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The approximating Hamiltonian method for the imperfect boson gas

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Abstract

The pressure for the imperfect (mean field) boson gas can be derived in several ways. The aim of the present paper is to provide a new method based on the approximating Hamiltonian argument which is extremely simple and very general.

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1. Set-up

Consider a system of identical bosons of mass m enclosed in a smooth, connected, bounded domain $\Lambda \subset \mathbb{R}^d$ (of volume $|\Lambda| = V$). Let $E_0^\Lambda < E_1^\Lambda \leqslant E_2^\Lambda \leqslant E_3^\Lambda \leqslant \cdots$ be the eigenvalues of $h_\Lambda := -\Delta/2m$ on Λ with some boundary conditions and let $\{\phi_l^\Lambda\}$ with $l = 0, 1, 2, 3, \ldots$ 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 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, i.e. $T_\Lambda = \sum_{l=0}^\infty E_l^\Lambda N_l$, 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 the *imperfect* or *mean field boson gas* is

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

where a is a positive coupling constant (see e.g. [1]).

Let $\mu_0 := \lim_{\Lambda \uparrow \mathbb{R}^d} E_0^\Lambda$, which may be *negative* in the case of *attractive* boundary conditions (see e.g. [2]). Let $p_0(\mu)$ and $\rho_0(\mu)$ be the grand-canonical pressure and mean density, respectively, for the free Bose gas at chemical potential $\mu < \mu_0$, i.e.

$$p_0(\mu) = -\int \ln(1 - \mathrm{e}^{-\beta(\eta-\mu)}) F(\mathrm{d}\eta) \quad \text{and} \quad \rho_0(\mu) = \int \frac{1}{\mathrm{e}^{\beta(\eta-\mu)} - 1} F(\mathrm{d}\eta), \tag{1.2}$$

where F is the integrated density of states of h_Λ in the limit $\Lambda \uparrow \mathbb{R}^d$. Let $\rho_c := \lim_{\mu \to \mu_0} \rho_0(\mu)$.

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The grand-canonical pressure of the mean field boson model with Hamiltonian (1.1) is

$$p_\Lambda(\mu) = \frac{1}{\beta V} \ln \text{ trace } \exp\{-\beta(H_\Lambda - \mu N_\Lambda)\} \tag{1.3}$$

and we put

$$p(\mu) = \lim_{\Lambda\uparrow\mathbb{R}^d} p_\Lambda(\mu). \tag{1.4}$$

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

$$p(\mu) = \begin{cases} \frac{1}{2}a\rho^2(\mu) + p_0(\mu - a\rho(\mu)) & \text{if } \mu \leqslant \mu_c, \\ \frac{(\mu-\mu_0)^2}{2a} + p_0(\mu_0) & \text{if } \mu > \mu_c, \end{cases} \tag{1.5}$$

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

This result, for special boundary conditions implying $\mu_0 = 0$, can be proved in at least three ways [3–5]; see also [6–8]. The aim of the present note is to provide yet another but extremely simple and very general way of proving this result. Moreover, since we allow $\mu_0 < 0$, our method covers also the case of *attractive* boundary conditions. The proof is based on the *approximating Hamiltonian* technique (see e.g. [9]).

We need the following auxiliary operators for $\rho \in \mathbb{R}$ and $\eta \in \mathbb{C}$:

$$H_\Lambda(\eta) = H_\Lambda + \sqrt{V}(\eta a_0^* + \eta^* a_0) \tag{1.6}$$

and

$$H_\Lambda(\rho,\eta) = T_\Lambda + a\rho N - \tfrac{1}{2}a\rho^2 V + \sqrt{V}(\eta a_0^* + \eta^* a_0), \tag{1.7}$$

so that

$$H_\Lambda(\eta) - H_\Lambda(\rho,\eta) = \frac{a}{2V}(N_\Lambda - V\rho)^2. \tag{1.8}$$

Let

$$p_\Lambda(\eta,\mu) = \frac{1}{\beta V} \ln \text{ trace } \exp\{-\beta(H_\Lambda(\eta) - \mu N_\Lambda)\} \tag{1.9}$$

and

$$p_\Lambda(\rho,\eta,\mu) = \frac{1}{\beta V} \ln \text{trace} \exp\{-\beta(H_\Lambda(\rho,\eta) - \mu N_\Lambda)\}. \tag{1.10}$$

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

$$H_\Lambda(\rho,\eta) - \mu N_\Lambda = \sum_{l=0}^{\infty} \epsilon_l^\Lambda a_l^* a_l + \sqrt{V}(\eta a_0^* + \eta^* a_0) - \frac{1}{2}a\rho^2 V, \tag{1.11}$$

where

$$\epsilon_l^\Lambda(\rho,\mu) := E_l^\Lambda - \mu + a\rho. \tag{1.12}$$

For convergence in (1.10) one must have $E_0^\Lambda - \mu + a\rho > 0$.

2. The Proof

The proof of the proposition consists of four straightforward lemmas. The idea is to show that, for $\eta \neq 0$, the pressure $p_\Lambda(\eta, \mu)$ in the limit coincides with $p_\Lambda(\rho, \eta, \mu)$ minimized with respect to ρ (lemmas 1 and 2) and that in turn this minimization can be performed after the thermodynamic limit (lemma 3). The final step is to switch off the source η to obtain the limiting pressure $p(\mu)$ (lemma 4).

We shall use the notation: $x_+ := \max(0, x)$ and $x_- := \max(0, -x)$ for $x \in \mathbb{R}$, so that $x = x_+ - x_-$.

Lemma 1. *For a given η, there is a compact subset of $((\mu - \mu_0)_+/a, \infty)$, independent of Λ, such that for Λ sufficiently large the infimum of $p_\Lambda(\rho, \eta, \mu)$ with respect to ρ is attained in this set.*

Proof. From (1.10) and (1.11) we can see that

$$p_\Lambda(\rho, \eta, \mu) = -\frac{1}{\beta V}\sum_{l=0}^{\infty}\{\ln(1 - \exp(-\beta\epsilon_l^\Lambda))\} + \frac{|\eta|^2}{\epsilon_0^\Lambda} + \frac{1}{2}a\rho^2 \tag{2.1}$$

and

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

Suppose $\eta \neq 0$. If $a\rho < (\mu - \mu_0)_+ + \delta$, with $\delta > 0$, then

$$\frac{\partial p_\Lambda}{\partial\rho}(\rho, \eta, \mu) \leqslant -\frac{a|\eta|^2}{(\epsilon_0^\Lambda)^2} + a\rho \leqslant -\frac{a|\eta|^2}{((\mu - \mu_0)_- + 2\delta)^2} + (\mu - \mu_0)_+ + \delta < 0 \tag{2.3}$$

if δ is sufficiently small and Λ large enough. On the other hand, for $a\rho > (\mu - \mu_0)_+ + \delta$, with $\delta > 0$,

$$\frac{\partial p_\Lambda}{\partial\rho}(\rho, \eta, \mu) > -\frac{a}{V}\sum_{l=0}^{\infty}\frac{1}{\exp\beta(E_l^\Lambda - (\mu_0 - \delta)) - 1} - \frac{4a|\eta|^2}{\delta^2} + a\rho$$

$$> -a(\rho_c + 1) - \frac{4a|\eta|^2}{\delta^2} + a\rho > 0 \tag{2.4}$$

for ρ and Λ sufficiently large and small δ. Therefore there exists $K < \infty$, independent of Λ, such that the infimum of $p_\Lambda(\rho, \eta, \mu)$ with respect to ρ is attained in $[((\mu - \mu_0)_+ + \delta)/a, K]$. □

Suppose the infimum of $p_\Lambda(\rho, \eta, \mu)$ with respect to ρ that is attained at $\bar{\rho}_\Lambda(\eta, \mu)$, which is not *a priori* unique. Then $\bar{\rho}_\Lambda \in [((\mu - \mu_0)_+ + \delta)/a, K]$.

Lemma 2. *If $\eta \neq 0$,*

$$\lim_{\Lambda\uparrow\mathbb{R}^d} p_\Lambda(\eta, \mu) = \lim_{\Lambda\uparrow\mathbb{R}^d} p_\Lambda(\bar{\rho}_\Lambda, \eta, \mu). \tag{2.5}$$

Proof. Since, by lemma 1, $\bar{\rho}_\Lambda$ is a interior point of $((\mu - \mu_0)_+/a, \infty)$, it satisfies

$$\frac{\partial p_\Lambda}{\partial\rho}(\bar{\rho}_\Lambda, \eta, \mu) = 0. \tag{2.6}$$

Now the mean particle density in the grand-canonical state with Hamiltonian (1.7) takes the form

$$\left\langle \frac{N_\Lambda}{V} \right\rangle_{H_\Lambda(\rho,\eta)} = \frac{\partial p_\Lambda}{\partial \mu}(\rho,\eta) = \frac{1}{V}\sum_{l=0}^{\infty} \frac{1}{\exp(\beta\epsilon_l^\Lambda)-1} + \frac{|\eta|^2}{(\epsilon_0^\Lambda)^2}. \tag{2.7}$$

Comparing this last equation (2.7) with (2.2) we see that $\bar{\rho}_\Lambda$ satisfies the equation $\bar{\rho}_\Lambda = (1/V)\langle N_\Lambda\rangle_{H_\Lambda(\bar{\rho}_\Lambda,\eta)}$. By Bogoliubov's convexity inequality (see e.g. [9]),

$$0 \leqslant p_\Lambda(\bar{\rho}_\Lambda,\eta,\mu) - p_\Lambda(\eta,\mu) \leqslant \frac{1}{2V^2}\Delta_\Lambda(\eta), \tag{2.8}$$

where

$$\Delta_\Lambda(\eta) = a\langle (N_\Lambda - V\bar{\rho}_\Lambda)^2\rangle_{H_\Lambda(\bar{\rho}_\Lambda,\eta)}. \tag{2.9}$$

We want to obtain an estimate for $\Delta_\Lambda(\eta)$ in terms of V. Since

$$\frac{\Delta_\Lambda(\eta)}{aV} = \frac{\partial^2 p_\Lambda}{\partial \mu^2}(\rho,\eta) = \frac{\beta}{V}\sum_{l=0}^{\infty} \frac{\exp(\beta\epsilon_l^\Lambda)}{(\exp(\beta\epsilon_l^\Lambda)-1)^2} + \frac{2|\eta|^2}{(\epsilon_l^\Lambda)^3}, \tag{2.10}$$

we use $e^x/(e^x-1) \leqslant 2(1+1/x)$ for $x \geqslant 0$ and $\epsilon_l^\Lambda(\bar{\rho}_\Lambda,\mu) \geqslant E_0^\Lambda + a\bar{\rho}_\Lambda - \mu > (\mu-\mu_0)_- + \delta + (E_0^\Lambda - \mu_0) > \frac{1}{2}\delta$, which is valid for large Λ, to obtain

$$\frac{\partial^2 p_\Lambda}{\partial \mu^2}(\bar{\rho}_\Lambda,\eta,\mu) \leqslant 2\left(\frac{2}{\delta}+\beta\right)\frac{1}{V}\sum_{l=0}^{\infty}\frac{1}{\exp(\beta\epsilon_l^\Lambda)-1} + \frac{4}{\delta}\frac{|\eta|^2}{(\epsilon_0^\Lambda)^2}. \tag{2.11}$$

By (2.2) and (2.6)

$$\frac{1}{V}\sum_{l=0}^{\infty}\frac{1}{(\exp(\beta\epsilon_l^\Lambda)-1)} \leqslant \bar{\rho}_\Lambda \tag{2.12}$$

and

$$\frac{|\eta|^2}{(\epsilon_0^\Lambda)^2} \leqslant \bar{\rho}_\Lambda. \tag{2.13}$$

Therefore

$$\frac{\partial^2 p_\Lambda}{\partial \mu^2}(\bar{\rho}_\Lambda,\eta,\mu) \leqslant 2\left(\frac{4}{\delta}+\beta\right)\bar{\rho}_\Lambda. \tag{2.14}$$

Thus since by lemma 1, $\bar{\rho}_\Lambda < K$,

$$\lim_{V\to\infty}\frac{1}{V^2}\Delta_\Lambda(\eta) = \lim_{V\to\infty}\frac{a}{V}\frac{\partial^2 p_\Lambda}{\partial \mu^2}(\bar{\rho}_\Lambda,\eta,\mu) = 0. \tag{2.15}$$

□

Lemma 3.

$$\lim_{\Lambda\uparrow\mathbb{R}^d} p_\Lambda(\eta,\mu) = \frac{1}{2}a\rho^2(\eta,\mu) + p_0(\mu - a\rho(\eta,\mu)) + \frac{|\eta|^2}{a\rho(\eta,\mu)-\mu}, \tag{2.16}$$

where $\rho(\eta,\mu)$ is the unique solution of the equation $\rho = \rho_0(\mu - a\rho) + |\eta|^2/(a\rho-\mu)^2$.

Proof. Let $\rho(\eta,\mu)$ be a limit point of $\bar{\rho}_\Lambda \in [((\mu-\mu_0)_+ + \delta)/a, K]$; $p_0(\mu - a\rho)$ and $\rho_0(\mu - a\rho)$ are convex in ρ. From (2.1) one can see that $p_\Lambda(\rho,\eta,\mu)$ is convex in ρ and thus as $\Lambda\uparrow\mathbb{R}^d$, $p_\Lambda(\rho,\eta,\mu)$ converges uniformly in ρ on compact subsets of $((\mu-\mu_0)_+/a,\infty)$ to

$$\frac{1}{2}a\rho^2 + p_0(\mu - a\rho) + \frac{|\eta|^2}{a\rho-\mu}. \tag{2.17}$$

Similarly, from (2.2), one can see that $(\partial p_\Lambda/\partial\rho)(\rho,\eta,\mu) + a|\eta|^2/(\epsilon_0^\Lambda)^2$ is also convex in ρ and thus by the same argument, it converges uniformly in ρ on compact subsets of $((\mu-\mu_0)_+/a,\infty)$. Since it is also clear that $a|\eta|^2/(\epsilon_0^\Lambda)^2$ converges uniformly on the same subsets, so does $(\partial p_\Lambda/\partial\rho)(\rho,\eta,\mu)$ with limit

$$a\rho - a\rho_0(\mu - a\rho) - \frac{a|\eta|^2}{(a\rho-\mu)^2}. \tag{2.18}$$

Since

$$\lim_{\Lambda\uparrow\mathbb{R}^d} p_\Lambda(\eta,\mu) = \lim_{\Lambda\uparrow\mathbb{R}^d} p_\Lambda(\bar{\rho}_\Lambda,\eta,\mu) \tag{2.19}$$

and

$$\frac{\partial p_\Lambda}{\partial\rho}(\bar{\rho}_\Lambda,\eta,\mu) = 0, \tag{2.20}$$

the lemma follows immediately. □

Lemma 4.

$$\lim_{\Lambda\uparrow\mathbb{R}^d} p_\Lambda(\mu) = \lim_{\eta\to 0}\lim_{\Lambda\uparrow\mathbb{R}^d} p_\Lambda(\eta,\mu). \tag{2.21}$$

Proof. By Bogoliubov's convexity inequality one has

$$-\frac{|\eta|}{\sqrt{V}}|\langle a_0 + a_0^*\rangle_{H_\Lambda}| \leqslant p_\Lambda(\mu) - p_\Lambda(\eta,\mu) \leqslant \frac{|\eta|}{\sqrt{V}}|\langle a_0 + a_0^*\rangle_{H_\Lambda(\eta)}|, \tag{2.22}$$

$$0 \leqslant p_\Lambda(\mu) - p_\Lambda(\eta,\mu) \leqslant \frac{2|\eta|}{\sqrt{V}}|\langle a_0^*\rangle_{H_\Lambda(\eta)}| \leqslant \frac{2|\eta|}{\sqrt{V}}\langle a_0^*a_0\rangle_{H_\Lambda(\eta)}^{1/2} \leqslant \frac{2|\eta|}{\sqrt{V}}\langle N_\Lambda\rangle_{H_\Lambda(\eta)}^{1/2}. \tag{2.23}$$

Now, by convexity of the pressure $p_\Lambda(\eta,\mu)$ with respect to μ we obtain

$$\left\langle\frac{N_\Lambda}{V}\right\rangle_{H_\Lambda(\eta)} \leqslant p_\Lambda(\eta,\mu+1) - p_\Lambda(\eta,\mu) \leqslant p_\Lambda(\eta,\mu+1). \tag{2.24}$$

Since

$$\begin{aligned}
H_\Lambda(\eta) - (\mu+1)N_\Lambda &= T_\Lambda + \frac{aN_\Lambda^2}{2V} - (\mu+1)N_\Lambda + (\sqrt{V}\bar{\eta} + a_0^*)(\sqrt{V}\eta + a_0) - a_0^*a_0 - V|\eta|^2 \\
&\geqslant T_\Lambda + \frac{aN_\Lambda^2}{2V} - (\mu+2)N_\Lambda - V|\eta|^2 \\
&= T_\Lambda - (\mu_0 - 1)N_\Lambda + \frac{a}{2V}\left(N_\Lambda - \frac{V(\mu-\mu_0+3)}{a}\right)^2 \\
&\quad - V|\eta|^2 - \frac{V(\mu-\mu_0+3)^2}{2a} \\
&\geqslant T_\Lambda - (\mu_0-1)N_\Lambda - V|\eta|^2 - \frac{V(\mu-\mu_0+3)^2}{2a},
\end{aligned} \tag{2.25}$$

we have the estimate

$$p_\Lambda(\eta, \mu+1) \leqslant p_0(\mu_0 - 1) + 1 + |\eta|^2 + \frac{(\mu - \mu_0 + 3)^2}{2a} \tag{2.26}$$

for large Λ. Thus the right-hand side of (2.23) tends to zero as η tends to zero. □

Proof of the Proposition. To prove proposition we combine lemmas 3 and 4. It is straightforward to check that as $\eta \to 0$, $\rho(\eta, \mu)$, as defined in lemma 3, tends to $(\mu - \mu_0)/a$ if $\mu \geqslant \mu_c$ and to the unique solution of $\rho = \rho_0(\mu - a\rho)$ if $\mu < \mu_c$. From (2.16) and (2.21) one then obtains the values in the proposition for the pressure. □

3. Remarks

Note that the proof in [3] is based on the equivalence between the canonical and the grand-canonical ensembles produced by the mean field interaction, $aN_\Lambda^2/2V$, and the use of explicit information about the grand-canonical free Bose gas.

In the proof presented in [4] the authors employ the device of shifting the spectrum to change the density of states removing the phase transition.

Thirdly, in [5], a probabilistic approach based on the theory of Large Deviations is used to treat the pressure for this model, amongst other things.

The essential feature of our proof is the addition of sources to make the grand-canonical critical mean density infinite so as to eliminate phase transitions. This allows us to linearize the mean field interaction and to control the particle number fluctuations. The limiting pressure is calculated in this regime and then the phase transition is restored by the removal of the sources.

We would like to remark that if one replaces the interaction term in (1.1) by the operator $V\phi(N_\Lambda/V)$ where ϕ is a non-negative smooth convex function, the arguments used here go through with minor modifications to obtain the limiting pressure, cf [3, 8].

Finally, we note that by standard arguments using convexity (see e.g. [4, 5]), our proposition implies that there is always *Generalized Bose Einstein Condensation* (GBEC) for $\mu > \mu_c$ in the imperfect boson gas. However, in spite of the fact that the proof in the present note is based on *forcing* by external sources the microscopic occupation of the ground state, $l = 0$, this does not guarantee that the condensate, after removal of the sources, is to be found only in this state (GBEC of type I). In fact, we know that in general this is not true, since the nature of the condensate in the imperfect boson gas depends crucially on the details of the spectrum of the free Bose gas (see e.g. [7, 10]).

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