Interacting electrons in a random background

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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

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

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

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

Thermodynamic limit

- Let $E^U_\omega(\Lambda,n)$ be the ground state energy of $H_\omega(\Lambda,n)$.
- Let $\Psi^U_\omega(\Lambda,n)$ be the associated eigenfunction.

Problem

Describe $E^U_\omega(\Lambda,n)$ and $\Psi^U_\omega(\Lambda,n)$ in the limit $|\Lambda|\to+\infty$ and $\dfrac{n}{|\Lambda|}\to\rho>0$.

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

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

- k-particle density matrix : $\gamma_\Psi^{(k)}(x,y) = \binom{n}{k} \int_{\Lambda^{n-1}} \Psi(x,\tilde{x})\Psi^*(y,\tilde{x})d\tilde{x}$.
- $\gamma_\Psi^{(k)}$ non negative trace class operator satisfying $\operatorname{tr}\gamma_\Psi^{(k)} = \binom{n}{k}$.

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

Define the counting fct per volume unit : $N_{H_\omega(\Lambda)}(E) = \dfrac{\#\{\text{e.v. of } H_\omega(\Lambda) \text{ in } (-\infty,E]\}}{|\Lambda|}$.

As $N_{H_\omega(\Lambda)}(E_n) = n/|\Lambda| \to \rho$, one has

$$\frac{E^0_\omega(\Lambda,n)}{n} = \frac{1}{n}\sum_{j=1}^n E_j = \frac{|\Lambda|}{n}\int_{-\infty}^{E_n} E\, dN_{H_\omega(\Lambda)}(E) \underset{\substack{|\Lambda|\to+\infty\\ n/|\Lambda|\to\rho}}{\longrightarrow} \frac{1}{\rho}\int_{-\infty}^{E_\rho} E\, dN(E)$$

where $N(E_\rho) = \rho$; E_ρ = Fermi energy and $N(E) := \lim_{|\Lambda|\to+\infty} N_{H_\omega(\Lambda)}(E)$ (IDS of H_ω).

Moreover, for non interacting ground state

$$\gamma^{(1)}_{\Psi^0_\omega(\Lambda,n)} = \sum_{k=0}^n |\psi_k\rangle\langle\psi_k| \underset{\substack{|\Lambda|\to+\infty\\ n/|\Lambda|\to\rho}}{\longrightarrow} \mathbf{1}_{(-\infty,E_\rho]}(H_\omega).$$

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

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

- Integrated density of states

$$N(E) := \lim_{L\to+\infty} \frac{\sharp\{\text{eigenvalues of } H_\omega(L) \text{ in } (-\infty,E]\}}{L}$$
$$= \frac{\exp(-\ell_E)}{1-\exp(-\ell_E)} 1_{E\geq 0} \text{ where } \ell_E := \frac{\pi}{\sqrt{E}}.$$

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

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

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

$$U\in L^p(\mathbb{R}) \text{ for some } p\in(1,+\infty] \quad \text{and} \quad x^3\cdot\int_x^{+\infty} U(t)dt \underset{x\to+\infty}{\longrightarrow} 0.$$

  Define

$$H^U_\omega(L,n) = H^0_\omega(L,n) + W_n, \quad \text{where} \quad W_n(x^1,\cdots,x^n) := \sum_{i<j} U(x^i-x^j).$$

The non interacting system : the ground state energy per particle

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

The non interacting ground state

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

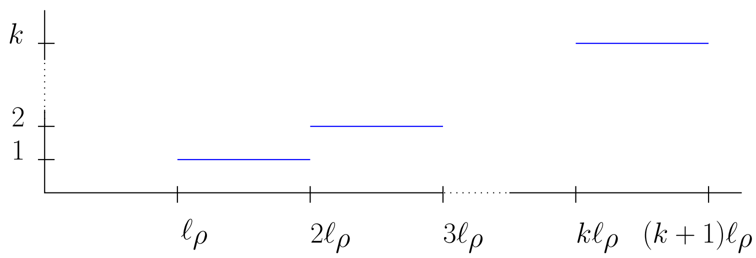
The reduced one-particle density matrix for the non interacting ground state

$$\gamma^{(1)}_{\Psi^0_\omega(L,n)} = \sum_{j\geq 1}\left[\sum_{j\ell_\rho\leq|\Delta_k|<(j+1)\ell_\rho}\left(\sum_{n=1}^{j}\gamma^{(1)}_{\varphi^n_{\Delta_k}}\right)\right]$$

$$= \sum_{\ell_\rho\leq|\Delta_k|<2\ell_\rho}\gamma^{(1)}_{\varphi^1_{\Delta_k}} + \sum_{2\ell_\rho\leq|\Delta_k|<3\ell_\rho}\left(\gamma^{(1)}_{\varphi^1_{\Delta_k}}+\gamma^{(1)}_{\varphi^2_{\Delta_k}}\right) + R^{(1)}$$

where

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



The 2 point correlation function

Theorem

Assume U cpct support. There exists $\rho_U > 0$ and $\mu > 0$ s.t. for $0 < \rho < \rho_U$ sufficiently small, one has

$$\sup_{\Lambda} \sup_{(x,x',y,y') \in \Lambda^4} \mathbb{E}(|\gamma^{(2)}_{\Psi^U_\omega(L,n)}(x,y;x',y')| e^{\mu(|x-y|+|x'-y'|)}) < +\infty.$$

Ground state energy per particle

Theorem (K.-Veniaminov)

Under our assumptions on U, $\omega-$almost surely, the following limit exists, is independent of ω and admits the asymptotic expansion

$$\mathcal{E}^U(\rho) := \lim_{\substack{L \to +\infty \\ n/L \to \rho}} \frac{E^U_\omega(L,n)}{n} = \mathcal{E}^0(\rho) + \frac{\pi^2 \gamma_*}{|\log \rho|^3} \rho + o\left(\frac{\rho}{|\log \rho|^3}\right),$$

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

Systems of two electrons within the same piece :

Lemma (K.-Veniaminov)

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 electrons in $[0,\ell]$ interacting via the pair potential U, i.e., on $L^2([0,\ell]) \wedge L^2([0,\ell])$, consider the Hamiltonian

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

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

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

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

Uniqueness of the ground state :

Theorem (K.-Veniaminov)

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

Interacting ground state : "optimal" approximation

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

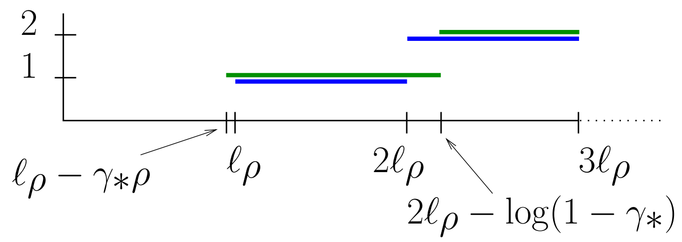
$$\gamma^{(1)}_{\Psi^{\text{opt}}_{L,n}} = \sum_{\ell_\rho - \rho\gamma_* \le |\Delta_k| \le 2\ell_\rho - \log(1-\gamma_*)} \gamma^{(1)}_{\varphi^1_{\Delta_k}} + \sum_{2\ell_\rho - \log(1-\gamma_*) \le |\Delta_k|} \gamma^{(1)}_{\zeta^1_{\Delta_k}},$$

Theorem (K.-Veniaminov)

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

$$\limsup_{\substack{L\to+\infty \\ n/L\to\rho}} \frac{1}{n} \left\| \gamma^{(1)}_{\Psi^U_\omega(L,n)} - \gamma^{(1)}_{\Psi^{opt}_{L,n}} \right\|_1 \lesssim \frac{\rho}{|\log \rho|},$$

$$\limsup_{\substack{L\to+\infty \\ n/L\to\rho}} \frac{1}{n^2} \left\| \gamma^{(2)}_{\Psi^U_\omega(L,n)} - \frac{1}{2}(Id - Ex)\left[\gamma^{(1)}_{\Psi^{opt}_{L,n}} \otimes \gamma^{(1)}_{\Psi^{opt}_{L,n}}\right] \right\|_1 \lesssim \frac{\rho}{|\log \rho|}.$$



Quantification of the influence of interactions

Influence of interactions on the ground state is essentially described by

$$\gamma^{(1)}_{\Psi^0_\omega(L,n)} - \gamma^{(1)}_{\Psi^{\text{opt}}_{L,n}} = \sum_{2\ell_\rho - \log(1-\gamma_*) \le |\Delta_k|} \left(\gamma^{(1)}_{\varphi^1_{\Delta_k}} + \gamma^{(1)}_{\varphi^2_{\Delta_k}} - \gamma^{(1)}_{\zeta^1_{\Delta_k}} \right)$$

$$- \sum_{\ell_\rho - \rho\gamma_* \le |\Delta_k| \le \ell_\rho} \gamma^{(1)}_{\varphi^1_{\Delta_k}} + \sum_{2\ell_\rho \le |\Delta_k| \le 2\ell_\rho - \log(1-\gamma_*)} \gamma^{(1)}_{\varphi^2_{\Delta_k}} + \widetilde{R}^{(1)}$$

In particular,

$$\lim_{\substack{L\to+\infty \\ n/L\to\rho}} \frac{1}{n} \left\| \gamma^{(1)}_{\Psi^0_\omega(L,n)} - \gamma^{(1)}_{\Psi^U_\omega(L,n)} \right\|_1 = 2\gamma_*\rho + O\left(\frac{\rho}{|\log \rho|}\right),$$

and

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

To be compared with

$$\limsup_{\substack{L\to+\infty \\ n/L\to\rho}} \frac{1}{n} \left\| \gamma^{(1)}_{\Psi^U_\omega(L,n)} - \gamma^{(1)}_{\Psi^{\text{opt}}_{L,n}} \right\|_1 \lesssim \frac{\rho}{|\log \rho|}.$$

A more realistic random model

The Poisson potential

- On $\mathbb{R}$, consider the Poisson point process $d\mu(\omega)$ of intensity 1

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

- Fix $v : \mathbb{R} \to \mathbb{R}^+$, $v \geq 0$, continuous compactly supported and define

$$H_\omega = -\Delta + \int_{\mathbb{R}} v(x-y)d\mu(y) = -\Delta + \sum_{k\in\mathbb{Z}} v(x - x_k(\omega)).$$

- Integrated density of states cannot be computed explicitly

Theorem

For E small, one has the asymptotic expansion

$$-\log N(E) = \ell_E - c_0 + \sum_{k\geq 1} c_k \ell_E^{-k} \quad \textit{where} \quad \ell_E = \frac{\pi}{\sqrt{E}}.$$

Ground state energy per particle

Theorem

For U repulsive and continuous of cpct support, $\omega-$almost surely, the following limit exists, is independent of ω and admits the asymptotic expansion

$$\mathscr{E}^U(\rho) := \lim_{\substack{L\to+\infty \\ n/L\to\rho}} \frac{E^U_\omega(L,n)}{n} = \mathscr{E}^0(\rho) + \frac{\pi^2\gamma_*}{|\log\rho|^3}\rho + o\left(\frac{\rho}{|\log\rho|^3}\right).$$

One also has description of ground states (not necessarily unique).

Some open questions

- Prove exponential decay of 2 point correlation for random Schrödinger model. (related work of Mastropietro (2014-16)).
- Study the influence of the range of the interaction U.
- What happens if ρ is increased ?
- What happens for random Schrödinger model in dimension $d \geq 2$?
- What happens when $T \neq 0$? (Mastropietro (2014-16)).