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 note is to provide a new method based on the Approximating Hamiltonian argument which is extremely simple and very general.
Consider a system of identical bosons of mass \( m \) enclosed in a cube \( \Lambda \subset \mathbb{R}^d \) of volume \( V \) centered at the origin. Let \( E_0^\Lambda < E_1^\Lambda \leq E_2^\Lambda \leq E_3^\Lambda \leq \ldots \) be the eigenvalues of \( h^\Lambda := -\Delta/2m \) on \( \Lambda \) 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 \( T_\Lambda \) 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 \( \Lambda \). The Hamiltonian of the interacting gas known as the Imperfect or Mean Field Boson Gas is

\[
H_\Lambda = T_\Lambda + \frac{a}{2V} N_\Lambda^2
\]

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

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

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

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

The grand-canonical pressure of the Mean Field Boson Model with Hamiltonian (1.1) is

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

and we put

\[
p(\mu) = \lim_{\Lambda \to \mathbb{R}^d} p_\Lambda(\mu).
\]

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

\[
p(\mu) = \begin{cases} 
\frac{1}{2} a \rho^2(\mu) + p_0(\mu - a \rho(\mu)) & \text{if } \mu \leq \mu_c; \\
\frac{(\mu - \mu_0)^2}{2a} + p_0(\mu_0) & \text{if } \mu > \mu_c,
\end{cases}
\]

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, can be proved in at least three ways [2–4], see also [5–7]. The aim of the present note is to provide yet another but extremely simple and very general way of proving this result. Our method covers also the case of attractive boundary conditions. The proof is based on the Approximating Hamiltonian technique, see e.g. [8].

We shall need the following auxiliary operators for \( \rho \in \mathbb{R} \) and \( \eta \in \mathbb{C} \),

\[
H_\Lambda(\eta) = H_\Lambda + \sqrt{V} (\eta a_0^* + \eta^* a_0),
\]

and

\[
H_\Lambda(\rho, \eta) = T_\Lambda + a \rho N - \frac{1}{2} a \rho^2 V + \sqrt{V} (\eta a_0^* + \eta^* a_0),
\]
so that
\[ H_\Lambda(\eta) - H_\Lambda(\rho, \eta) = \frac{a}{2V}(N_\Lambda - V\rho)^2. \] (1.8)

Let
\[ p_\Lambda(\eta, \mu) = \frac{1}{\beta V} \ln \text{trace} \exp\{-\beta(H_\Lambda(\eta) - \mu N_\Lambda)\} \] (1.9)
and
\[ p_\Lambda(\rho, \eta, \mu) = \frac{1}{\beta V} \ln \text{trace} \exp\{-\beta(H_\Lambda(\rho, \eta) - \mu N_\Lambda)\}. \] (1.10)

We can write \( H_\Lambda(\rho, \eta) - \mu N_\Lambda \) in the form
\[ H_\Lambda(\rho, \eta) - \mu N_\Lambda = \sum_{l=0}^{\infty} \epsilon^\Lambda_l a^*_l a_l + \sqrt{V} (\eta a^*_0 + \eta^* a_0) - \frac{1}{2} a\rho^2 V \] (1.11)
where
\[ \epsilon^\Lambda_l(\rho, \mu) := E^\Lambda_l - \mu + a\rho. \] (1.12)

For convergence in (1.10) must have \( a\rho - \mu + E^\Lambda_0 > 0. \)

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 \( \rho \) (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 \( \eta \) to obtain the limiting pressure \( p(\mu) \) (Lemma 4).

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

Proof: From (1.10) we can see that
\[ p_\Lambda(\rho, \eta, \mu) = -\frac{1}{\beta V} \sum_{l=0}^{\infty} \left\{ \ln \left( 1 - \exp(-\beta \epsilon^\Lambda_l) \right) \right\} + \frac{\eta_0^2}{\epsilon^\Lambda_0} + \frac{1}{2} a\rho^2. \] (2.1)
and
\[ \frac{\partial p_\Lambda}{\partial \rho}(\rho, \eta, \mu) = -\frac{a}{V} \sum_{l=0}^{\infty} \frac{1}{\exp(\beta \epsilon^\Lambda_l) - 1} - \frac{a|\eta|^2}{(\epsilon^\Lambda_0)^2} + a\rho. \] (2.2)
Suppose \( \eta \neq 0 \). If \( a\rho < \mu - \mu_0 + \delta \), with \( \delta > 0 \), then
\[ \frac{\partial p_\Lambda}{\partial \rho}(\rho, \eta, \mu) \leq -\frac{a|\eta|^2}{(\epsilon^\Lambda_0)^2} + a\rho \leq -\frac{a|\eta|^2}{(2\delta)^2} + \mu - \mu_0 + \delta < 0 \] (2.3)
if \( \delta \) is sufficiently small and \( \Lambda \) large enough. On the other hand for \( a\rho > \mu - \mu_0 + \alpha \), with \( \alpha > 0 \),
\[ \frac{\partial p_\Lambda}{\partial \rho}(\rho, \eta, \mu) > -\frac{a}{V} \sum_{l=0}^{\infty} \frac{1}{\exp(\beta (E^\Lambda_l - (\mu_0 - \alpha))) - 1} - \frac{4a|\eta|^2}{\alpha^2} + a\rho > -a(\rho_c - 1) - \frac{4a|\eta|^2}{\alpha^2} + a\rho > 0 \] (2.4)
for \( \rho \) and \( \Lambda \) sufficiently large. Therefore there exists \( K < \infty \), independent of \( \Lambda \) such that the infimum of \( p_\Lambda(\rho, \eta, \mu) \) with respect to \( \rho \) is attained in \([(\mu - \mu_0 + \delta)/a, K]\).

\[\square\]

Suppose the infimum of \( p_\Lambda(\rho, \eta, \mu) \) with respect to \( \rho \) that is attained at \( \bar{\rho}_\Lambda(\eta, \mu) \), which is not a priori unique.

**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 an 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

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

Comparing this last equation (2.7) with (2.2) we see that \( \bar{\rho}_\Lambda \) satisfies the equation

\[
\bar{\rho}_\Lambda = \frac{1}{V} \langle N_\Lambda \rangle_{H_\Lambda(\bar{\rho}_\Lambda, \eta)}. \tag{2.8}
\]

By Bogoliubov’s convexity inequality, see e.g. [8],

\[
0 \leq p_\Lambda(\bar{\rho}_\Lambda, \eta, \mu) - p_\Lambda(\eta, \mu) \leq \frac{1}{2V^2} \Delta_\Lambda(\eta). \tag{2.9}
\]

where

\[
\Delta_\Lambda(\eta) = a \langle (N_\Lambda - V\bar{\rho}_\Lambda)^2 \rangle_{H_\Lambda(\bar{\rho}_\Lambda, \eta)}. \tag{2.10}
\]

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

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

we use \( e^x/(e^x - 1) \leq 2(1 + 1/x) \) for \( x \geq 0 \) and \( \epsilon_l^\Lambda(\bar{\rho}_\Lambda, \mu) \geq E_0^\Lambda + a\bar{\rho}_\Lambda - \mu > E_0^\Lambda - \mu_0 + \delta > \frac{1}{2}\delta \) to obtain

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

By (2.2) and (2.6)

\[
\frac{1}{V} \sum_{l=0}^{\infty} \frac{1}{\exp(\beta \epsilon_l^\Lambda) - 1} \leq \bar{\rho}_\Lambda \tag{2.11}
\]

and

\[
\frac{|\eta|^2}{(\epsilon_0^\Lambda)^2} \leq \bar{\rho}_\Lambda. \tag{2.12}
\]

Therefore

\[
\frac{\partial^2 p_\Lambda}{\partial \mu^2}(\bar{\rho}_\Lambda, \eta, \mu) \leq 2 \left( \frac{4}{\delta} + \beta \right) \bar{\rho}_\Lambda. \tag{2.13}
\]
Thus since by Lemma $\bar{\rho}_\Lambda < K$, 
\[ \lim_{V \to \infty} \frac{1}{V^2} \Delta_\Lambda(\eta) = \lim_{V \to \infty} \frac{a}{V} \frac{\partial^2 p_\Lambda}{\partial \mu^2}(\bar{\rho}_\Lambda, \eta, \mu) = 0. \] (2.14)

Lemma 3
\[ \lim_{\Lambda \uparrow \mathbb{R}^d} p_\Lambda(\eta, \mu) = \frac{1}{2} a \rho^2(\eta, \mu) + p_0(\mu - a \rho(\eta, \mu)) + \frac{a}{a \rho(\eta, \mu) - \mu} \frac{|\eta|^2}{a \rho(\eta, \mu) - \mu} \] (2.15)
where $\rho(\eta, \mu)$ is the unique solution of the equation $\rho = p_0(\mu - a \rho) + \frac{|\eta|^2}{(a \rho - \mu)^2}$.

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 $\rho$. From (2.1) one can see that $p_\Lambda(\rho, \eta, \mu)$ is convex and thus as $\Lambda \uparrow \mathbb{R}^d$, $p_\Lambda(\rho, \eta, \mu)$ converges uniformly in $\rho$ on compact subsets of $((\mu - \mu_0)/a, \infty)$ to
\[ \frac{1}{2} a \rho^2 + p_0(\mu - a \rho) + \frac{|\eta|^2}{a \rho - \mu}. \] (2.16)
Similarly from (2.2), one can see that $\frac{\partial p_\Lambda}{\partial \rho}(\rho, \eta, \mu) + \frac{a|\eta|^2}{(\epsilon_0^\Lambda)^2}$ is also convex and thus by the same argument, it converges uniformly in $\rho$ on compact subsets of $((\mu - \mu_0)/a, \infty)$. Since it is also clear that $\frac{a|\eta|^2}{(\epsilon_0^\Lambda)^2}$ converges uniformly on the same subsets, so does $\frac{\partial p_\Lambda}{\partial \rho}(\rho, \eta, \mu)$ with limit
\[ a \rho - a \rho_0(\mu - a \rho) - \frac{a|\eta|^2}{(a \rho - \mu)^2}. \] (2.17)
Since
\[ \lim_{\Lambda \uparrow \mathbb{R}^d} p_\Lambda(\eta, \mu) = \lim_{\Lambda \uparrow \mathbb{R}^d} p_\Lambda(\bar{\rho}_\Lambda, \eta, \mu) \] (2.18)
and
\[ \frac{\partial p_\Lambda}{\partial \rho}(\bar{\rho}_\Lambda, \eta, \mu) = 0, \] (2.19)
the lemma follows immediately.

Lemma 4
\[ \lim_{\Lambda \uparrow \mathbb{R}^d} p_\Lambda(\mu) = \lim_{\eta \to 0} \lim_{\Lambda \uparrow \mathbb{R}^d} p_\Lambda(\eta, \mu). \] (2.20)

Proof: By Bogoliubov's convexity inequality one has
\[ -\frac{|\eta|}{\sqrt{V}} \langle a_0 + a_0^* \rangle_{H_\Lambda(\mu)} \leq p_\Lambda(\mu) - p_\Lambda(\eta, \mu) \leq \frac{|\eta|}{\sqrt{V}} \langle a_0 + a_0^* \rangle_{H_\Lambda(\eta, \mu)}. \] (2.21)
\[0 \leq p_{\Lambda}(\mu) - p_{\Lambda}(\eta, \mu) \leq \frac{2|\eta|}{\sqrt{V}} |\langle a_0^* \rangle_{H_{\Lambda}(\eta, \mu)}| \leq \frac{2|\eta|}{\sqrt{V}} \langle a_0^* a_0 \rangle_{H_{\Lambda}(\eta, \mu)}^{\frac{1}{2}} \leq \frac{2|\eta|}{\sqrt{V}} \langle N_{\Lambda} \rangle_{H_{\Lambda}(\eta, \mu)}^{\frac{1}{2}}. \] (2.22)

Now, by convexity with respect to \(\mu\):

\[\left\langle \frac{N_{\Lambda}}{V} \right\rangle_{H_{\Lambda}(\eta, \mu)} \leq p_{\Lambda}(\eta, \mu + 1) - p_{\Lambda}(\eta, \mu) \leq p_{\Lambda}(\eta, \mu + 1). \] (2.23)

Since

\[H_{\Lambda}(\eta) - (\mu + 1)N_{\Lambda} = T_{\Lambda} + \frac{aN^2_{\Lambda}}{2V} - (\mu + 1)N_{\Lambda} + (\sqrt{V}\eta + a_0^*)(\sqrt{V}\eta + a_0) - a_0^* a_0 - V|\eta|^2\]
\[\geq T_{\Lambda} + \frac{aN^2_{\Lambda}}{2V} - (\mu + 2)N_{\Lambda} - V|\eta|^2\]
\[= T_{\Lambda} - (\mu_0 - 1)N_{\Lambda} + \frac{a}{2V} \left( N_{\Lambda} - \frac{V(\mu - \mu_0 + 3)}{a} \right)^2\]
\[\geq T_{\Lambda} - (\mu_0 - 1)N_{\Lambda} - V|\eta|^2 - \frac{V(\mu - \mu_0 + 3)^2}{2a}, \] (2.24)

we have the estimate

\[p_{\Lambda}(\eta, \mu + 1) \leq p_0(\mu_0 - 1) + 1 + |\eta|^2 + \frac{(\mu - \mu_0 + 3)^2}{2a} \] (2.25)

for large \(\Lambda\). Thus the righthand side of (2.22) tends to zero as \(\eta\) tends to zero.

\[\square\]

Finally as \(\eta \rightarrow 0\), \(\rho(\eta, \mu)\) tends to \((\mu - \mu_0)/a\) if \(\mu \geq \mu_c\) and to the unique solution of \(\rho = \rho_0(\mu - a\rho)\) if \(\mu < \mu_c\), proving the Proposition.

\[\square\]

3 Remarks

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

In the proof presented in [3] the authors employ the device of shifting the spectrum to change the density of states removing the phase transition.

Thirdly, in [4] 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 critical 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.

Finally we remark that if we replace the interaction term in (1.1) by the operator $V\phi(N_\Lambda/V)$
where $\phi$ is a non-negative smooth convex function, the arguments used here go through with
minor modifications to obtain the limiting pressure.

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