

The thermodynamic limit for interacting quantum fermions in a random environment: the random pieces model

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IMJ - UPMC

Microlocal analysis and spectral theory
In honor of J. Sjöstrand
CIRM, Luminy, 23/09/2013

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The n particle system

- On Λ large cube of \mathbb{R}^d , consider $H_\omega(\Lambda)$ a random Schrödinger operator (single particle model).
- On $\bigwedge_{j=1}^n L^2(\Lambda) = L^2_-(\Lambda^n)$, consider the free operator

$$H_\omega^0(\Lambda, n) = \sum_{i=1}^n \underbrace{1 \otimes \dots \otimes 1}_{i-1 \text{ times}} \otimes H_\omega(\Lambda) \otimes \underbrace{1 \otimes \dots \otimes 1}_{n-i \text{ times}}.$$

- Pick $U : \mathbb{R}^d \rightarrow \mathbb{R}^+$ pair interaction potential
Define

$$H_\omega^U(\Lambda, n) = H_\omega^0(\Lambda, n) + W_n, \quad \text{where} \quad W_n(x^1, \dots, x^n) := \sum_{i < j} U(x^i - x^j).$$

Thermodynamic limit

- Let $E_\omega^U(\Lambda, n)$ be the ground state energy of $H_\omega^U(\Lambda, n)$.
- Let $\Psi_\omega^U(\Lambda, n)$ be the associated eigenfunction.

Problem

Describe $E_\omega^U(\Lambda, n)$ and $\Psi_\omega^U(\Lambda, n)$ in the limit $|\Lambda| \rightarrow +\infty$ and $\frac{n}{|\Lambda|} \rightarrow \rho > 0$.

Description of the ground state : the (reduced) density matrices :

Let $\Psi \in L^2_-(\Lambda^n)$ be a normalized n -fermion wave function.

- One-particle density matrix is an operator on $L^2(\Lambda)$ with kernel

$$\gamma_\Psi^{(1)}(x, y) = n \int_{\Lambda^{n-1}} \Psi(x, \tilde{x}) \Psi^*(y, \tilde{x}) d\tilde{x}.$$

- Two-particle density matrix is an operator on $L^2_-(\Lambda^2)$ with kernel

$$\gamma_\Psi^{(2)}(x^1, x^2, y^1, y^2) = \frac{n(n-1)}{2} \int_{\Lambda^{n-2}} \Psi(x^1, x^2, \tilde{x}) \Psi^*(y^1, y^2, \tilde{x}) d\tilde{x}.$$

Both $\gamma_\Psi^{(1)}$ and $\gamma_\Psi^{(2)}$ are positive trace class operators satisfying

$$\text{tr} \gamma_\Psi^{(1)} = n \quad \text{and} \quad \text{tr} \gamma_\Psi^{(2)} = \frac{n(n-1)}{2}.$$

The non interacting system

Let $(E_p)_{p \geq 1} = (E_p(\omega, \Lambda))_{p \geq 1}$ (resp. $(\psi_p)_{p \geq 1} = (\psi_p(\omega, \Lambda))_{p \geq 1}$) be the eigenvalues (resp. associated eigenfunctions) of $H_\omega(\Lambda)$.

Set $\mathbb{N}_n^+ = \{\alpha = (\alpha_1, \dots, \alpha_n); \forall i, \alpha_i < \alpha_{i+1}\}$. Then,

- eigenvalues of $H_\omega^0(\Lambda, n)$ given by $E_\alpha := \sum_{1 \leq j \leq n} E_{\alpha_j}$ where $\alpha \in \mathbb{N}_n^+$,
- eigenfunction of $H_\omega^0(\Lambda, n)$ associated to E_α given by Slater determinant

$$\Psi_\alpha(x^1, x^2, \dots, x^n) = \frac{1}{\sqrt{n!}} \det(\psi_{\alpha_k}(x^j))_{1 \leq j, k \leq n}.$$

Ground state energy per particle for non interacting particles : Define

$$N_{H_\omega(\Lambda)}(E) = \frac{\#\{\text{e.v. of } H_\omega(\Lambda) \text{ in } (-\infty, E]\}}{|\Lambda|}$$

Thus, as $N_{H_\omega(\Lambda)}(E_n) = n/|\Lambda| \rightarrow \rho$, one has

$$\frac{E_\omega^0(\Lambda, n)}{n} = \frac{1}{n} \sum_{j=1}^n E_j = \frac{|\Lambda|}{n} \int_{-\infty}^{E_n} E dN_{H_\omega(\Lambda)}(E) \xrightarrow[n/|\Lambda| \rightarrow \rho]{|\Lambda| \rightarrow +\infty} \frac{1}{\rho} \int_{-\infty}^{E_\rho} E dN(E)$$

where $N(E_\rho) = \rho$; E_ρ is the Fermi energy and N IDS of H_ω .

The non interacting ground state

We describe the one-particle density matrix of $\Psi_\omega^0(\Lambda, n)$, the non interacting ground state :

$$\gamma_{\Psi_\omega^0(\Lambda, n)}^{(1)} = \sum_{p=1}^n \gamma_{\psi_p(\omega, \Lambda)}^{(1)} = \sum_{p=1}^n \psi_p(\omega, \Lambda) \otimes \overline{\psi_p(\omega, \Lambda)}.$$

One proves that, in the thermodynamic limit, one has

$$\gamma_{\Psi_\omega^0(\Lambda, n)}^{(1)} \xrightarrow[n/|\Lambda| \rightarrow \rho]{|\Lambda| \rightarrow +\infty} \mathbf{1}_{(-\infty, E_\rho]}(H_\omega).$$

Depending on the model under consideration, the limit can be proved in the strong operator topology, or for the trace norm par particle.

A simple one-dimensional random model

The pieces (or Luttinger-Sy) model

- On \mathbb{R} , consider Poisson process $d\mu(\omega)$ of intensity μ i.e.

$$d\mu(\omega) = \sum_{k \in \mathbb{Z}} \delta_{x_k(\omega)}.$$

- For $\Lambda = [-L/2, L/2]$, on $L^2(\Lambda)$, define

$$H_\omega(L) = \bigoplus_{k \in \mathbb{Z}} -\frac{d^2}{dx^2} \Big|_{\Delta_k \cap \Lambda}^D \quad \text{where} \quad \Delta_k = \Delta_k(\omega) = [x_k, x_{k+1}]$$

- Integrated density of states

$$\begin{aligned} N(E) &:= \lim_{L \rightarrow +\infty} \frac{\#\{\text{eigenvalues of } H_\omega(L) \text{ in } (-\infty, E]\}}{L} \\ &= \frac{\exp(-\ell_E)}{1 - \exp(-\ell_E)} 1_{E \geq 0} \quad \text{where } \ell_E := \frac{\pi}{\sqrt{E}}. \end{aligned}$$

Why did we choose the pieces model ?

It shares the common characteristics of a general random one particle system in the localized phase :

- the model exhibits Lifshitz tail asymptotics,
- the eigenfunctions are localized (on a scale $\log L$),
- the localization centers and the eigenvalues satisfy Poisson statistics,

Description of spectral characteristics are much better than for a general random one particle system in the localized phase

- eigenfunctions and eigenvalues are known explicitly,
- the density of states is known explicitly i.e. given by a closed formula.

Main difference compared to more realistic models :

tunnel effect is missing for a single particle.

The n particle system

- On $\bigwedge_{j=1}^n L^2([-L/2, L/2]) = L^2([-L/2, L/2]^n)$, consider the free operator

$$H_\omega^0(L, n) = \sum_{i=1}^n \underbrace{1 \otimes \dots \otimes 1}_{i-1 \text{ times}} \otimes H_\omega(L) \otimes \underbrace{1 \otimes \dots \otimes 1}_{n-i \text{ times}}.$$

- Pick $U : \mathbb{R} \rightarrow \mathbb{R}^+$ not identically vanishing, even, bounded.

We assume $U \in L^p(\mathbb{R})$ for some $p \in (1, +\infty]$ and $x^3 \cdot \int_x^{+\infty} U(t) dt \xrightarrow{x \rightarrow +\infty} 0$.

Recall $H_\omega^U(L, n) = H_\omega^0(L, n) + W_n$ where $W_n(x^1, \dots, x^n) := \sum_{i < j} U(x^i - x^j)$.

Thermodynamic limit at small density : $n/L \rightarrow \rho$ as $L \rightarrow +\infty$ where $\rho > 0$ small.

Note : by scaling $x \rightarrow \mu x$, $H_\omega^U(L, n)$ on $[0, L]^n$ becomes $\mu^2 H_{\omega_\mu}^U(\mu L, n)$ on $[0, \mu L]^n$ thus, $(\rho, \mu) \rightarrow (\rho/\mu, 1)$ (up to rescaling energy).

The non interacting system : the ground state energy per particle

$$\mathcal{E}^0(\rho) = \lim_{\substack{L \rightarrow +\infty \\ n/L \rightarrow \rho}} \frac{E_\omega^0(L, n)}{n} = E_\rho (1 + O(\sqrt{E_\rho})) = \pi^2 |\log \rho|^{-2} \left(1 + O(|\log \rho|^{-1}) \right).$$

The non interacting ground state

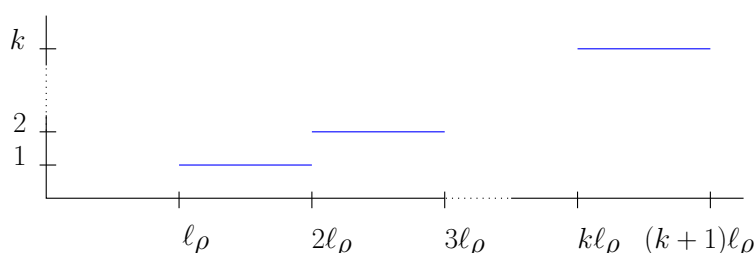
- Pick all the pieces $\Delta_k = [x_k(\omega), x_{k+1}(\omega)]$ of length larger than $\ell_\rho = \pi/\sqrt{E_\rho}$.
- For each piece, take all the states associated to levels below E_ρ .
- Form the Slater determinant to get the non interacting ground state.

The reduced one-particle density matrix for the non interacting ground state

$$\begin{aligned} \gamma_{\Psi_\omega^0(L, n)}^{(1)} &= \sum_{j \geq 1} \left[\sum_{j\ell_\rho \leq |\Delta_k| < (j+1)\ell_\rho} \left(\sum_{n=1}^j \gamma_{\varphi_{\Delta_k}^n}^{(1)} \right) \right] \\ &= \sum_{\ell_\rho \leq |\Delta_k| < 2\ell_\rho} \gamma_{\varphi_{\Delta_k}^1}^{(1)} + \sum_{2\ell_\rho \leq |\Delta_k| < 3\ell_\rho} \left(\gamma_{\varphi_{\Delta_k}^1}^{(1)} + \gamma_{\varphi_{\Delta_k}^2}^{(1)} \right) + R^{(1)} \end{aligned}$$

where

- for an interval I , we let φ_I^j be the j -th normalized eigenvector of $-\Delta_I^D$,
- the operator $R^{(1)}$ is trace class and $\|R^{(1)}\|_1 \leq C\rho^2 n$.



Theorem

Under our assumptions on U , ω -almost surely, the following limit exists and is independent of ω

$$\mathcal{E}^U(\rho) := \lim_{\substack{L \rightarrow +\infty \\ n/L \rightarrow \rho}} \frac{E_\omega^U(L, n)}{n}.$$

Ground state energy asymptotic expansion

Theorem

Under our assumptions on U , one has

$$\mathcal{E}^U(\rho) = \mathcal{E}^0(\rho) + \frac{\pi^2 \gamma_*}{|\log \rho|^3} \rho + o\left(\frac{\rho}{|\log \rho|^3}\right),$$

where $\gamma_* = 1 - \exp\left(-\frac{\gamma}{8\pi^2}\right)$.

Systems of two fermions : within the same piece :

Lemma

Assume that $U \in L^p(\mathbb{R})$ for some $p \in (1, +\infty]$ and that $\int_{\mathbb{R}} x^2 U(x) dx < +\infty$. Consider two fermions in $[0, \ell]$ interacting via the pair potential U , i.e., on $L^2([0, \ell]) \wedge L^2([0, \ell])$, consider the Hamiltonian

$$-\frac{d^2}{dx_1^2} - \frac{d^2}{dx_2^2} + U(x_1 - x_2). \tag{1}$$

Then, for large ℓ , $E^{2,U}(\ell)$, its ground state energy admits the following expansion

$$E^{2,U}(\ell) = \frac{5\pi^2}{\ell^2} + \frac{\gamma}{\ell^3} + o(\ell^{-3})$$

where $\gamma := \frac{5\pi^2}{2} \left\langle u \sqrt{U(u)}, \left(Id + \frac{1}{2} U^{1/2} (-\Delta_1)^{-1} U^{1/2} \right)^{-1} u \sqrt{U(u)} \right\rangle$.

Uniqueness of the ground state :

Theorem

Assume U is analytic. Then, for any L and n , $H_\omega^U(L, n)$ has a unique ground state ω -almost surely.

Interacting ground state : “optimal” approximation

Let ζ_l^1 be the ground state of $-\Delta|_{l^2}^D + U$ acting on $L_-^2(I^2)$. Define

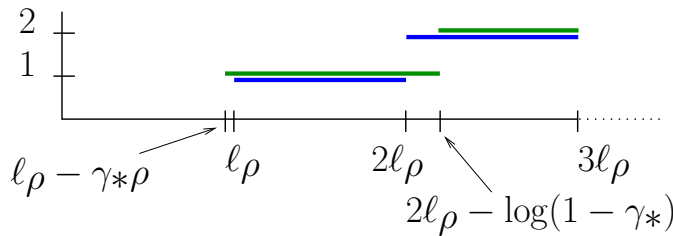
$$\gamma_{\Psi_{L,n}^{\text{opt}}}^{(1)} = \sum_{\ell\rho - \rho\gamma_* \leq |\Delta_k| \leq 2\ell\rho - \log(1-\gamma_*)} \gamma_{\varphi_{\Delta_k}^1}^{(1)} + \sum_{2\ell\rho - \log(1-\gamma_*) \leq |\Delta_k|} \gamma_{\zeta_{\Delta_k}^1}^{(1)},$$

Theorem

We assume U cpct support. There exists $\rho_0 > 0$ s.t. for $\rho \in (0, \rho_0)$, ω -a.s., one has

$$\limsup_{\substack{L \rightarrow +\infty \\ n/L \rightarrow \rho}} \frac{1}{n} \left\| \gamma_{\Psi_{\omega}^U(L,n)}^{(1)} - \gamma_{\Psi_{L,n}^{\text{opt}}}^{(1)} \right\|_1 \lesssim \frac{\rho}{|\log \rho|},$$

$$\limsup_{\substack{L \rightarrow +\infty \\ n/L \rightarrow \rho}} \frac{1}{n^2} \left\| \gamma_{\Psi_{\omega}^U(L,n)}^{(2)} - \frac{1}{2} (\text{Id} - Ex) \left[\gamma_{\Psi_{L,n}^{\text{opt}}}^{(1)} \otimes \gamma_{\Psi_{L,n}^{\text{opt}}}^{(1)} \right] \right\|_1 \lesssim \frac{\rho}{|\log \rho|}.$$



Quantification of the influence of interactions

Influence of interactions on the ground state is essentially described by

$$\gamma_{\Psi_{\omega}^0(L,n)}^{(1)} - \gamma_{\Psi_{L,n}^{\text{opt}}}^{(1)} = \sum_{2\ell\rho - \log(1-\gamma_*) \leq |\Delta_k|} \left(\gamma_{\varphi_{\Delta_k}^1}^{(1)} + \gamma_{\varphi_{\Delta_k}^2}^{(1)} - \gamma_{\zeta_{\Delta_k}^1}^{(1)} \right) - \sum_{\ell\rho - \rho\gamma_* \leq |\Delta_k| \leq \ell\rho} \gamma_{\varphi_{\Delta_k}^1}^{(1)} + \sum_{2\ell\rho \leq |\Delta_k| \leq 2\ell\rho - \log(1-\gamma_*)} \gamma_{\varphi_{\Delta_k}^2}^{(1)} + \tilde{R}^{(1)}$$

In particular,

$$\lim_{\substack{L \rightarrow +\infty \\ n/L \rightarrow \rho}} \frac{1}{n} \left\| \gamma_{\Psi_{\omega}^0(L,n)}^{(1)} - \gamma_{\Psi_{\omega}^U(L,n)}^{(1)} \right\|_1 = 2\gamma_*\rho + O\left(\frac{\rho}{|\log \rho|}\right),$$

and

$$\lim_{\substack{L \rightarrow +\infty \\ n/L \rightarrow \rho}} \frac{1}{n^2} \left\| \gamma_{\Psi_{\omega}^0(L,n)}^{(2)} - \gamma_{\Psi_{\omega}^U(L,n)}^{(2)} \right\|_1 = 2\gamma_*\rho + O\left(\frac{\rho}{|\log \rho|}\right).$$

To be compared with

$$\limsup_{\substack{L \rightarrow +\infty \\ n/L \rightarrow \rho}} \frac{1}{n} \left\| \gamma_{\Psi_{\omega}^U(L,n)}^{(1)} - \gamma_{\Psi_{L,n}^{\text{opt}}}^{(1)} \right\|_1 \lesssim \frac{\rho}{|\log \rho|}.$$

Some open questions

- ① For U compactly supported, we have a description of ground state.

When $x^3 \int_x^{+\infty} U(t) dt \xrightarrow{x \rightarrow +\infty} 0$ not too fast, changes induced by these “long” range interactions difficult to control. Get a good description of the ground state.

- ② For U compactly supported, we actually have a better expansion for $\mathcal{E}^U(\rho)$. And we have a more precise description of the ground state.

Does $\gamma_{\Psi_\omega^U(L,n)}^{(1)}$ converge as $L \rightarrow +\infty$?

- ③ What happens if $x^3 \int_x^{+\infty} U(t) dt \xrightarrow{x \rightarrow +\infty} +\infty$? One may expect

- ▶ if $\int_{\mathbb{R}} U(t) dt < +\infty$: interactions at a distance become more important than local interactions in the same piece.
- ▶ if $\int_{\mathbb{R}} U(t) dt = +\infty$, interactions become more important than non interacting energy term.

In our model, no tunneling for a single particle. How to take tunneling into account ?

The work of **Helffer and Sjöstrand** (and successors) on multiple wells !

In dimension 1, preliminary computations suggest same picture.

What happens in higher dimensions ?