QMath10 - Moeciu, September 10–15, 2007 "Simon Stoilow" Institute of Mathematics Bucarest, Romania

BOSON GAS with BCS INTERACTION

Valentin A. ZAGREBNOV

Université Aix-Marseille II - Luminy Centre de Physique Théorique - UMR 6207

CONTENTS

- Introduction, Motivation and Pair Boson Model
- BCS-Bose Hamiltonian
- Thermodynamics of the BCS-Bose Hamiltonian
- CCR and Quasi-Free States
- Equilibrium States of the BCS-Bose Hamiltonian
- Condensations, Pairing and Type III BEC

(Based on joint works with Joe Pulé - UC Dublin, and André Verbeure - KU Leuven)

0. Introduction, Motivation and Pair Boson Model

• The first version of Hamiltonian with BCS-Bose interaction, (Pair Boson Hamiltonian (PBH), or BCS-Bose model) was proposed by *Zubarev* and *Tserkovnikov* [Sov.Phys.Acad.Docl.1958]. Intention was to *generalize* the Bogoliubov model of the Weakly Imperfect Bose Gas by including more terms of the total interaction, without losing the possibility of having an "exact" solution.

• Two-body v(x-y) interacting Bose-gas in $\Lambda \subset \mathbb{R}^{\nu}$:

$$H_{\Lambda} = \sum_{k \in \Lambda^*} \varepsilon(k) a_k^* a_k + \frac{1}{2V} \sum_{k_1, k_2, q \in \Lambda^*} \widehat{v}(q) a_{k_1 + q}^* a_{k_2 - q}^* a_{k_2} a_{k_1},$$

• Truncations: (a) WIBG "2-zero-momentum" BEC cut: $\{k_1 = k_2 = 0\}$, $\{k_1 = -q, k_2 = q\}$, $\{k_1 = 0, k_2 = q\}$,..., $\{k_{1,2} = q = 0\}$. (b)"BCS" 1-constraint: $\{k_1 = -k_2 = p\}$ $(p = 0 \text{ cut} \Rightarrow \text{WIBG}) \Rightarrow$ $\frac{1}{2V} \sum_{p,p' \in \Lambda^*} \hat{v}(p - p') a_{p'}^* a_{-p'}^* a_{-p} a_p (\text{If } \hat{v}(p - p') \Rightarrow \overline{\lambda_p} \lambda_p' = \text{BCS} - \text{Bose})$

1

1.1 BCS-Bose Hamiltonian

• Let $\Lambda \subset \mathbb{R}^{\nu}$ be a cube of volume $V = |\Lambda|$ centered at the origin. The kinetic energy operator for a particle of mass m enclosed into the cubic box Λ , is a self-adjoint extension of the operator $t_{\Lambda} = (-\Delta/2m)$ in $\mathfrak{H}_{\Lambda} = L^2(\Lambda)$ with **e.g., periodic boundary conditions**, i.e. with eigenvalues and eigenfunctions:

$$\varepsilon(k) = ||k||^2 / 2m, \ f_k(x) = e^{ikx} / \sqrt{V}, \ k \in \Lambda^* := \{2\pi s / V^{1/\nu} | s \in \mathbb{Z}^\nu\}.$$

• Let $f_k \mapsto a^*(f_k)(=a_k^*)$ and $f_k \mapsto a(f_k)(=a_k)$ be CCR representation by the creation and annihilation operators in the **boson Fock space** $\mathfrak{F}(\mathfrak{H}_{\Lambda})$: $[a^*(f_k), a(f_{k'})] = (f_k, f_{k'})_{\mathfrak{H}_{\Lambda}}$. Then $N_k := a_k^* a_k$ is the k-mode particle number operator and $N_{\Lambda} := \sum_{k \in \Lambda^*} N_k$ is the total number operator. The kinetic-energy operator $T_{\Lambda} := d\Gamma(t_{\Lambda})$ (*Perfect Bose-gas* Hamiltonian), is

$$T_{\Lambda} := \sum_{k \in \Lambda^*} \varepsilon(k) a_k^* a_k.$$

• To introduce a *pairing term* in the BCS-Bose Hamiltonian we need the **operators** $A_k = A_{-k} := a_k a_{-k}, k \in \Lambda^*$ and

$$\tilde{Q}_{\Lambda} := \sum_{k \in \Lambda^*} \tilde{\lambda}(k) A_k$$

• The function $\tilde{\lambda} : \mathbb{R}^{\nu} \mapsto \mathbb{C}$ satisfies the following conditions:

$$|\tilde{\lambda}(k)| \leq |\tilde{\lambda}(0)| = 1, \ \tilde{\lambda}(k) = \tilde{\lambda}(-k) \text{ for all } k \in \mathbb{R}^{\nu},$$

and there exists $\mathfrak{C}<\infty\text{, }\delta>0$ such that

$$|\tilde{\lambda}(k)| \leq rac{\mathfrak{C}}{1+\|k\|^{\max(
u,\,
u/2+1)+\delta}}.$$

This implies that $\tilde{\lambda} \in L^1(\mathbb{R}^{\nu})$ and existence of $M < \infty$ that

$$\mathfrak{m}_{\Lambda} := \sum_{k \in \Lambda^*} |\tilde{\lambda}(k)| \le MV, \ \mathfrak{n}_{\Lambda} := \sum_{k \in \Lambda^*} \varepsilon(k) |\tilde{\lambda}(k)|^2 \le MV,$$

$$\mathfrak{c}_{\Lambda} := \sup_{k \in \Lambda^*} \varepsilon(k) |\tilde{\lambda}(k)|^2 \le M$$

• The constant couplings u, v Pair Boson Hamiltonian is :

$$H_{\Lambda} := T_{\Lambda} - \frac{u}{2V} \tilde{Q}_{\Lambda}^* \tilde{Q}_{\Lambda} + \frac{v}{2V} N_{\Lambda}^2$$

• Let $\varphi := \arg \tilde{\lambda}(0)$ and $\lambda(k) := \tilde{\lambda}(k)e^{-i\varphi}$. Then $\lambda(0) = 1$ and

$$H_{\Lambda} = T_{\Lambda} - \frac{u}{2V} Q_{\Lambda}^* Q_{\Lambda} + \frac{v}{2V} N_{\Lambda}^2$$

with $Q_{\Lambda} := \sum_{k \in \Lambda^*} \lambda(k) A_k$, where $|\lambda(k)| \le \lambda(0) = 1$.

• We shall assume that v > 0 and $\alpha := v - u > 0$. This condition ensures the (super)stability of the model.

• **REMARK:** In the case $u \leq 0$ (BCS repulsion), the second condition $\alpha > 0$ is satisfied and the **PBH** gives the same thermodynamics as the Mean-Field (MF) Bose-gas Hamiltonian:

$$H^{MF}_{\Lambda} := T_{\Lambda} + \frac{v}{2V} N^2_{\Lambda},$$

but not the same Bose-Einstein Condensation (BEC) !!!

1.2 Thermodynamics of the BCS-Bose Hamiltonian

• The grand-canonical pressure corresponding to Hamiltonian H_{Λ}

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

• Theorem 1: The limiting pressure for the PBH model with u > 0 (BCS attraction) has the form

$$p := \lim_{\Lambda} p_{\Lambda}[H_{\Lambda}] = \sup_{q \ge 0} \inf_{\rho : \sigma(q,\rho) \ge 0} p[H_{\Lambda}^{(2)}(q,\rho)] ,$$

while with $u \leq 0$ (BCS repulsion) it has the form

$$p := \lim_{\Lambda} p_{\Lambda}[H_{\Lambda}] = \inf_{q \ge 0} \inf_{\rho : \sigma(q,\rho) \ge 0} p[H_{\Lambda}^{(2)}(q,\rho)] ,$$

$$H_{\Lambda}^{(2)}(q,\rho) := T_{\Lambda} + v\rho N_{\Lambda} - \frac{1}{2}u(Q_{\Lambda}^{*}q + Q_{\Lambda}q^{*}) - \frac{V}{2}v\rho^{2} + \frac{V}{2}u|q|^{2} ,$$

where $q \in \mathbb{C}$, $\rho \in \mathbb{R}_+$ and the function: $\sigma(q,\rho) := \inf_{k \in \mathbb{R}^{\nu}} (f(k,\rho) - |h(k,q)|) = v\rho - \mu - |u|q.$

2.1 CCR and Quasi-Free States

• Let $f \mapsto b(f) := a(f) + a^*(f)$ on the Fock space $\mathfrak{F}(L^2(\mathbb{R}^{\nu}))$ and (*Weyl operators*) $W(f) := \exp(ib(f))$. Then CCR take the form

$$W(f)W(g) = e^{-i\sigma(f,g)}W(f+g), \ \sigma(f,g) = \Im\mathfrak{m}(f,g).$$

• Truncated states on $\mathfrak{A}(b)$ are defined recursively:

 $\omega(b(f))_t = \omega(b(f)), \ \omega(b(f)b(g)) = \omega(b(f)b(g))_t + \omega(b(f))_t \omega(b(g))_t,$ $\omega(b(f_1)...b(f_n)) = \sum \omega(b(f_k)...)_t ... \omega(...b(f_l))_t,$

• Quasi-Free states(QF) on the Weyl algebra $\mathfrak{A}(b)$ are :

$$\omega(W(f)) = \exp\{i\omega(b(f)) - \frac{1}{2}\omega(b(f)b(f))_t\}.$$

For them all truncated functions of order n > 2 vanish: $\phi(f) = \omega(a^*(f)), \langle f, Rg \rangle = \omega(a^*(f)a(g)) - \omega(a^*(f))\omega(a(g)), \langle f, Sg \rangle = \omega(a(f)a(\overline{g})) - \omega(a(f))\omega(a(\overline{g})).$

2.2 Equilibrium States of the BCS-Bose Hamiltonian

• Theorem 2: Pure Gibbs state $\omega_{\alpha}(-) = \lim_{\Lambda} \omega_{H_{\Lambda}}(-)$ generated by the BCS-Bose Hamiltonian is Quasi-Free with parameters defined by Theorem 1: $c = \sqrt{\rho_0}e^{i\alpha} = \lim_{\Lambda} \omega_{H_{\Lambda}}(a_{k=0}/\sqrt{V})$

 $\omega(a_k^*a_k) = \langle f_k, Rf_k \rangle + |c|^2 V \delta_{k,0}, \quad \omega(a_k a_{-k}) = \langle \phi_k, S\phi_k \rangle + c^2 V \delta_{k,0},$ for $V \to \infty$ with $\rho(k) = r(k), \ \overline{\rho} = \int \mathrm{d}k \,\rho(k) + \rho_0$ and $\sigma = \int \mathrm{d}k \,\lambda(k) s(k).$ • Since $f(k) = \epsilon(k) - \mu + v\overline{\rho}, \ E(k) = \left\{ f^2(k) - u^2 |\lambda(k)|^2 (\rho_0 + |\sigma|)^2 \right\}^{1/2}.$

$$\overline{\rho} = \frac{1}{2} \int_{\mathbb{R}^{\nu}} \frac{d^{\nu}k}{(2\pi)^{\nu}} \left\{ \frac{f(k)}{E(k)} \operatorname{coth} \frac{1}{2} \beta E(k) - 1 \right\} + \rho_{0} ,$$
$$(|\sigma| + \rho_{0}) = \frac{u(|\sigma| + \rho_{0})}{2} \int_{\mathbb{R}^{\nu}} \frac{d^{\nu}k}{(2\pi)^{\nu}} \frac{|\lambda(k)|^{2}}{E(k)} \operatorname{coth} \frac{1}{2} \beta E(k) + \rho_{0} .$$

• Chemical potential and the "spectrum":

$$\mu = v\overline{\rho} + u(\rho_0 + |\sigma|)) \Leftrightarrow E(k = 0) = 0.$$

3. Condensations, Pairing and Type III BEC

3.1 Let u > 0 (BCS-Bose attraction), v > 0 and v - u > 0 (stability).

• For large u there is $\mu_c^-(u) < \mu_c$: $\sigma \neq 0$, $\rho_0 = 0$ and "gap", when $\mu_c^-(u) < \mu < \mu_c = v \overline{\rho}_c^{PBG}$.

• For $\mu_c \leq \mu$: $\rho_0 > 0$ (one-mode BEC) $\Rightarrow \sigma \neq 0$ and no "gap".

3.2 Let u < 0 (BCS-Bose repulsion).

- Pressure for BCS-Bose = Mean-Field model (v > 0).
- Condensations: $\sigma = 0$ and $\rho_0 = 0$!
- BEC \neq 0 for $\mu > \mu_c = v \overline{\rho}_c^{PBG}$ and is type III.