Symmetry breaking in quantum 1D jellium

Sabine Jansen
Ruhr-Universität Bochum

joint work with Paul Jung (University of Alabama at Birmingham)

Warwick University, March 2014

Context

Setting: quantum statistical mechanics. Charged fermions move on a line, homogeneous neutralizing background.

Wigner '34: in order to understand the effect of electronic interactions in solids, crude approximation: periodic charge distribution (atoms) $\approx$ homogeneous positive charge distribution. Keep electronic interactions. Jellium, one-component plasma.

Possible scenario: at low density, electrons minimize repulsive Coulomb energy by forming a periodic lattice. Wigner crystal.

Dimension one: Wigner crystallization proven for the classical jellium at all densities (Kunz '74, Brascamp-Lieb '75, Aizenman-Martin '80), for the quantum and classical jellium at low densities Brascamp-Lieb '75.

This talk: Wigner crystallization for quantum 1D jellium at all densities. Proof combines arguments of cited works, notably Kunz's transfer matrix approach.

Outline

1. Setting
2. Main result
   - existence of the thermodynamic limit of all correlation functions
   - translational symmetry breaking at all $\beta, \rho > 0$
3. Proof ideas
   - path integrals
   - transfer matrix, Perron-Frobenius

Electrostatic energy and Hamiltonian

- N particles of charge -1, positions $x_1, \dots, x_N \in [a, b] \subset \mathbb{R}$
- one-dimensional Coulomb potential $V(x-y) = -|x-y|$
- neutralizing background of homogeneous charge density $\rho = N/(b-a)$
- total potential energy

$$U(x_1, \dots, x_N) := -\sum_{1 \leq j \leq k \leq N} |x_j - x_k| + \rho \sum_{j=1}^{N} \int_a^b |x_j - x| \mathrm{d}x - \frac{\rho^2}{2} \int_a^b \int_a^b |x - x'| \mathrm{d}x \mathrm{d}x'.$$

- $\mathcal{H}_N$ Hilbert space for N fermions $=$ antisymmetric functions in $L^2([a, b]^N)$.
- Hamilton operator

$$H_N := -\frac{1}{2} \sum_{j=1}^{N} \frac{\partial^2}{\partial x_j^2} + U(x_1, \dots, x_N).$$

Dirichlet boundary conditions at $x = a$ and $x = b$.

Free energy and reduced density matrices

- $\beta > 0$ inverse temperature
- Thermodynamic limit

$$N \to \infty, \; a \to -\infty, \; b \to +\infty, \; \frac{N}{b-a} \to \rho.$$

- Canonical partition function

$$Z_N(\beta) := \mathrm{Tr}\, \exp(-\beta H_N) = \frac{1}{N!} \int_{[a,b]^N} \exp(-\beta H_N)(\mathbf{x}, \mathbf{x}) \mathrm{d}x_1 \dots \mathrm{d}x_N,$$

  $\exp(-\beta H_N)(\mathbf{x}; \mathbf{y})$ integral kernel of $\exp(-\beta H_N)$.

- Free energy

$$f(\beta, \rho) = -\lim \frac{1}{\beta N} \log Z_N(\beta).$$

- n-particle reduced density matrices

$$\rho_n^N(x_1, \dots, x_n; y_1, \dots, y_n) \propto \int_{[a,b]^{N-n}} \exp(-\beta H_N)(\mathbf{x}, \mathbf{x}'; \mathbf{y}, \mathbf{x}') \mathrm{d}\mathbf{x}'$$

  proportionality constant fixed by

$$\int_{[a,b]^n} \rho_n^N(\mathbf{x}; \mathbf{x}) \mathrm{d}x_1 \cdots \mathrm{d}x_n = N(N-1) \cdots (N-n+1)$$

Results

Theorem (Free energy)

$$f(\beta,\rho) = \frac{1}{12\rho} + \left(\sqrt{\frac{\rho}{2}} + \frac{1}{\beta}\log(1 - e^{-\beta\sqrt{2\rho}})\right) - \frac{1}{\beta}\log z_0(\beta,\rho).$$

$z_0(\beta,\rho)$ principal eigenvalue of a transfer operator.

Free energy of independent harmonic oscillators + a correction term.

Theorem (Symmetry breaking)

(i) *In the thermodynamic limit along $a, b \in \rho^{-1}\mathbb{Z}$, all reduced density matrices have uniquely defined limits*

$$\rho_n(x_1,\dots,x_n;y_1,\dots,y_n) = \lim \rho_n^N(x_1,\dots,x_n;y_1,\dots,y_n).$$

The convergence is uniform on compact subsets of $\mathbb{R}^n \times \mathbb{R}^n$, and ρ_n^N and ρ_n are continuous functions of $\mathbf{x}$ and $\mathbf{y}$.

(ii) *The limit is periodic with respect to shifts by $\lambda = \rho^{-1}$,*

$$\rho_n(x_1 - \lambda,\dots;\dots,y_n - \lambda) = \rho_n(x_1,\dots;\dots,y_n)$$

for all $n \in \mathbb{N}$ and $\mathbf{x},\mathbf{y} \in \mathbb{R}^n$. For every $\theta \notin \lambda\mathbb{Z}$ there is some $n \in \mathbb{N}$ and some $\mathbf{x} \in \mathbb{R}^n$ such that $\rho_n(\mathbf{x}-\theta;\mathbf{x}-\theta) \neq \rho_n(\mathbf{x};\mathbf{x})$: λ is the smallest period.

Periodicity of the one-particle density

Limit state on fermionic observable algebra has smallest period $\lambda = \rho^{-1}$.

Question: periodicity visible at the level of the one-particle density?

Brascamp, Lieb '75: one-particle density is

$$\rho_1(x;x) = \sum_{k=-\infty}^{\infty} F(x-k\lambda)\exp\Big(-\frac{(x-k\lambda)^2}{2\sigma^2}\Big)$$

F even, log-concave function, $2\sigma^2 = [\sqrt{2\rho}\tanh(\beta\sqrt{\rho/2})]^{-1}$. At low density ($\lambda = \rho^{-1} \gg \sigma$), one-particle density has smallest period $\lambda = \rho^{-1}$.

At high density, we do not know whether this is true.

Note A state can have a non-trivial period but constant one-particle density. Example

$$\Psi_N = \cdots \wedge \mathbf{1}_{[-1,0)} \wedge \mathbf{1}_{[0,1)} \wedge \cdots \wedge \mathbf{1}_{[n,n+1)} \wedge \cdots$$

One-particle density $\sum_n \mathbf{1}_{[n,n+1)}(x) \equiv 1$, periodicity visible only at the level of two-point correlation functions.

Energy as a sum of squares

Observation: when particles are labelled from left to right

$$a \leq x_1 \leq \cdots \leq x_N \leq b,$$

energy is a sum of squares

$$U(x_1, \ldots, x_N) = \rho \sum_{j=1}^{N} (x_j - m_j)^2 + \frac{N}{12\rho}, \quad m_j = a + (j - \frac{1}{2})\lambda.$$

BAXTER '63. Elementary computation:

$$- \sum_{j<k} (x_k - x_j) + \rho \sum_j (x_j - \frac{a+b}{2})^2$$
$$= \sum_k (k-1)x_k - \sum_j (N - j + 1)x_j + \rho \sum_j (x_j - \frac{a+b}{2})^2,$$

then complete the squares.

Remark: Boltzmann weight: a Gaussian times a characteristic function (of a convex set). Starting point for BRASCAMP, LIEB '75.

Transfer matrix for the classical jellium

Partition function for the classical system:

$$Z_N(\beta) \propto \int_a^b \mathrm{d}x_1 \cdots \int_a^b \mathrm{d}x_N \exp\Big(-\beta\rho \sum_{j=1}^{N} (x_j - m_j)^2\Big) \mathbf{1}(x_1 \leq \cdots \leq x_N).$$

Three easy steps:

1. change variables $y_j = x_j - m_j$
2. define Gaussian measure $\mu(\mathrm{d}y) = \exp(-\beta\rho y^2)\mathrm{d}y$
3. write indicator that particles are ordered as product of pair terms

$$\boxed{\mathbf{1}(x_1 \leq \cdots \leq x_N) = \prod_{j=2}^{N} \mathbf{1}(y_{j-1} \leq y_j + \lambda) = \prod_{j=2}^{N} K(y_{j-1}, y_j)}$$

Remember $m_j - m_{j-1} = \lambda = \rho^{-1}$.

Partition function becomes

$$Z_N(\beta) \propto \int_{\mathbb{R}^N} \mu(\mathrm{d}y_1) \cdots \mu(\mathrm{d}y_N) F(y_1) K(y_1, y_2) \cdots K(y_{N-1}, y_N) G(y_N).$$

Functions $F(y_1) = \mathbf{1}(y_1 + m_1 \geq a)$ and $G(y_N) = \mathbf{1}(y_N + m_N \leq b)$ encode boundary conditions. Representation used in Kunz's proof.

Path integrals I

Work in L^2(Weyl chamber) instead of antisymmetric wave functions.

$$W_N(a,b) = \{\mathbf{x} \mid a \leq x_1 \leq \cdots \leq x_N \leq b\},$$

Fermionic Hilbert space is isomorphic to $L^2(W_N(a,b))$. Hamiltonian becomes

$$\boxed{H_N = \sum_{1\leq j\leq N} \Big(-\frac{1}{2}\frac{\partial^2}{\partial x_j^2} + \rho(x_j - m_j)^2\Big) + \frac{N}{12\rho}.}$$

Fermi statistics $\Rightarrow$ Dirichlet boundary conditions at $x_j = x_{j+1}$.

Apply Feynman-Kac formula in Weyl chamber. Path space

$$E = \{\gamma : [0,\beta] \to \mathbb{R} \mid \gamma \text{ continuous}\}$$

μ_{xy} = Brownian bridge measure on E (not normalized). Non-colliding paths

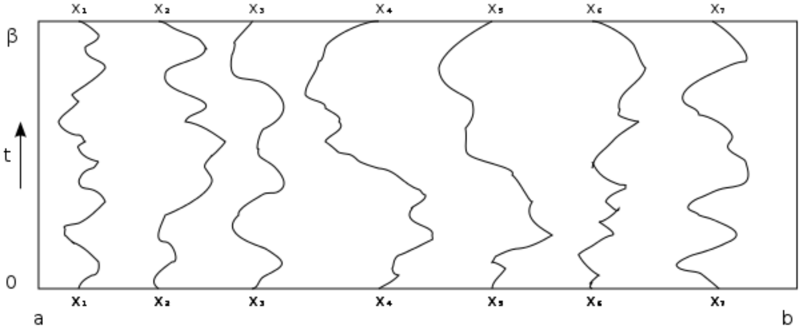
$$W_N^\beta(a,b) := \{(\gamma_1,\ldots,\gamma_N) \in E^N \mid \forall t \in [0,\beta]: \ a < \gamma_1(t) < \cdots < \gamma_N(t) < b\}.$$

Feynman-Kac formula:

$$\boxed{e^{-\beta H_N}(\mathbf{x};\mathbf{y}) \propto \mu_{x_1 y_1} \otimes \cdots \otimes \mu_{x_N y_N}\Big(e^{-\rho\sum_{j=1}^N \int_0^\beta (\gamma_j(t) - m_j)^2 \mathrm{d}t}\mathbf{1}_{W_N^\beta(a,b)}(\gamma)\Big)}$$

Path integrals II

$$Z_N(\beta) \propto \int_{W_N(a,b)} \mu_{x_1 x_1} \otimes \cdots \otimes \mu_{x_N x_N} \left(e^{-\rho \sum_{j=1}^{N} \int_0^{\beta} (\gamma_j(t) - m_j)^2 \mathrm{d}t} \mathbf{1}_{W_N^{\beta}(a,b)}(\gamma) \right) \mathrm{d}x_1 \cdots \mathrm{d}x_N .$$



Probability measure on non-colliding paths $W_N^{\beta}(a,b) \subset E^N$. Gaussian measure conditioned on non-collision. Particle positions recovered as path starting points $x_j = \gamma_j(0)$.

Transfer matrix for the quantum jellium

Step 1: change variables $\eta_j(t) = \gamma_j(t) - m_j$.

Step 2: Define Gaussian measure ν on 1-particle path space

$$\int_E \nu(\mathrm{d}\eta) f(\eta) = \frac{1}{c(\beta,\rho)} \int_{\mathbb{R}} \mathrm{d}x \int_E \mu_{xx}(\mathrm{d}\eta) \exp\Big(-\rho \int_0^\beta \eta(t)^2 \mathrm{d}t\Big) f(\gamma).$$

Step 3: Transfer operator in $L^2(E,\nu)$ encoding non-collision:

$$(\mathbb{K}f)(\eta) = \int_E K(\eta,\xi) f(\xi) \nu(\mathrm{d}\xi), \quad K(\eta_1,\eta_2) = \mathbf{1}\Big(\forall t:\ \eta_1(t) < \eta_2(t) + \lambda\Big).$$

Partition function

$$Z_N(\beta) \propto \langle F, \mathbb{K}^{N-1} G \rangle,$$

suitable $F, G \in L^2(E,\nu)$. Operator $\mathbb{K}$ is compact (Hilbert-Schmidt), irreducible $\Rightarrow ||\mathbb{K}|| =$ largest eigenvalue $z_0(\beta,\rho) > 0$ (Krein-Rutman / Perron-Frobenius).

Asymptotics of the partition function $\leftrightarrow$ principal eigenvalue $z_0(\beta,\rho)$ of $\mathbb{K}$.
Infinite volume measure on $E^{\mathbb{Z}}$: Shift-invariant, ergodic.

Theorems on free energy, existence and uniqueness of the limits of correlation functions follow.

Symmetry breaking I

- It is enough to look at "diagonal" correlation functions $\rho(\mathbf{x};\mathbf{x})$ / expectations of multiplication operators. Instead of dealing with full quantum state, look at probability measure $\mathbb{P}$ on point configurations

$$\omega = \{x_j \mid j \in \mathbb{Z}\}.$$

  Shifted configuration is

$$\tau_\theta \omega = \{x_j + \theta \mid j \in \mathbb{Z}\}.$$

- Correlation functions are factorial moment densities of $\mathbb{P}$

$$\int_{I\times\cdots\times I} \rho_n(\mathbf{x};\mathbf{x}) \mathrm{d}x_1 \cdots \mathrm{d}x_n = \mathbb{E}\big[N_I(N_I-1)\cdots(N_I-n+1)\big],$$

  $N_I = \#\omega \cap I = \#\{j \mid x_j \in I\}$ number of particles in interval I.
  Correlation functions determine measure $\mathbb{P}$ uniquely (moment problem).
- If measure $\mathbb{P}$ and shifted measure $\mathbb{P}\circ\tau_\theta$ are mutually singular, then there must be some correlation function ρ_n and some $x_1,\dots,x_n$ such that $\rho_n(x_1-\theta,\dots;\dots,x_n-\theta) \neq \rho_n(x_1,\dots;\dots,x_n)$.

We prove $\mathbb{P}\circ\tau_\theta \perp \mathbb{P}$ **whenever** $\theta \notin \lambda\mathbb{Z}$.

Symmetry breaking II

Label particles in infinite point configuration ω as

$$\cdots < x_{-1}(\omega) < x_0(\omega) \leq 0 \leq x_1(\omega) < \cdots$$

$\mathbb{P}$ limit along $a, b \in \lambda\mathbb{Z}$. Preferred positions: half-integer multiples of λ.

Lemma: ergodicity of measure for infinitely many paths $\Rightarrow$

$$\lim_{n\to\infty} \exp\left(\mathrm{i}\frac{2\pi}{\lambda}\frac{1}{n}\sum_{j=1}^{n}\Big(x_k(\omega) - (k - \frac{1}{2})\lambda\Big)\right) = 1 \quad \mathbb{P}\text{-almost surely.}$$

W.r.t. shifted measure $\mathbb{P}\circ\tau_\theta$, almost sure limit is instead $\exp(\mathrm{i}2\pi\theta/\lambda)$.
Measure and shifted measure are mutually singular when $\theta \notin \lambda\mathbb{Z}$.

Related to arguments in Aizenman, Martin '80, Aizenman, Goldstein, Lebowitz '01.

Conclusion

Symmetry is not limited to low temperature or low density.

Proofs combine standard tools from statistical mechanics: path integrals & transfer matrices.

Ref,:
S. Jansen and P. Jung,
Wigner crystallization for the quantum 1D jellium at all densities.
arXiv: 1306.6906 [math-ph]