

Boson gas mean field models in weak trapping potentials by means of random point fields

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概要

We study a mean field model of boson gases trapped in a harmonic potential. The behaviors of the position distribution in the weak potential limit are classified into two types. In the high temperature region and in the weak potential limit, the position distributions converge to that of the free boson gas. In the low temperature region, the position distributions is not uniform (diverge) because of the Bose condensation.

1 Introduction and the Result

The mean field models are the simplified models of quantum statistical mechanics of boson gases, where constituent particles are supposed to interact each other by homogeneous repulsive force with a coupling constant $\lambda > 0$.

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We start with the one particle Hamiltonian

$$H_\kappa = \frac{1}{2} \sum_{j=1}^d \left(-\frac{\partial^2}{\partial x_j^2} + \frac{x_j^2}{\kappa^2} - \frac{1}{\kappa} \right),$$

which is self-adjoint operator in $L^2(\mathbb{R}^d)$ for $\kappa > 0$. We assume $d > 2$. It is well known that

$$\text{Spec } H_\kappa = \{ |n|_1/\kappa \mid n = (n_1, \dots, n_d) \in \mathbb{Z}_+^d \}$$

holds, where $|n|_1 = \sum_{j=1}^d n_j$ and \mathbb{Z}_+ is the set of all non-negative integers. The wave function of the ground state is

$$\Omega_0^\kappa(x) = \frac{1}{(\pi\kappa)^{d/4}} e^{-|x|^2/2\kappa}, \quad (1.1)$$

where $x = (x_1, \dots, x_d) \in \mathbb{R}^d$ and $|x|^2 = \sum_{j=1}^d x_j^2$. The Boltzmann factor $G_\kappa = e^{-\beta H_\kappa}$ has the integral kernel

$$G_\kappa(x, y) = \frac{\exp\left(- (2\kappa)^{-1} \tanh(\beta/2\kappa) (|x|^2 + |y|^2) - |x - y|^2 / (2\kappa \sinh(\beta/\kappa))\right)}{(\pi\kappa(1 - e^{-2\beta/\kappa}))^{d/2}} \quad (1.2)$$

(Mehler's formula), the trace $\text{Tr } G_\kappa = 1/(1 - e^{-\beta/\kappa})^d = O(\kappa^d)$ and the largest eigenvalue $\|G_\kappa\| = 1$. Here, $\beta > 0$ is the inverse temperature.

The partition function of our mean field model is given by

$$\begin{aligned} \Xi_\kappa &= \sum_{n=0}^{\infty} e^{\beta\mu n - \beta\lambda n^2/2\kappa^d} \text{Tr}_{\otimes_s^n L^2(\mathbb{R}^d)} [\otimes^n G_\kappa] \\ &= \sum_{n=0}^{\infty} \frac{e^{\beta\mu n - \beta\lambda n^2/2\kappa^d}}{n!} \int_{(\mathbb{R}^d)^n} \text{per} \{G_\kappa(x_i, x_j)\}_{1 \leq i, j \leq n} dx_1 \cdots dx_n, \end{aligned}$$

where $\otimes_s^n L^2(\mathbb{R}^d)$ is the n -fold symmetric Hilbert space tensor product of $L^2(\mathbb{R}^d)$, "per" represents the permanent for matrices, and the zeroth term of Ξ_κ is 1 by definition.

We are interesting in the limit $\kappa \rightarrow \infty$. This can be considered as a procedure of thermodynamic limit(TDL). Consider the general Hamiltonian

$$\tilde{H}_\kappa = \frac{1}{2} \sum_{j=1}^d \left(-\frac{\partial^2}{\partial x_j^2} + V\left(\frac{x}{\kappa}\right) \right).$$

In the usual TDL procedure, we take V as a infinitely deep well potential. By generalizing the potential V , we expect that we can obtain various theories in the limit $\kappa \rightarrow \infty$ and we may regard them as those for free boson gases. As the first case of the possibility, we take the harmonic potential for V in this note. We can also regard that the model

will yield the description of the behavior of the boson gases in macroscopic vessels. This is experimentally more realistic than that of boson gases in the unbounded space \mathbb{R}^d .

In this note, we announce the result concerning the behavior of the position distributions of the mean field boson gas models in the weak potential limit $\kappa \rightarrow \infty$. We also illustrate some ideas which was used in the proof of the result. The detailed proof will be published elsewhere. [TZ]

We study the system in terms of random point fields which describe the position distribution of the constituent particles of the gases. Here, let us try to make an brief introduction of the theory of random point fields adapted to our system.

Let $Q(\mathbb{R}^d)$ be the set of all the locally finite subsets of \mathbb{R}^d , i.e., the space of all the sets of sparsely distributed points in \mathbb{R}^d . A probability measure on $Q(\mathbb{R}^d)$ is called a random point field (RPF) on \mathbb{R}^d . We make the identification between the set of points $\{x_1, x_2, \dots, x_n, \dots\}$ and the point measure $\sum_j \delta_{x_j} = \xi$. Then, $Q(\mathbb{R}^d)$ is considered as the space of all the integer valued Radon measures on \mathbb{R}^d . In this scheme, we may introduce the natural functionals on $Q(\mathbb{R}^d)$:

$$\langle f, \xi \rangle = \sum_j f(x_j)$$

for $f : \mathbb{R}^d \rightarrow \mathbb{R}$. By using this functional, various quantities are described. For examples,

$$\langle \chi_A, \xi \rangle = \sum_j \chi_A(x_j) = \#\{x_j \in A\}$$

represents the number of points in the intersection of A and the set identified by ξ , and

$$\lim_{A \uparrow \mathbb{R}^d} \frac{\langle \chi_A, \xi \rangle}{\text{vol}(A)}$$

represents the average density of ξ , and so on. Especially, the generating functionals or Laplace functional of a RPF plays an important role in the theory of RPFs. A RPF μ on \mathbb{R}^d is characterize by its generating (or Laplace) functional

$$\int_{Q(\mathbb{R}^d)} e^{-\langle f, \xi \rangle} d\nu,$$

for $f \in C_0(\mathbb{R}^d)$, $f \geq 0$. Moreover the weak convergence of any sequence of RPF is established if the point-wise convergence of corresponding sequence of generating functionals is shown. For details description of the theory of RPFs, see e.g., [DV].

Now let us see how to represent RPFs on \mathbb{R}^d which describe the position distribution of our mean field model and to calculate their generating functionals.

A RPF is determined if the exclusion measures are given. That is to say,

$$\text{Prob} \left\{ \begin{array}{l} \text{The total number of points is equal to } n \\ \text{and one point is contained in each} \\ d\text{-dimensional rectangle } (x_j, x_j + dx_j] \\ = \prod_{k=1}^d (x_j^{(k)}, x_j^{(k)} + dx_j^{(k)}], (j = 1, \dots, n) \end{array} \right\} \equiv J_n(x_1, \dots, x_n) dx_1 \cdots dx_n,$$

where $x_j = (x_j^{(k)})_{k=1}^d$. The partition function Ξ_κ suggests that the position distribution of constituent particles of our system is given by

$$J_n(x_1, \dots, x_n) = e^{\beta\mu n - \beta\lambda n^2/2\kappa^d} \text{per} \{G_\kappa(x_i, x_j)\}_{1 \leq i, j \leq n} / \Xi_\kappa.$$

Then the resulting RPF ν_κ has the generating functional

$$\begin{aligned} \int_{Q(\mathbb{R}^d)} d\nu_\kappa(\xi) e^{-\langle f, \xi \rangle} &= \sum_{n=0}^{\infty} \int_{(\mathbb{R}^d)^n} e^{-\sum_j f(x_j)} \frac{J_n(x_1, \dots, x_n)}{n!} dx_1 \cdots dx_n \\ &= \frac{1}{\Xi_\kappa} \sum_{n=0}^{\infty} e^{\beta\mu n - \beta\lambda n^2/2\kappa^d} \text{Tr}_{\otimes_n^2 L^2(\mathbb{R}^d)} [(\otimes^n G_\kappa)(\otimes^n e^{-f})] = \frac{\tilde{\Xi}_\kappa}{\Xi_\kappa}, \end{aligned} \quad (1.3)$$

where

$$\tilde{\Xi}_\kappa = \sum_{n=0}^{\infty} e^{\beta(\mu n - \lambda n^2/2\kappa^d)} \text{Tr}_{\otimes_n^2 L^2(\mathbb{R}^d)} [\otimes^n \tilde{G}_\kappa]$$

and $\tilde{G}_\kappa = G_\kappa^{1/2} e^{-f} G_\kappa^{1/2}$. See the arguments in [TIa, TIb, TIc] for detail.

Put

$$m = \int_{[0, \infty)^d} \frac{dp}{e^{|p|_1} - 1},$$

where $|p|_1 = \sum_{j=1}^d |p_j|$ for $p = (p_1, \dots, p_d)$. Note that m is finite, since $d > 2$. Our main result is

Theorem 1.1 (i) *If $\beta^d \mu < m\lambda$ holds, the random point fields ν_κ defined above converge weakly to the random point field ν_∞ having the generating functional*

$$\int_{Q(\mathbb{R}^d)} e^{-\langle f, \xi \rangle} d\nu_\infty(\xi) = \text{Det} [1 + \sqrt{1 - e^{-f}} r_* G (1 - r_* G)^{-1} \sqrt{1 - e^{-f}}]^{-1} \quad (1.4)$$

with $\kappa \rightarrow \infty$, where $G = e^{\beta\Delta/2}$ is the heat operator on $L^2(\mathbb{R}^d)$ and $r_* \in (0, 1)$ is uniquely determined by

$$\beta\mu = \lambda \log r_* + \frac{\lambda}{\beta^{d-1}} \int_{[0, \infty)^d} \frac{r_* dp}{e^{|p|_1} - r_*}.$$

Here Det stands for the Fredholm determinant.

(ii) *If $\beta^d \mu > m\lambda$ holds, the generating functional (1.3) has the behavior*

$$\lim_{\kappa \rightarrow \infty} \frac{1}{\kappa^{d/2}} \log \int_{Q(\mathbb{R}^d)} e^{-\langle f, \xi \rangle} d\nu_\kappa(\xi) = -\frac{\beta^d \mu - m\lambda}{\pi^{d/2} \beta^d \lambda} (\sqrt{1 - e^{-f}}, (1 + K_f)^{-1} \sqrt{1 - e^{-f}}), \quad (1.5)$$

where $K_f = (G^{1/2}(1 - G)^{-1/2} \sqrt{1 - e^{-f}})^* (G^{1/2}(1 - G)^{-1/2} \sqrt{1 - e^{-f}})$.

Remark 1. K_f is a positive trace class operator on $L^2(\mathbb{R}^d)$, (see [Tib]).

Remark 2. There is a sharp contrast in the particle density distribution between two regimes (i) and (ii). Heuristic understanding of this difference is the following:

In the case (i) (normal phase), let us suppose that each constituent particle may be considered independently distributed according to the Gibbs factor $G_\kappa = e^{-\beta H_\kappa}$. Then the particles are located in the region of radius κ around the origin almost uniformly as the kernel of G_κ (1.2) indicates. While in the case (ii) (condensed phase), let us suppose that a substantial part of particles are in the ground state and the other part of particles behave as in (i). Then the former part distributes in the region of radius $\kappa^{1/2}$ around the origin according to the profile of the square of the ground state wave function of the harmonic oscillator (1.1). Since we focus our attention to the distribution of particles near the origin in the limit $\kappa \rightarrow \infty$, the density is dominated by the particles condensed in the ground state.

Corollary 1.2 (i) *If $\beta^d \mu < m\lambda$ holds, the mean and the covariance of the (random) point measure $\{\xi(x)\}_{x \in \mathbb{R}^d}$ are given by*

$$E[\xi(x)] = \int_{\mathbb{R}^d} \frac{dp}{(2\pi)^d} \frac{r_*}{e^{\beta|p|^2} - r_*},$$

$$Cov[\xi(x), \xi(y)] = \delta(x-y) \int_{\mathbb{R}^d} \frac{dp}{(2\pi)^d} \frac{r_*}{e^{\beta|p|^2} - r_*} + \left| \int_{\mathbb{R}^d} \frac{dp}{(2\pi)^d} \frac{r_* e^{ip \cdot (x-y)}}{e^{\beta|p|^2} - r_*} \right|^2$$

in the limiting distribution.

(ii) *If $\beta^d \mu > m\lambda$ holds, the leading term of the mean and the covariance of the point measure $\xi(x)$ are given by*

$$E[\xi(x)] = \frac{\beta^d \mu - m\lambda}{\pi^{d/2} \beta^d \lambda} \kappa^{d/2} + o(\kappa^{d/2}),$$

$$Cov[\xi(x), \xi(y)] = \frac{\beta^d \mu - m\lambda}{\pi^{d/2} \beta^d \lambda} \kappa^{d/2} \left(\delta(x-y) + 2 \int_{\mathbb{R}^d} \frac{dp}{(2\pi)^d} \frac{e^{ip \cdot (x-y)}}{e^{\beta|p|^2} - 1} \right) + o(\kappa^{d/2}).$$

2 Strategy of the Proof

In this section, we give an sketch of the proof of the main theorem. First we use the following formula to handle the integrations of permanents

$$\frac{1}{n!} \int \text{per} \{J(x_i, x_j)\}_{1 \leq i, j \leq n} dx_1 \cdots dx_n = \oint_{S_r(0)} \frac{dz}{2\pi i z^{n+1} \text{Det}(1 - zJ)},$$

where $r > 0$ satisfies $\|rJ\| < 1$. This comes from the generalized *Vere-Jones' formula* [V, ST]

$$\text{Det}(1 - zJ)^{-1} = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int \text{per} \{J(x_i, x_j)\}_{1 \leq i, j \leq n} dx_1 \cdots dx_n.$$

To calculate the sum of n , we use

$$e^{-\beta\lambda n^2/2\kappa^d} = \sqrt{\frac{\beta\lambda}{2\pi\kappa^d}} \int_{\mathbb{R}} dx e^{-\frac{\beta\lambda}{2\kappa^d}((x+is)^2 - 2in(x+is))}.$$

If

$$e^{\beta\mu - \beta\lambda s/\kappa^d} < r$$

holds, we get

$$\Xi_\kappa = \sqrt{\frac{\kappa^d}{2\pi\beta\lambda} \frac{e^{\beta\lambda s^2/2\kappa^d}}{\text{Det}[1 - rG_\kappa]}} \int_{\mathbb{R}} dx \frac{e^{-isx - \kappa^d x^2/2\beta\lambda}}{\text{Det}[1 - (e^{ix} - 1)rG_\kappa(1 - rG_\kappa)^{-1}]}.$$

It is convenient to choose $(r, s) = (r_\kappa, s_\kappa)$ which is the solution of

$$\begin{cases} r = \exp(\beta\mu - \beta\lambda s/\kappa^d) \\ s = \text{Tr}[rG_\kappa(1 - rG_\kappa)^{-1}]. \end{cases}$$

Similarly, we have

$$\tilde{\Xi}_\kappa = \sqrt{\frac{\kappa^d}{2\pi\beta\lambda} \frac{e^{\beta\lambda \tilde{s}_\kappa^2/2\kappa^d}}{\text{Det}[1 - \tilde{r}_\kappa \tilde{G}_\kappa]}} \int_{\mathbb{R}} dx \frac{e^{-i\tilde{s}_\kappa x - \kappa^d x^2/2\beta\lambda}}{\text{Det}[1 - (e^{ix} - 1)\tilde{r}_\kappa \tilde{G}_\kappa(1 - \tilde{r}_\kappa \tilde{G}_\kappa)^{-1}]},$$

where $(\tilde{r}_\kappa, \tilde{s}_\kappa)$ satisfies

$$\begin{cases} \tilde{r} = \exp(\beta\mu - \beta\lambda \tilde{s}/\kappa^d) \\ \tilde{s} = \text{Tr}[\tilde{r}\tilde{G}_\kappa(1 - \tilde{r}\tilde{G}_\kappa)^{-1}]. \end{cases}$$

The conditions for $r_\kappa, \tilde{r}_\kappa$ can be written as

$$\frac{1}{\kappa^d} \text{Tr}[r_\kappa G_\kappa(1 - r_\kappa G_\kappa)^{-1}] = \frac{\beta\mu - \log r_\kappa}{\beta\lambda}, \quad (2.1)$$

$$\frac{1}{\kappa^d} \text{Tr}[\tilde{r}_\kappa \tilde{G}_\kappa(1 - \tilde{r}_\kappa \tilde{G}_\kappa)^{-1}] = \frac{\beta\mu - \log \tilde{r}_\kappa}{\beta\lambda}. \quad (2.2)$$

The behavior of r_κ for large κ can be deduced from (2.1):

Proposition 2.1 (a) $\{r_\kappa\}$ converges to $r_* \in (0, 1)$ as $\kappa \rightarrow \infty$, if and only if $\beta^d \mu < m\lambda$ (high temperature region).

(b) $\kappa^d(1 - r_\kappa) \rightarrow \beta^d \lambda / (\beta^d \mu - m\lambda)$, and hence $\lim_{\kappa \rightarrow \infty} r_\kappa = 1$, if and only if $\beta^d \mu > m\lambda$ (low temperature region).

(c) $\lim_{\kappa \rightarrow \infty} r_\kappa = 1$ and $\kappa^d(1 - r_\kappa) \rightarrow +\infty$, if and only if $\beta^d \mu = m\lambda$ (critical point).

The proposition gives the phase structure.

For this type of work, we must need some estimates of the spirit of

$$H_\kappa = \frac{1}{2} \left(-\Delta + \frac{x^2}{\kappa^2} - \frac{d}{\kappa} \right) \rightarrow -\frac{1}{2} \Delta$$

or

$$G_\kappa = e^{-\beta H_\kappa} \rightarrow G = e^{\beta \Delta/2}$$

in some sense. The following lemma gives such estimates suitable to the work.

Lemma 2.2 For any $r \in (0, 1)$,

$$\|\sqrt{1 - e^{-f}} [rG_\kappa(1 - rG_\kappa)^{-1} - rG(1 - rG)^{-1}] \sqrt{1 - e^{-f}}\|_1 \rightarrow 0,$$

$$\|\sqrt{1 - e^{-f}} Q_\kappa G_\kappa Q_\kappa (1 - Q_\kappa G_\kappa Q_\kappa)^{-1} \sqrt{1 - e^{-f}} - K_f\|_1 \rightarrow 0$$

hold in the limit $\kappa \rightarrow \infty$, where $\|\cdot\|_1$ denotes the trace norm and Q_κ the projection onto the orthogonal subspace to the ground state.

We use the lemma to calculate the following ratio appeared in $\tilde{\Xi}_\kappa/\Xi_\kappa$. For the high temperature phase, we get

$$\begin{aligned} \frac{\text{Det}[1 - \tilde{r}_\kappa \tilde{G}_\kappa]}{\text{Det}[1 - \tilde{r}_\kappa G_\kappa]} &= \text{Det}[1 + \tilde{r}_\kappa (G_\kappa - \tilde{G}_\kappa) (1 - \tilde{r}_\kappa G_\kappa)^{-1}] \\ &= \text{Det}[1 + \sqrt{1 - e^{-f}} \frac{\tilde{r}_\kappa G_\kappa}{1 - \tilde{r}_\kappa G_\kappa} \sqrt{1 - e^{-f}}] \rightarrow \text{Det}[1 + \sqrt{1 - e^{-f}} \frac{r_* G}{1 - r_* G} \sqrt{1 - e^{-f}}]. \end{aligned}$$

For low temperature phase, the lemma is used in the second factor of the right-hand side of

$$\begin{aligned} \frac{\text{Det}[1 - r_\kappa G_\kappa]}{\text{Det}[1 - \tilde{r}_\kappa \tilde{G}_\kappa]} &= \frac{\text{Det}[1 - \tilde{r}_\kappa Q_\kappa \tilde{G}_\kappa Q_\kappa]}{\text{Det}[1 - \tilde{r}_\kappa \tilde{G}_\kappa]} \\ &\times \frac{\text{Det}[1 - \tilde{r}_\kappa Q_\kappa G_\kappa Q_\kappa]}{\text{Det}[1 - \tilde{r}_\kappa Q_\kappa \tilde{G}_\kappa Q_\kappa]} \frac{\text{Det}[1 - r_\kappa G_\kappa]}{\text{Det}[1 - r_\kappa Q_\kappa G_\kappa Q_\kappa]} \end{aligned} \quad (2.3)$$

to get

$$\begin{aligned} \frac{\text{Det}[1 - \tilde{r}_\kappa Q_\kappa G_\kappa Q_\kappa]}{\text{Det}[1 - \tilde{r}_\kappa Q_\kappa \tilde{G}_\kappa Q_\kappa]} &= \frac{1}{\text{Det}[1 + \tilde{r}_\kappa Q_\kappa (G_\kappa - \tilde{G}_\kappa) Q_\kappa (1 - \tilde{r}_\kappa Q_\kappa G_\kappa Q_\kappa)^{-1}]} \\ &= \text{Det}[1 + \tilde{r}_\kappa \sqrt{1 - e^{-f}} Q_\kappa G_\kappa Q_\kappa (1 - \tilde{r}_\kappa Q_\kappa G_\kappa Q_\kappa)^{-1} \sqrt{1 - e^{-f}}]^{-1} \rightarrow \text{Det}[1 + K_f]^{-1}. \end{aligned}$$

However this factor yields a contribution of $O(1)$. A part of the leading contributions comes from the third factors. The first factor is calculated by means of the Feshbach formula. For these factors, we need estimates about the difference between the largest eigenvalues of G_κ and \tilde{G}_κ . Put the eigenvalues of G_κ in decreasing order:

$$g_0^{(\kappa)} = 1 > g_1^{(\kappa)} = e^{-\beta/\kappa} \geq g_2^{(\kappa)} \geq \dots$$

and those of \tilde{G}_κ in the decreasing order:

$$\tilde{g}_0^{(\kappa)} = \|\tilde{G}_\kappa\| \geq \tilde{g}_1^{(\kappa)} \geq \dots$$

Then the following lemma holds.

Lemma 2.3 (i) $g_j^{(\kappa)} \geq \tilde{g}_j^{(\kappa)} \quad (j = 0, 1, 2, \dots)$
(ii) $g_0^{(\kappa)} = 1 > \tilde{g}_0^{(\kappa)} = 1 - \hat{O}(\kappa^{-d/2}) > g_1^{(\kappa)} = 1 - \hat{O}(\kappa^{-1}) \geq \tilde{g}_1^{(\kappa)}$.

The first part is immediate from the min-max principle. However, the second needs some analysis for the perturbation.

The above properties about \tilde{G}_κ and G_κ and (2.2) give the following behavior of $\tilde{r}_\kappa - r_\kappa$.

Lemma 2.4 (a) If $\beta^d \mu < m\lambda$ (high temperature),
 $0 < \tilde{r}_\kappa - r_\kappa = O(\kappa^{-d})$.
(b) If $\beta^d \mu > m\lambda$ (low temperature),
 $0 < \tilde{r}_\kappa - r_\kappa = O(\kappa^{-d/2})$.

Finally we must calculate the integration

$$\int_{\mathbf{R}} dx \frac{e^{-is_\kappa x - \kappa^d x^2 / 2\beta\lambda}}{\text{Det}[1 - (e^{ix} - 1)r_\kappa G_\kappa(1 - r_\kappa G_\kappa)^{-1}]} \quad (2.4)$$

and the corresponding one for \tilde{G} . Note that the poles of the integrand are contained in the lower half plane. In the high temperature region ($\beta^d \mu < m\lambda$), the poles are bounded away from the real line. In this case, expanding $\log \text{Det}(1 - X)$, we get the Gaussian integral in the limit $\kappa \rightarrow \infty$ (the saddle point method). In the low temperature region ($\beta^d \mu > m\lambda$), some part of those poles come infinitesimally close to the real axis. And it turn out that the residue of the pole nearest to the origin is dominant for the integral.

These calculations are straightforward for (2.4). For the corresponding integrals for \tilde{G} , we obtain the same leading terms using above Lemmas 2.3 and 2.4. Thus the contributions of those complex integrals are reduced in the calculation of leading term of $\tilde{\Xi}_\kappa / \Xi_\kappa$.

For the critical case ($\beta^d \mu = m\lambda$), we have not ever obtained a corresponding result. In this case, the poles also come infinitesimally close to the real axis. However, the residues of infinitely many poles contribute to the integral comparably. So we need other idea to study the case.

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