotes the appropriate grand-canonical average with respect to the Hamiltonian Γ, and $\bar\rho_\Lambda$ satisfies the self-consistency equation

$$\bar\rho_\Lambda = \frac{1}{V}\langle N_\Lambda\rangle_{H_\Lambda^{\rm appr}(\bar\rho_\Lambda)}.$$

One can see that the right-hand side of (5) does not tend to zero as $V\to\infty$ for all $\mu\in\mathbb{R}$. It tends to $a\rho_0^2/2$, where ρ_0 is the Bose condensate density. Thus, the thermodynamical equivalence of the model Hamiltonian (1) and the approximating Hamiltonian (4) takes place only in the domain, where there is no Bose condensate. One easily obtains that this domain is $\mu \le \mu_{\rm c}$, and

$$p(\mu) = \inf_{\alpha<\mu_0}\left[\frac{(\mu-\alpha)^2}{2a} + p_0(\alpha)\right]. \qquad (6)$$

Curiously, that expressions (3) and (6) are equal for any μ. This fact holds out a hope for the chance to use, nevertheless, the approximating Hamiltonian method for the mean field model. It is clearly necessary to construct a different approximating Hamiltonian. This idea was realized in [3].

First, the authors of [3] constructed the auxiliary Hamiltonian for $\eta\in\mathbb{C}$,

$$H_\Lambda^{\rm P-Z}(\eta) = H_\Lambda + \sqrt{V}(\eta a_0^\dagger + \eta^* a_0). \qquad (7)$$

A convenient approximating Hamiltonian has the form

$$H_\Lambda^{\rm P-Z}(\rho,\eta) = T_\Lambda + a\rho N_\Lambda - \frac{a\rho^2}{2}V +$$

$$+\sqrt{V}(\eta a_0^\dagger + \eta^* a_0), \qquad (8)$$

where the self-consistency parameter $\rho\in\mathbb{R}$.

Next, to prove Proposition 1, the authors showed that, for $\eta\ne 0$, the pressure

$$p_\Lambda^{\rm P-Z}(\eta,\mu) = \frac{1}{\beta V}\ln{\rm Tr}\exp[-\beta(H_\Lambda^{\rm P-Z}(\eta) - \mu N_\Lambda)]$$

in the thermodynamic limit coincides with the pressure

$$p_\Lambda^{\rm P-Z}(\rho,\eta,\mu) = \frac{1}{\beta V}\ln{\rm Tr}\exp[-\beta(H_\Lambda^{\rm P-Z}(\rho,\eta) - \mu N_\Lambda)]$$

minimized with respect to ρ (Lemmata 1 and 2 in [3]) and that, in turn, this minimization can be performed after the passage to the limit (Lemma 3 in [3]).

Finally, the authors switched off the source η ($\eta\to 0$) in Lemma 4 to obtain the limiting pressure $p(\mu)$.

For Hamiltonians (7) and (8), the Bogolyubov's convexity inequality is

$$0 \le p_\Lambda^{\rm P-Z}(\bar\rho_\Lambda,\eta,\mu) - p_\Lambda^{\rm P-Z}(\eta,\mu) \le \frac{1}{2V^2}\Delta_\Lambda(\eta),$$

where

$$\Delta_\Lambda(\eta) = a\langle (N_\Lambda - V\bar\rho_\Lambda)^2\rangle_{H_\Lambda^{\rm P-Z}(\bar\rho_\Lambda,\eta)},$$

and $\bar\rho_\Lambda$ satisfies the equation

$$\bar\rho_\Lambda = \frac{1}{V}\langle N_\Lambda\rangle_{H_\Lambda^{\rm P-Z}(\bar\rho_\Lambda,\eta)}.$$

In this case, as distinct from case (5), the authors proved that

$$\lim_{V\to\infty}\frac{1}{V^2}\Delta_\Lambda(\eta) = 0$$

for $\eta\ne 0$. Therefore (Lemma 2 of [3]),

$$\lim_{\Lambda\uparrow\mathbb{R}^d} p_\Lambda^{\rm P-Z}(\eta,\mu) = \lim_{\Lambda\uparrow\mathbb{R}^d} p_\Lambda^{\rm P-Z}(\bar\rho_\Lambda,\eta,\mu) \qquad (9)$$

for $\eta\ne 0$. This is the benefit of the Pulé–Zagrebnov approach.

2. Application of the Approximating Hamiltonian Method to the Mean Field Model

Let us first restrict our discussion to the cases of periodic, Dirichlet, Neumann, and repulsive-wall boundary conditions. In the case of attractive walls, there are two negative eigenvalues for the free Bose gas. Owing to this fact, we have some features in the thermodynamical properties of the model. We consider the case of attractive boundary conditions separately.

We suggest to take advantage of the macroscopic occupation of the zero momentum one-particle state to replace the corresponding operators $a_0, a_0^\dagger$ by c-numbers [6–8]. Therefore, we define

$$\mathcal{H}_\Lambda(c) = \sum_{l=1}^{\infty} \left[E_l^\Lambda - \mu + |c|^2 a\right] N_l + \frac{a}{2V} N_\Lambda^{'2} +$$

$$+\frac{a|c|^2}{2} + \frac{a|c|^4}{2} V + (E_0^\Lambda - \mu)|c|^2 V, \tag{10}$$

where $c \in \mathbb{C}$, $N_\Lambda^{'} = \sum_{l=1}^{\infty} N_l$, and the Hamiltonian $\mathcal{H}_\Lambda(c)$ contains the term $-\mu N_\Lambda$. This is the Bogolyubov approximation which was proposed as early as 1947 [2, 9]. The replacement is exact in the thermodynamic limit [10]. Therefore, we have

$$\lim_{\Lambda\uparrow\mathbb{R}^d} p_\Lambda(\mu) = \lim_{\Lambda\uparrow\mathbb{R}^d} \sup_c p_\Lambda(c,\mu) \equiv p(\bar{c},\mu), \tag{11}$$

where

$$p_\Lambda(c,\mu) = \frac{1}{\beta V} \ln \mathrm{Tr}' \exp[-\beta \mathcal{H}_\Lambda(c)],$$

and $|\bar{c}|^2$ is the density of the Bose condensate. Tr' means trace in $\mathcal{F}_\Lambda^{'}$, where $\mathcal{F}_\Lambda^{'}$ is the boson Fock space constructed on the orthogonal complement of the one-dimensional subspace of $L^2(\Lambda)$ generated by Φ_0^Λ.

Starting from Hamiltonian (10), we get the following approximating Hamiltonian for $\rho' \in \mathbb{R}$:

$$\mathcal{H}_\Lambda(\bar{c},\rho') = \sum_{l=1}^{\infty} \left(E_l^\Lambda - \mu + |\bar{c}|^2 a\right) N_l +$$

$$+\frac{a|\bar{c}|^2}{2} + \frac{a|\bar{c}|^4}{2} V + (E_0^\Lambda - \mu)|\bar{c}|^2 V + a\rho' N_\Lambda' - \frac{a\rho'^2}{2} V. \tag{12}$$

Now, we are going to apply the Bogolyubov's convexity inequality

$$0 \le p_\Lambda(\bar{\rho}_\Lambda', \bar{c}, \mu) - p_\Lambda(\bar{c},\mu) \le \frac{1}{2V^2} \Delta_\Lambda'(\bar{c}), \tag{13}$$

where

$$p_\Lambda(\rho', c, \mu) = \frac{1}{\beta V} \ln \mathrm{Tr}' \exp\left[-\beta \mathcal{H}_\Lambda(c,\rho')\right],$$

$$\Delta_\Lambda'(\bar{c}) = a\langle (N_\Lambda' - V\bar{\rho}_\Lambda')^2 \rangle_{\mathcal{H}_\Lambda(\bar{c},\bar{\rho}_\Lambda')},$$

and $\bar{\rho}_\Lambda'$ satisfies the equation

$$\bar{\rho}_\Lambda' = \frac{1}{V} \langle N_\Lambda' \rangle_{\mathcal{H}_\Lambda(\bar{c},\bar{\rho}_\Lambda')}.$$

One calculates

$$\Delta_\Lambda'(\bar{c}) = a \sum_{l=1}^{\infty} \frac{\exp(\beta\epsilon_l^\Lambda)}{[\exp(\beta\epsilon_l^\Lambda) - 1]^2},$$

where $\epsilon_l^\Lambda = E_l^\Lambda - \mu + a(\bar{\rho}_\Lambda' + |\bar{c}|^2)$. Referring to the inequality $\coth x < 1 + x^{-1}$ with $x \ge 0$, we get

$$\Delta_\Lambda'(\bar{c}) < a \sum_{l=1}^{\infty} \frac{1}{\exp(\beta\epsilon_l^\Lambda) - 1} \left(1 + \frac{2}{\beta\epsilon_l^\Lambda}\right). \tag{14}$$

Use inequality [11] $\left\langle [A,[H,A^\dagger]] \right\rangle \ge 0$ which is valid for any operator A and for any self-conjugate Hamiltonian H. Take $A = a_l^\dagger$, $H = \mathcal{H}_\Lambda(\bar{c},\rho')$. One gets $E_0^\Lambda + a(\bar{\rho}_\Lambda' + |\bar{c}|^2) - \mu \ge 0$ for large V. So we obtain that

$$\epsilon_l^\Lambda > E_1^\Lambda - E_0^\Lambda \ge \frac{\pi^2}{2m} V^{-2/3} \qquad \text{for } l = 1,2,3,\ldots. \tag{15}$$

Inserting this estimate into (14), we have

$$\Delta_\Lambda'(\bar{c}) < a\bar{\rho}_\Lambda' V \left(1 + \frac{4m}{\pi^2\beta} V^{2/3}\right).$$

Therefore,

$$\lim_{V\to\infty} \frac{\Delta_\Lambda'(\bar{c})}{V^2} = 0,$$

and we conclude that

$$\lim_{\Lambda\uparrow\mathbb{R}^d} p_\Lambda(\mu) = \lim_{\Lambda\uparrow\mathbb{R}^d} p_\Lambda(\bar{\rho}_\Lambda', \bar{c}, \mu).$$

Hence, the grand-canonical pressure of the mean field model is

$$p(\mu) = -\frac{a|\bar{c}|^4}{2} + (\mu - \mu_0)|\bar{c}|^2 +$$

$$+ \inf_{\rho\ge 0} \left[\frac{a\rho^2}{2} + p_0(\mu - a(|\bar{c}|^2 + \rho))\right].$$

Finally, for $\mu \le \mu_c$, we have $|\bar{c}| = 0$, and $\rho'(\mu)$ is the unique solution of $\rho' = \rho_0(\mu - a\rho')$; for $\mu > \mu_c$, we have $\mu - a(|\bar{c}|^2 + \rho') = \mu_0$. Proposition 1 is proved.

From the very beginning, we consider the case of a cubic box Λ. If we take a parallelepiped of the same volume with sides of length $L_j = V^{\alpha_j}$, $j = 1, 2, 3$, such that $\alpha_1 \ge \alpha_2 \ge \alpha_3 > 0$ and $\alpha_1 + \alpha_2 + \alpha_3 = 1$, the situation changes. We can prove estimate (15) for $\alpha_1 < 1/2$ only. For a long parallelepiped in the direction $j = 1$, there is the generalized condensation in Girardeau's sense [12], and the proposed method must be improved.

Consider the case of attractive walls in the dimension $d = 1$. The $d > 1$ generalization becomes more tedious but is not hard. The spectrum of the one-dimensional Schrödinger equation $-\frac{1}{2m}\Phi'' = \varepsilon^\Lambda \Phi$ with attractive boundary conditions $\Phi'(-L/2) = \sigma\Phi(-L/2), \Phi'(L/2) = -\sigma\Phi(L/2)$, where $\sigma < 0$, consists of two negative eigenvalues tending to the same limit (when $L \to \infty$) and an infinite number of positive eigenvalues (for $L|\sigma| > 2$), namely

$$\varepsilon_0^\Lambda = -\frac{\sigma^2}{2m} - O(e^{-L|\sigma|}),$$

$$\varepsilon_1^\Lambda = -\frac{\sigma^2}{2m} + O(e^{-L|\sigma|}),$$

$$\frac{1}{2m}\left(\frac{(k-1)\pi}{L}\right)^2 < \varepsilon_k^\Lambda < \frac{1}{2m}\left(\frac{k\pi}{L}\right)^2 \qquad \text{for } k \ge 2.$$

We take this fact into account in the Bogolyubov approximation, replacing the operators $a_0^\#$, as well as $a_1^\#$, by c-numbers. Thus, instead of the approximating Hamiltonian (10), we can write

$$\mathcal{H}_\Lambda(c) = (\varepsilon_0^\Lambda - \mu)|c|^2 L + \frac{a|c|^4}{2} L + \sum_{l=2}^{\infty} \big(\varepsilon_l^\Lambda - \mu +$$

$$+|c|^2 a\big) N_l + \frac{a}{2L}\widetilde{N}_\Lambda^2 + \frac{a|c|^2}{2} + \Delta\varepsilon^\Lambda |c_1|^2 L, \qquad (16)$$

where $\Delta\varepsilon^\Lambda \doteq \varepsilon_1^\Lambda - \varepsilon_0^\Lambda \sim O(e^{-L|\sigma|}), \widetilde{N}_\Lambda = \sum_{l=2}^\infty N_l$ and $|c|^2 = |c_0|^2 + |c_1|^2$ with $|c_i|^2 = \langle a_i^\dagger a_i / L\rangle_{\mathcal{H}_\Lambda(c)}, i = 0, 1$. Obviously, the last term in (16) is inessential in the thermodynamic limit. Reiterating our previous consideration, we prove Proposition 1 in the case of attractive walls. The only difference in comparison with the above-stated cases of boundary conditions is connected with the replacement of the operator N'_Λ by $\widetilde{N}_\Lambda$. Thus, we must begin to sum over l from 2 in the appropriate formulae, and the main estimate (15) is

$$\epsilon_l^\Lambda > \varepsilon_2^\Lambda - \varepsilon_0^\Lambda > \frac{\sigma^2}{2m}$$

for $l = 2, 3, \ldots$.

In [13], Vandevenne and Verbeure rigorously studied the imperfect Bose gas with attractive boundary conditions, where

$$\tilde{H}_\Lambda = T_\Lambda + \frac{a}{2V}\tilde{N}_\Lambda^2. \qquad (17)$$

The authors gave a proof of the occurrence of Bose condensation in the one-dimensional case. The condensation is equally distributed over the two negative energy levels and is localized in the same area as that for the free Bose gas with attractive boundary conditions [14]. Remark that the interaction in (17) is not of the usual form (1). The reason for choosing (17) instead of (1) is the breaking of the spatial translation invariance in the terms with N_0 and N_1.

The model Hamiltonian (17) can be treated by the stereotyped approximating Hamiltonian method, so long as we have

$$\lim_{V\to\infty} \langle \tilde{H}_\Lambda - \tilde{H}_\Lambda^{\rm appr}(\bar{\rho}_\Lambda)\rangle_{\tilde{H}_\Lambda^{\rm appr}(\bar{\rho}_\Lambda)} = 0,$$

where

$$\tilde{H}_\Lambda^{\rm appr}(\rho) = T_\Lambda + a\rho\tilde{N}_\Lambda - \frac{a\rho^2}{2}V,$$

and $\bar{\rho}_\Lambda$ satisfies the self-consistency equation

$$\bar{\rho}_\Lambda = \frac{1}{V}\langle \tilde{N}_\Lambda\rangle_{\tilde{H}_\Lambda^{\rm appr}(\bar{\rho}_\Lambda)}.$$

As distinct from the usual Hamiltonian (1), Hamiltonian (17) is not superstable, and $\mu \le \mu_0 = -d\sigma^2/(2m)$. Consequently, one must take this restriction into account in the formula for the pressure of model (17),

$$\tilde{p}(\mu) = \lim_{\Lambda\uparrow\mathbb{R}^d} \tilde{p}_\Lambda^{\rm appr}(\bar{\rho}, \mu) = \inf_{\rho\ge 0}\left[\frac{a\rho^2}{2} + p_0(\mu - a\rho)\right],$$

where

$$\tilde{p}_\Lambda^{\rm appr}(\rho, \mu) = \frac{1}{\beta V}\ln \operatorname{Tr}\exp\left[-\beta\left(\tilde{H}_\Lambda^{\rm appr}(\rho) - \mu N_\Lambda\right)\right].$$

We conclude by remarking that, in the case of attractive boundary conditions, the condensate has essentially infinite density and occupies essentially zero volume near the walls as for the free Bose gas.

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БОГОЛЮБОВСЬКА АПРОКСИМАЦІЯ ДЛЯ БОЗОНОВ

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Р е з ю м е

Проаналізовано метод апроксимуючого гамільтоніана для бозе-систем. У межах цього методу знайдено тиск для моделі середнього поля неідеального бозе-газу. Задачу розглянуто за допомогою послідовного застосування апроксимації Боголюбова–Жінібра.