Existence of the thermodynamic limit for disordered Coulomb quantum systems

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joint work with X. Blanc (CEA, Paris), based on previous works with C. Hainzl (Tuebingen) & J.P. Solovej (Copenhagen)

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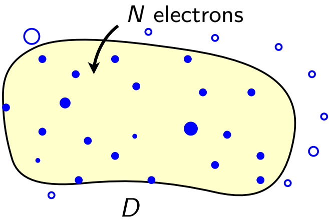
Key references for this talk

	short range	Coulomb
stability of matter $\mathcal{F}(D) \geq C\|D\|$	*Ruelle & Fisher (66)*	*Dyson & Lenard (67)* *Lieb & Thirring (75)*
$\exists$ thermo limit, deterministic $\mathcal{F}(D) \sim f\,\|D\|$	*Ruelle (63)* *Fisher (64)*	*Lebowitz & Lieb (72)* *Fefferman (85)* *Hainzl, M.L. & Solovej (09)*
$\exists$ thermo limit, stochastic $\mathcal{F}(\omega, D) \sim f\,\|D\|$	*Veniaminov (11)*	

Main difficulty with Coulomb: quantify screening

Conlon-Lieb-Yau (88), Graf-Schenker (95): lower bounds on classical Coulomb systems when $\mathbb{R}^3$ split using a tiling

Grand canonical energy



Nuclei: $\mathcal{K} = \{(R,z)\} \subset \mathbb{R}^3 \times (0,\infty)$

$$H^N_{\mathcal{K}}(D) := -\sum_{i=1}^N \Delta_{x_i} + V_{\mathcal{K},D}(x_1,\dots,x_N)$$

where $-\Delta=$ Dirichlet Laplacian

$$V_{\mathcal{K},D}(x) = \sum_{i=1}^N \sum_{(R,z)\in\mathcal{K}\cap D} \frac{-z}{|R-x_i|} + \frac{1}{2}\sum_{1\le i\neq j\le N} \frac{1}{|x_i-x_j|} + \frac{1}{2}\sum_{R\neq R'\in\mathcal{K}\cap D} \frac{zz'}{|R-R'|}$$

- Ground state energy for N electrons:

$$\mathcal{F}^N_{\mathcal{K}}(D) = \inf\left\{\left\langle\Psi, H^N_{\mathcal{K}}(D)\Psi\right\rangle,\ \Psi \text{ antisymm.},\ \|\Psi\|_{L^2(D^N)} = 1\right\} > -\infty$$

- Grand canonical energy:

$$\mathcal{F}_{\mathcal{K}}(D) := \inf_{N\geq 0} \mathcal{F}^N_{\mathcal{K}}(D) \qquad \left[= \inf \operatorname{Spec}_{\bigoplus_{N\geq 0}\bigwedge_1^N L^2(D)} \bigoplus_{N\geq 0} H^N_{\mathcal{K}}(D)\right]$$

Stability of matter

Theorem (Stability of matter)

There exists a constant C, depending on $\max_{(R,z)\in\mathcal{K}} z$ but not on $\mathcal{K}$, such that

$$\mathcal{F}_{\mathcal{K}}(D) \geq -C|D|$$

for every bounded open set D.

Modern proof based on:

- Lieb-Yau (88) classical electrostatic estimate on many-body Coulomb $\rightsquigarrow$ nearest neighbor one-body
- Lieb-Thirring (75) and Sobolev inequalities

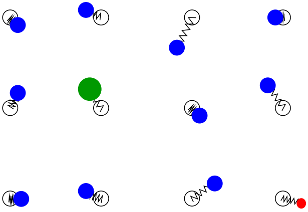
[Sol-06] Solovej, *Stability of Matter*, Encyclopedia of Mathematical Physics, Elsevier (2006).

[LieSei-10] Lieb & Seiringer, *The stability of matter in quantum mechanics*, Cambridge Univ. Press, 2010.

[HaiLewSol-09] Hainzl, M. L. & Solovej, *Advances in Math.*, **221** (2009), pp. 454–487 & 488–546.

Disordered crystal

Typical situation:



$$\mathcal{K}(\omega) = \Big\{ \big(k + \delta_k(\omega), z_k(\omega)\big),\ k \in \mathbb{Z}^3 \Big\}$$

with δ_k and z_k i.i.d. random variables

Example: $\delta_k \sim$ gaussian and $z_k \sim$ Bernouilli

$\Rightarrow$
- random many-body Schrödinger operator $H^N(\omega, D)$
- random grand-canonical energy $\mathcal{F}(\omega, D)$

Ergodicity of nuclei

- **General situation:**
  - translation group $\mathbb{Z}^3 \curvearrowright$ probability space $(\Omega, \mathscr{T}, \mathbb{P})$
  - ergodicity: $\tau_k A = A$, $\forall k \in \mathbb{Z}^3 \Rightarrow \mathbb{P}(A) = 0$ or 1
  - $\mathcal{K}(\omega)$= countable subset of $\mathbb{R}^3 \times [z_{\min}, z_{\max}]$ with

$$\mathcal{K}(\tau_k\omega) = \mathcal{K}(\omega) + k, \quad \text{for all } k \in \mathbb{Z}^3 \text{ and a.s. in } \omega$$

- **Example:** $\Omega = (\Omega_0)^{\mathbb{Z}^3}$, $\delta_k(\omega) = \delta(\omega_k)$, $z_k(\omega) = z(\omega_k)$ and $\tau_k(\omega_\ell) = (\omega_{k+\ell})$

- **Local distribution of nuclei:** with $Q := [0,1)^3$, define

$$X_0(\omega) := \#\big(\mathcal{K}(\omega) \cap Q\big) = \sum_{(R,z)\in\mathcal{K}(\omega)\cap Q} 1$$

$$X_1(\omega) := \sum_{(R,z)\in\mathcal{K}(\omega)\cap Q} \frac{1}{\min_{(R',z')\in\mathcal{K}(\omega)\setminus(R,z)} |R-R'|}$$

Existence of the thermodynamic limit

Theorem (Existence of thermo limit [BlaLew-12])

Assume that

$$\mathbb{E}\,|X_1|^p < \infty \quad \text{for some } p \geq 2.$$

There exists a cst f such that, for all 'regular' sequences (D_n) with $|D_n| \to \infty$,

$$\lim_{n\to\infty} \mathbb{E}\left|\frac{\mathcal{F}(\cdot, D_n)}{|D_n|} - f\right|^q = 0$$

for $q = 1$ if $p = 2$ and all $1 \leq q < p/2$ if $p > 2$.

Rmk.

- Almost sure CV expected as well if (D_n) does not escape to infinity
- Neutrality in average:

$$\lim_{n\to\infty} \mathbb{E}\left|\frac{N(\cdot, D_n)}{|D_n|} - \mathbb{E}\left(\sum_{(R,z)\in\mathcal{K}\cap Q} z\right)\right|^2 = 0$$

- Same result at finite temperature

[BlaLew-12] X. Blanc & M.L. arXiv:1201.4670

Remarks on the assumptions on nuclei

Simple i.i.d. case, ν=law of displacement, charges all $=z$

- (Lieb-Yau '88) $\mathbb{E}\,\dfrac{\mathcal{F}(\cdot,D)}{|D|} \geq -C + \dfrac{z^2}{8}\mathbb{E}\,X_1$, so X_1 must be in $L^1(\Omega)$
- If ν decays fast, then $\mathbb{E}\,|X_0|^p < \infty\ \forall 1 \leq p < \infty$ and $\mathbb{E}\,|X_1|^p < \infty\ \forall 1 \leq p < 3$
- If the support of ν is not compact, then $X_0 \notin L^\infty(\Omega)$
- If $\nu \geq \varepsilon > 0$ on $B(x,\varepsilon) \cup B(x+k,\varepsilon)$ for some $0 \neq k \in \mathbb{Z}^3$, then $X_1 \notin L^3(\Omega)$

Corollary (Harmonic oscillators)

For $\nu(x) = (2\pi\sigma)^{-3/2}\exp(-|x|^2/(2\sigma))$, *then*

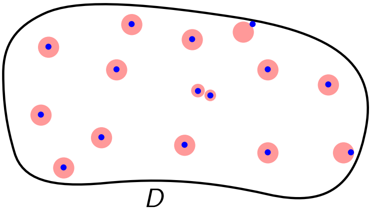
- $\mathbb{E}\,|X_0|^p < \infty$ *for all* $1 \leq p < \infty$ *and* $\mathbb{E}\,|X_1|^p < \infty$ *for all* $1 \leq p < 3$;
- X_0 *is not bounded and* $\mathbb{E}\,|X_1|^3 = \infty$;
- $\mathbb{E}\,|\mathcal{F}(\cdot,D)|^3 = \infty$ *for all fixed* D;
- *the thermo limit exists in* $L^q(\Omega)$ *for all* $1 \leq q < 3/2$.

Strategy of proof

In [HaiLewSol-09], abstract method based on Graf-Schenker inequality

1. Stability of matter: uniform lower bound on $\mathcal{F}$;

2. Prove upper bounds $\mathbb{E}\,|\mathcal{F}(\cdot, D)|^q \leq C|D|^q$, for $q \leq p/2$



Screen the nuclei with radial electrons
Radius $\sim \delta_R =$ distance to the nearest nucleus
Cost in kinetic energy: $\sum_{(R,z)\in\mathcal{K}(\omega)\cap D} \delta_R^{-2} \in L^{p/2}(\Omega)$ when $\mathbb{E}\,|X_1|^p < \infty$

Strategy of proof

3. Prove that periodic $D \mapsto \mathbb{E}\,\mathcal{F}(\cdot, D)$ satisfies abstract (deterministic) assumptions of [HaiLewSol-09]. Requires much more precise upper bounds

   $\Rightarrow$ thermo limit exists for $\mathbb{E}\,\mathcal{F}(\cdot, D)$

4. Graf-Schenker inequality together with ergodic thm:

$$\liminf_{n\to\infty} \frac{\mathcal{F}(\omega, D_n)}{|D_n|} \geq \lim_{n\to\infty} \frac{\mathbb{E}\,\mathcal{F}(\cdot, D_n)}{|D_n|} := f, \quad \text{almost surely}$$

5. Simple lemma: if (Y_n) bd in $L^1(\Omega)$ is such that $\mathbb{E}\,Y_n \to e$, $Y_n \geq C$ and $\liminf Y_n \geq e$, then $\mathbb{E}\,|Y_n - e| \to 0$

6. The result follows in $L^q(\Omega)$ by interpolation