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COMMENT

Comments on the approximating Hamiltonian method for imperfect boson gas

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Abstract

In the recent paper (Pulé J V and Zagrebnov V A 2004 The approximating Hamiltonian method for the imperfect boson gas *J. Phys. A: Math. Gen.* **45** 3565–83) the pressure for the imperfect (mean field) boson gas is derived by a method based on the approximating Hamiltonian argument. We give some comments about this derivation.

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1. Approximating Hamiltonian

For the reader's convenience we recall the set-up of the problem. Below we follow essentially the notations of the paper [1]. Consider a system of identical bosons of mass m enclosed in a smooth connected bounded domain $\Lambda \subset \mathbb{R}^d$ (of volume $|\Lambda| = V$) containing the origin of coordinates. Let $E_0^\Lambda \leqslant E_1^\Lambda \leqslant E_2^\Lambda \leqslant E_3^\Lambda \leqslant \cdots$ be the eigenvalues of $h_\Lambda := -\Delta/2m$ on Λ with some boundary conditions and let $\{\phi_l^\Lambda\}$ with $l = 0, 1, 2, 3, \dots$ be the corresponding eigenfunctions. Let $a_l := a(\phi_l^\Lambda)$ and $a_l^* := a^*(\phi_l^\Lambda)$ be the boson annihilation and creation operators respectively on the Fock space $\mathcal{F}_\Lambda$, satisfying $[a_l, a_{l'}^*] = \delta_{l,l'}$. Let T_Λ be the Hamiltonian of the *free* Bose gas, that is $T_\Lambda = \sum_{l=0}^\infty E_l^\Lambda N_l$, where $N_l = a_l^* a_l$. Let $N_\Lambda = \sum_{l=0}^\infty N_l$ be the operator corresponding to the number of particles in Λ. The Hamiltonian of interacting bosons,

$$H_\Lambda = T_\Lambda + \frac{a}{2V} N_\Lambda^2 \tag{1.1}$$

with $a > 0$, is known as *imperfect* or *mean field* boson gas. The grand-canonical pressure of the mean field boson model with Hamiltonian (1.1) is

$$p_\Lambda(\mu) = \frac{1}{\beta V} \ln \operatorname{Tr} \exp\{-\beta(H_\Lambda - \mu N_\Lambda)\},$$

and we put in the thermodynamic limit

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

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Here we consider, for simplicity, the *Dirichlet* boundary conditions; then $\mu_0 := \lim_{\Lambda\uparrow\mathbb{R}^d} E_0^\Lambda = 0$. Generalization to other types of conditions is identical to that in [1]. Put $p_0(\mu)$ and $\rho_0(\mu)$ for the grand-canonical pressure and mean density respectively for the free Bose gas at chemical potential $\mu < \mu_0 = 0$, that is

$$p_0(\mu) = -\int \ln(1 - \mathrm{e}^{-\beta(\eta-\mu)}) F(\mathrm{d}\eta) \qquad \text{and} \qquad \rho_0(\mu) = \int \frac{1}{\mathrm{e}^{\beta(\eta-\mu)} - 1} F(\mathrm{d}\eta),$$

$F(\eta)$ being the integrated density of states of h_Λ in the limit $\Lambda \uparrow \mathbb{R}^d$. Let $\rho_c := \lim_{\mu\to 0} \rho_0(\mu)$ denote the free boson gas critical density, which is *bounded*, if $d > 2$. The main property of the mean field boson gas is resumed by

Proposition. *The pressure in the thermodynamic limit $p(\mu)$ exists and is given by*

$$p(\mu) = \begin{cases} \dfrac{1}{2} a\rho^2(\mu) + p_0(\mu - a\rho(\mu)) & \text{if} \quad \mu \leqslant \mu_c; \\ \dfrac{\mu^2}{2a} + p_0(\mu_0 = 0) & \text{if} \quad \mu > \mu_c, \end{cases} \tag{1.2}$$

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

It is known that this result, for special boundary conditions implying $\mu_0 = 0$, can be proved in several ways. The proof in [1] is more general than others and is based on a simple application of the *approximating* Hamiltonian technique. To this end they use the following *auxiliary* Hamiltonians for $\rho \in \mathbb{R}$ and $\eta \in \mathbb{C}$, with sources in zero mode $l = 0$:

$$H_\Lambda(\eta) = H_\Lambda + \sqrt{V}(\eta a_0^* + \eta^* a_0)$$

and

$$H_\Lambda(\rho, \eta) = T_\Lambda + a\rho N - \tfrac{1}{2} a\rho^2 V + \sqrt{V}(\eta a_0^* + \eta^* a_0), \tag{1.3}$$

so that

$$H_\Lambda(\eta) - H_\Lambda(\rho, \eta) = \frac{a}{2V}(N_\Lambda - V\rho)^2.$$

The corresponding grand-canonical pressures are

$$p_\Lambda(\eta, \mu) = \frac{1}{\beta V} \ln \operatorname{Tr} \exp\{-\beta(H_\Lambda(\eta) - \mu N_\Lambda)\}$$

and

$$p_\Lambda(\rho, \eta, \mu) = \frac{1}{\beta V} \ln \operatorname{Tr} \exp\{-\beta(H_\Lambda(\rho, \eta) - \mu N_\Lambda)\}. \tag{1.4}$$

We can write $H_\Lambda(\rho, \eta) - \mu N_\Lambda$ in the form

$$H_\Lambda(\rho, \eta) - \mu N_\Lambda = \sum_{l=0}^{\infty} \epsilon_l^\Lambda a_l^* a_l + \sqrt{V}(\eta a_0^* + \eta^* a_0) - \frac{1}{2} a\rho^2 V, \tag{1.5}$$

where $\epsilon_l^\Lambda(\rho, \mu) := E_l^\Lambda - \mu + a\rho$. For convergence in (1.4) one must have $E_0^\Lambda - \mu + a\rho > 0$.

2. Comments

The proof of the proposition is essentially based on the following:

Lemma. *If* $\eta \neq 0$, *then*

$$\lim_{\Lambda\uparrow\mathbb{R}^d} p_\Lambda(\eta,\mu) = \lim_{\Lambda\uparrow\mathbb{R}^d} \min_{\rho\geqslant 0} p_\Lambda(\rho,\eta,\mu) = \lim_{\Lambda\uparrow\mathbb{R}^d} p_\Lambda(\bar\rho_\Lambda,\eta,\mu). \tag{2.1}$$

The aim of the present note is to show that this lemma is correct in spite of the fact that relation (2.10) used in [1] for its proof is not *valid.*

Proof. Lemma 1 of [1] implies that for the given parameters (β,μ,η) the minimizer $\bar\rho_\Lambda$ in (2.1) is an interior point of a finite interval $(\mu/a, K)$, where $K := K(\beta,\mu,\eta))$. This point $\bar\rho_\Lambda$ satisfies the equation

$$\frac{\partial p_\Lambda}{\partial\rho}(\rho,\eta,\mu) = -\frac{a}{V}\sum_{l=0}^{\infty}\frac{1}{\exp\left(\beta\epsilon_l^\Lambda\right)-1} - a\frac{|\eta|^2}{\left(\epsilon_0^\Lambda\right)^2} + a\rho = 0. \tag{2.2}$$

Since in the *grand-canonical state* for Hamiltonian (1.3) the particle density operator has the value

$$\left\langle\frac{N_\Lambda}{V}\right\rangle_{H_\Lambda(\rho,\eta)} = \frac{\partial p_\Lambda}{\partial\mu}(\rho,\eta,\mu) = \frac{1}{V}\sum_{l=0}^{\infty}\frac{1}{\exp\left(\beta\epsilon_l^\Lambda\right)-1} + \frac{|\eta|^2}{\left(\epsilon_0^\Lambda\right)^2}, \tag{2.3}$$

(2.2) is equivalent to the equation $\rho = \langle N_\Lambda\rangle_{H_\Lambda(\rho,\eta)}\big/V$. Let $\bar\rho_\Lambda := \bar\rho_\Lambda(\mu,\eta)$ denote a solution of this equation (minimizer). Then $\lim_{\Lambda\uparrow\mathbb{R}^d}\bar\rho_\Lambda(\mu,\eta) = \bar\rho(\mu,\eta) < K$ exists and verifies the limiting equation (2.2):

$$\rho = \rho_0(\mu - a\rho) + \frac{|\eta|^2}{(a\rho-\mu)^2}. \tag{2.4}$$

Now by Bogoliubov's convexity inequality one gets

$$0 \leqslant p_\Lambda(\bar\rho_\Lambda,\eta,\mu) - p_\Lambda(\eta,\mu) \leqslant \frac{1}{2V^2}\Delta_\Lambda(\eta), \tag{2.5}$$

where

$$\Delta_\Lambda(\eta) := a\left\langle\left(N_\Lambda - \langle N_\Lambda\rangle_{H_\Lambda(\bar\rho_\Lambda,\eta)}\right)^2\right\rangle_{H_\Lambda(\bar\rho_\Lambda,\eta)}, \tag{2.6}$$

and as in [1] we want to obtain an estimate for $\Delta_\Lambda(\eta)$ in terms of V.

Comment 1. Since for $\eta \neq 0$ the commutator $[H_\Lambda(\rho_\Lambda,\eta), N_\Lambda] \neq 0$, we get

$$\frac{\Delta_\Lambda(\eta)}{aV} \neq \frac{1}{\beta}\frac{\partial^2 p_\Lambda}{\partial\mu^2}(\bar\rho_\Lambda,\eta,\mu),$$

which breaks equation (2.10) in [1]. In fact, one gets for the second derivative the Bogoliubov–Duhamel formula, see e.g. [2]

$$\frac{1}{\beta}\frac{\partial^2 p_\Lambda}{\partial\mu^2}(\bar\rho_\Lambda,\eta,\mu) = \frac{1}{V\beta}\int_0^\beta \mathrm{d}s\,\langle\tau_s(\widehat{\delta N_\Lambda})\widehat{\delta N_\Lambda}\rangle_{H_\Lambda(\bar\rho_\Lambda,\eta)}, \tag{2.7}$$

where we denote $\widehat{\delta N_\Lambda} := N_\Lambda - \langle N_\Lambda\rangle_{H_\Lambda(\bar\rho_\Lambda,\eta)}$ and $\tau_s(A) := \mathrm{e}^{sH_\Lambda(\bar\rho_\Lambda,\eta)}A\,\mathrm{e}^{-sH_\Lambda(\bar\rho_\Lambda,\eta)}$. Using (2.7) one can check that in fact we have

$$\frac{\Delta_\Lambda(\eta)}{aV} \geqslant \frac{1}{\beta}\frac{\partial^2 p_\Lambda}{\partial\mu^2}(\bar\rho_\Lambda,\eta,\mu),$$

i.e. the second derivative with respect to the chemical potential is not very useful for estimation of the right-hand side of (2.5).

Comment 2. In this note we show that one can do a simple direct calculation to estimate $\Delta_\Lambda(\eta)$. To this end, we split the approximating Hamiltonian (1.3) and the difference $\widehat{\delta N}_\Lambda$ into terms which depend on the $(l = 0)$-mode and the others:

$$H_\Lambda(\bar\rho_\Lambda, \eta) := H^0_\Lambda(\bar\rho_\Lambda, \eta) + H'_\Lambda(\bar\rho_\Lambda),$$
$$\widehat{\delta N}_\Lambda := \widehat{\delta N}^0_\Lambda + \widehat{\delta N}'_\Lambda = N^0_\Lambda - \langle N^0_\Lambda\rangle_{H^0_\Lambda(\bar\rho_\Lambda,\eta)} + N'_\Lambda - \langle N'_\Lambda\rangle_{H'_\Lambda(\bar\rho_\Lambda)}.$$

Then we get for (2.6)

$$\frac{1}{a}\Delta_\Lambda(\eta) = \left\langle\left(\widehat{\delta N}^0_\Lambda\right)^2\right\rangle_{H^0_\Lambda(\bar\rho_\Lambda,\eta)} + \left\langle\left(\widehat{\delta N}'_\Lambda\right)^2\right\rangle_{H'_\Lambda(\bar\rho_\Lambda)} + 2\left\langle\widehat{\delta N}^0_\Lambda\right\rangle_{H^0_\Lambda(\bar\rho_\Lambda,\eta)}\left\langle\widehat{\delta N}'_\Lambda\right\rangle_{H'_\Lambda(\bar\rho_\Lambda)}.$$

By a standard diagonalization of $H^0_\Lambda(\bar\rho_\Lambda, \eta)$, which absorbs the linear zero-mode source terms, and after elementary calculations we obtain (cf (2.10) in [1])

$$\frac{1}{aV}\Delta_\Lambda(\eta) = \frac{1}{V}\sum_{l=0}^{\infty}\frac{\exp\left(\beta\bar\epsilon^\Lambda_l\right)}{\left(\exp\left(\beta\bar\epsilon^\Lambda_l\right)-1\right)^2} + \frac{|\eta|^2}{\left(\bar\epsilon^\Lambda_0\right)^2}\frac{\exp\left(\beta\bar\epsilon^\Lambda_0\right)}{\left(\exp\left(\beta\bar\epsilon^\Lambda_0\right)-1\right)}. \tag{2.8}$$

Here $\bar\epsilon^\Lambda_l := E^\Lambda_l - \mu + a\bar\rho_\Lambda \geqslant E^\Lambda_0 - \mu + a\bar\rho_\Lambda$. Since by virtue of equation (2.2) we obviously have $\bar\rho_\Lambda \geqslant |\eta|^2/\left(\bar\epsilon^\Lambda_0\right)^2$, this implies for $\bar\epsilon^\Lambda_l$ the uniform (in volume) estimate from below:

$$\bar\epsilon^\Lambda_l \geqslant \bar\epsilon^\Lambda_0 \geqslant \frac{|\eta|}{K^{1/2}} =: \delta > 0 \tag{2.9}$$

for non-zero sources. Now, we can follow the same line of reasoning as in [1]. By (2.9) and by the inequality $e^x/(e^x - 1) \leqslant 2(1 + 1/x)$ for $x \geqslant 0$, we find for (2.8) the estimate from above:

$$\frac{1}{aV}\Delta_\Lambda(\eta) \leqslant 2\left(1 + \frac{1}{\beta\delta}\right)\left[\frac{1}{V}\sum_{l=0}^{\infty}\frac{1}{\exp\left(\beta\epsilon^\Lambda_l\right)-1} + \frac{|\eta|^2}{\delta^2}\right]. \tag{2.10}$$

Since equations (2.2), (2.4) imply for $\eta \neq 0$ the uniform bound

$$\frac{1}{V}\sum_{l=0}^{\infty}\frac{1}{\exp\left(\beta\epsilon^\Lambda_l\right)-1} \leqslant \bar\rho_\Lambda \leqslant K, \tag{2.11}$$

by estimate (2.10) we get

$$\lim_{V\to\infty}\frac{1}{V^2}\Delta_\Lambda(\eta) = 0. \tag{2.12}$$

So, we see that this lemma stays true, independent of (2.10) in [1]. □

Comment 3. The rest of the proof of (1.5) is the same as in [1].

References

[1] Pulé J V and Zagrebnov V A 2004 The approximating Hamiltonian method for the imperfect boson gas *J. Phys. A: Math. Gen.* **45** 3565–83

[2] Bratelli O and Robinson D W 2002 *Operator Algebras and Quantum Statistical Mechanics* vol 2, 2nd edn (Berlin: Springer)