LONG RANGE ORDER IN ATOMISTIC MODELS FOR SOLIDS (LECTURE 1)

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Key problem in solid state physics: prove that typically systems of interacting particles at low temperatures form crystalline solids (crystallization problem).

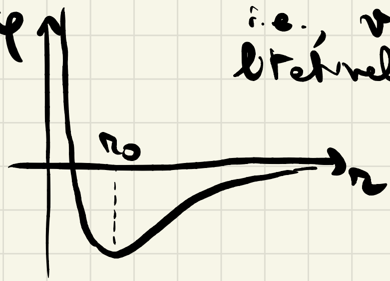
Prototypical problem, in the classical setting:

Consider a potential energy $V(\underline{Q}^{(N)})$

$\underline{Q}^{(N)} = (\underline{q}_1, \dots, \underline{q}_N) \in \mathbb{R}^{dN}$ and

$$V(\underline{q}) = \sum_{1 \le i < j \le N} v(\underline{q}_i - \underline{q}_j)$$

electrostatic potential, radial, i.e., $v(\underline{q}) = \varphi(|\underline{q}|)$, with φ qualitatively of the form:



NOTE: The energy function $V(\underline{Q}^{(N)})$ is invariant under two global continuous symmetries:

- TRANSLATIONS: $\underline{Q}^{(N)} \to \underline{Q}^{(N)} + \underline{\tau} \equiv (\underline{q}_1 + \underline{\tau}, \dots, \underline{q}_N + \underline{\tau})$ where $\underline{\tau}$ is a generic element of $\mathbb{R}^d$
- ROTATIONS: $\underline{Q}^{(N)} \to R\underline{Q}^{(N)} \equiv (R\underline{q}_1, \dots, R\underline{q}_N)$ where R is a generic element of $O(d)$

In order to define the model in a finite box, consider e.g. a torus Λ_L of sides $L\underline{a}_1, \dots, L\underline{a}_d$ and let $V_{\Lambda_L}(\underline{Q}^{(N)}) = \sum_{1 \le i < j \le N} v_{\Lambda_L}(\underline{q}_i - \underline{q}_j)$, where

$$v_{\Lambda_L}(\underline{q}) = \sum_{n \in \mathbb{Z}^d} v(\underline{q} + n_1 L_1 \underline{a}_1 + \dots + n_d L \underline{a}_d)$$

CRYSTALLIZATION PROBLEM: Prove that, for an appropriate choice of v, $\{\underline{a}_1, \dots, \underline{a}_d\}$, $n \in \mathbb{N}$

1) For any $L \in \mathbb{N}$, if $N = nL^d$, the minimum in $\min_{\underline{Q}^{(N)} \in \Lambda_L^N} V_{\Lambda_L}(\underline{Q}^{(N)})$ is realized by a periodic configuration obtained by translating a basic configuration $(\underline{q}_1^0, \dots, \underline{q}_n^0)$ on the elementary cell Λ_1 (i.e., $\underline{q}_j^0 \in \Lambda_1 \ \forall j = 1, \dots, n$) by integer multiples of $\underline{a}_1, \dots, \underline{a}_d$.

2) There exists $\beta_0 > 0$ s.t., for any $\beta > \beta_0$ $\exists\ \underline{a}_1(\beta), \dots, \underline{a}_d(\beta)$, continuous in β, such that $\underline{a}_i(\beta) \xrightarrow[\beta \to +\infty]{} \underline{a}_i$ and, letting Λ_L be the torus of sides $L\underline{a}_1(\beta), \dots, L\underline{a}_d(\beta)$ and $\mathcal{N}(\underline{q}; \underline{Q}^{(N)})$ the number operator $\mathcal{N}(\underline{q}; \underline{Q}^{(N)}) = \sum_{i=1}^{N} \delta(\underline{q} - \underline{q}_i)$, the

function $\rho(\underline{q}) := \lim_{\epsilon \to 0^+} \lim_{L \to \infty} \langle \mathcal{N}(\underline{q}; \cdot) \rangle_{\beta, \Lambda_L, \epsilon}$ (*)

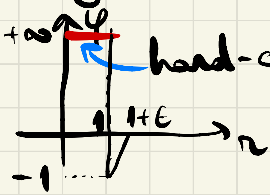
is non-constant and periodic under translations by integer multiples of $\underline{a}_1(\beta), \dots, \underline{a}_d(\beta)$.

[In (*), $\langle A \rangle_{\beta, \Lambda_L, \epsilon}$ indicates the average of the observable $A(\underline{Q}^{(N)})$ with respect to the Gibbs measure $\propto d\underline{Q}^{(N)} e^{-\beta V_{\Lambda_L}(\underline{Q}^{(N)}) - \beta \epsilon W_{\Lambda_L}(\underline{Q}^{(N)})}$ where $d\underline{Q}^{(N)}$ is the Lebesgue measure on Λ_L^N and $W_{\Lambda_L}(\underline{Q}^{(N)})$ is a smooth "symmetry breaking potential" with nL^d degenerate minima located at n appropriate positions in the elementary cell Λ_1 (which are continuous deformations of the ground state positions $\underline{q}_1^0, \dots, \underline{q}_n^0$, tending to these positions as $\beta \to \infty$) and to the translations thereof by integer multiples of $\underline{a}_1(\beta), \dots, \underline{a}_d(\beta)$.]

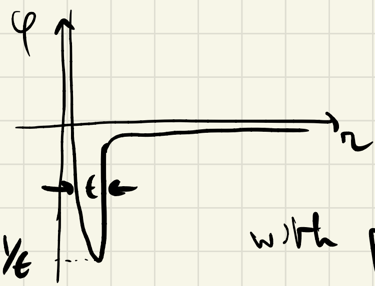
There are surprisingly few rigorously known results about this fundamental problem. I limit myself to mention just a couple:

• About problem (1) [crystalline GROUND STATES]:

- C. Radin (1981) proved that the ground states of a 2D particle system with pair interaction potential consist of triangular lattices of bond length 1.



- F. Theil (2006) extended Radin's result to Lennard-Jones-like potentials of the form:



where ϵ is sufficiently small, $\varphi(r) \underset{r\to 0^+}{\sim} C r^{-p}$, $\varphi(r) \underset{r\to+\infty}{\sim} -C' r^{-p'}$ with p, p' sufficiently large (still in 2D)

- Flatley - Theil (2015) proved that the ground states of a 3D system of particles interacting via a potential similar to the one considered by Theil in 2006 plus an appropriate 3-body potential form an FCC lattice.

• About problem (2) [crystalline states at LOW TEMPERATURES].

- Mermin (1968) proved that in 2D the system cannot exhibit long range positional order of a specific type (i.e., $\rho(q)$ cannot be non-trivially periodic) using Bogolubov's inequality

- Fröhlich - Pfister (1981, 1986) strengthened Mermin's result by showing that, for C^2 potentials, all Gibbs states are translationally-invariant. The result was further extended by Richthammer (2007, 2016) who proved the same for the hard-disk model, among others.

NOTE: These rigorous results do not exclude the possibility that 2D particle systems in the continuum exhibit long-range orientational order. The exactly solvable harmonic model actually predicts existence of orientational order (and of positional & orientational order in $d \geq 3$),

but it does not account for effects due to the presence of dislocations, which are lattice defects interacting via an effective Coulomb-like interactions. They are the main source of difficulty (and of interesting phenomena) in any proof of existence of positional/orientational order in 3D/2D (in more or less realistic models of crystallization).
Dislocations behave a bit like the vortices of the XY model, with the important difference that the "charges" (i.e., the analogue of the winding number in the XY model) are vectorial here and correspond to the Burger's vector (I will come back to this)
In this perspective, the crystallization problem at positive temperatures can be translated into a problem of interacting dislocations (i.e., vortices with "vectorial charges"):

- at high T, uniqueness of Gibbs measure and exponential decay of correlations should follow from the screening phenomenon, analogous to the one in the lattice Coulomb gas (proved by Brydges - Federbush 1980, Yang 1987)
- at low T, order emerges due to the formation of dipoles, in analogy with the analysis of the XY model and the lattice Coulomb gas (Fröhlich - Spencer 1981, 1982). The analysis suggests:
  - Existence of positional & orientational order in $d=3$
  - polynomial decay of positional correlations in $d=2$ and, presumably, existence of orientational order (unclear, due to the formation of "grains", to be discussed).

PLAN of these lectures:

- Mermin's proof of absence of positional order in 2D
- Definition of the harmonic model and picture emerging from its solution
- Dislocations and the Koster-Thouless-Halperin-Nelson-Young model for a gas of interacting dislocations
- Grains, grain boundaries and the Read-Shockley law (to orient or not to orient in 2D?)
- The Aizenman-Ortiz model: definition and "phenomenology": dislocations and grains; main results (Giuliani-Theil 2021).
- Proof of main results.

MERMIN'S proof of absence of positional order in 2D. Let me consider for simplicity the case of a simple Bravais lattice with basis vectors $\underline{a}_1, \underline{a}_2$ (e.g., triangular lattice of lattice spacing δ: $\underline{a}_1 = \delta\begin{pmatrix}1\\0\end{pmatrix}$, $\underline{a}_2 = \delta\begin{pmatrix}1/2\\ \sqrt{3}/2\end{pmatrix}$)

Recall: $\Lambda_L = \{ \underline{q} \in \mathbb{R}^2 : \underline{q} = \xi_1 L \underline{a}_1 + \xi_2 L \underline{a}_2 ,\ \xi_1, \xi_2 \in [0,1) \}$ with periodic boundary conditions.

Pair potential $v(\underline{q}_i - \underline{q}_j)$ stable (i.e., $V(\underline{q}_1, \dots, \underline{q}_N) \geq -BN$ for some $B \in \mathbb{R}^+$), smooth and suff. fast decaying at infinity (e.g., it is sufficient that $|\underline{q}\,\underline{q}\,\underset{\sim}{\partial}\underset{\sim}{\partial} v(\underline{q})| \leq \frac{C}{|\underline{q}|^{d+\alpha}}$ for some $C, \alpha > 0$ and $|\underline{q}| \geq r_0$).

Let $V_\Lambda(\underline{q}_1, \dots, \underline{q}_N) = \sum_{1 \leq i < j \leq N} v_\Lambda(\underline{q}_i - \underline{q}_j)$ with

$$v_\Lambda(\underline{q}) = \sum_{n \in \mathbb{Z}^2} v(\underline{q} + n_1 L \underline{a}_1 + n_2 L \underline{a}_2).$$

$$\rho_{\Lambda,\epsilon}(\underline{q}) = \langle \mathcal{N}(\underline{q}; \cdot) \rangle_{\beta,\Lambda,\epsilon} \quad \text{with}$$

$$\mathcal{N}(\underline{q}; (\underline{q}_1, \dots, \underline{q}_N)) = \sum_{i=1}^{N} \delta(\underline{q} - \underline{q}_i)$$

and $\langle \cdot \rangle_{\beta,\Lambda,\epsilon}$ the Gibbs measure at inverse temperature β, in the box $\Lambda = \Lambda_L$ and with "symmetry breaking potential" $\varepsilon W_\Lambda(\underline{q}_1 \dots \underline{q}_N)$ where $W_\Lambda(\underline{q}_1 \cdots \underline{q}_N) = \sum_i w_\Lambda(\underline{q}_i)$ with w_Λ a Λ-periodic function with degenerate minima at $n_1 \underline{a}_1 + n_2 \underline{a}_2$, e.g. $w_\Lambda(\underline{q}) = \left(\sin^2\left(\frac{\underline{G}_1 \cdot \underline{q}}{2}\right) + \sin^2\left(\frac{\underline{G}_2 \cdot \underline{q}}{2}\right)\right)$ where $\underline{G}_1, \underline{G}_2$ are the basis vectors of the reciprocal lattice:

$$\underline{G}_i \cdot \underline{a}_j = 2\pi \delta_{i,j} \quad , \quad i,j = 1,2.$$

We also let $\rho(\underline{q}) = \lim_{\epsilon \to 0^+} \lim_{L \to \infty} \rho_{\Lambda_L, \epsilon}(\underline{q})$ (possibly along a subsequence).

We would like to exclude the possibility that $\rho(\underline{q})$ is periodic by translations by integer multiples of $\underline{a}_1, \underline{a}_2$, in the following sense. Recall that $\rho_{\Lambda_L, \epsilon}$ is normalized so that $\int_{\Lambda_L} \rho_{\Lambda_L, \epsilon}(\underline{q})\, d\underline{q} = N = L^2$. If $\rho(\underline{q})$ is non-trivially periodic we thus expect that:

1) For any bounded function $\gamma : B \to \mathbb{R}$ on $B := \{\xi_1 \underline{G}_1 + \xi_2 \underline{G}_2 : \xi_1, \xi_2 \in [0,1)\}$ and any $p > 0$:

$$\lim_{N = L^2 \to \infty} \int \frac{d\underline{k}}{|B|}\, \gamma(\underline{k}) |\hat{\rho}_{\Lambda_L, \epsilon}(\underline{k})|^p = 0, \text{ where } \hat{\rho}_{\Lambda_L, \epsilon}(\underline{k}) := $$
$$= \frac{1}{L^2} \int d\underline{q}\, \rho_{\Lambda_L, \epsilon}(\underline{q})\, e^{-i\underline{k}\underline{q}} = \frac{1}{L^2} \langle \textstyle\sum_i e^{-i\underline{k} \cdot \underline{q}_i} \rangle$$

and $\int \frac{dk}{|B|}$ is a shorthand notation for $\frac{1}{L^2} \sum_{k \in B_L \setminus \{0\}}$

where $B_L = \{ n_1 \underline{G}_1/L + n_2 \underline{G}_2/L : 0 \le n_1, n_2 < L \}$.

2) $\lim_{N=L^2 \to \infty} \frac{1}{L^2} \int_{\Lambda_L} d\underline{q}\, \rho_{\Lambda,\epsilon}(\underline{q})\, e^{-i \underline{G}\cdot\underline{q}} \equiv \hat{\rho}_\epsilon(\underline{G})$ is non-zero and s.t. $\lim_{\epsilon \to 0^+} |\hat{\rho}_\epsilon(\underline{G})| > 0$ for at least one non-zero vector $\underline{G} \in \Lambda^*_\infty := \{ n_1 \underline{G}_1 + n_2 \underline{G}_2 : n_i \in \mathbb{Z} \}$

We now prove that (1)+(2) cannot hold, as a consequence of the following "Bogoliubov's inequality" (an example of an infrared bound):

$$\langle |\Sigma_i \psi_i|^2 \rangle \ge \frac{|\Sigma_i \langle \varphi_i \underline{\partial} \psi_i \rangle|^2}{\langle \frac{\beta}{2} \Sigma_{ij} \Delta v_{ij} |\varphi_i - \varphi_j|^2 + \epsilon\beta \Sigma_i \Delta w_i \varphi_i^2 + \Sigma_i |\underline{\partial} \varphi_i|^2 \rangle} \quad (*)$$

where $\psi_i \equiv \psi(\underline{q}_i)$, $\varphi_i \equiv \varphi(\underline{q}_i)$ and $w_i = w(\underline{q}_i)$

[The proof of (*) is elementary: just define

$$A = \Sigma_i \psi_i \,, \quad \underline{B} = -\beta^{-1} e^{\beta\phi_\Lambda} \Sigma_i \underline{\partial}_i (\varphi_i e^{-\beta\phi_\Lambda})$$

with $\phi_\Lambda(\underline{q}_1 \cdots \underline{q}_N) = V_\Lambda(\underline{q}_1 \cdots \underline{q}_N) + \varepsilon W_\Lambda(\underline{q}_1 \cdots \underline{q}_N)$,

use Cauchy-Schwartz inequality:

$$\langle |A|^2 \rangle \ge \frac{|\langle A \underline{B} \rangle|^2}{\langle |\underline{B}|^2 \rangle} \quad \text{with } \langle \cdot \rangle =$$

$$\langle \cdot \rangle = \frac{1}{Z} \int d\underline{q}_1 \cdots d\underline{q}_N\, e^{-\beta\phi_\Lambda(\underline{q}_1 \cdots \underline{q}_N)} (\cdot) \text{ and,}$$

in the RHS, integrate by parts once in the numerator and twice in the denominator:

- $\langle A \underline{B} \rangle = -\frac{\beta^{-1}}{Z} \int dq_1 \cdots dq_N \sum_{i,j} \varphi_i \partial_j (\varphi_j e^{-\beta\phi_\Lambda})$

$$= \beta^{-1} \langle \Sigma_i \varphi_i \partial \varphi_i \rangle$$

- $\langle |\underline{B}|^2 \rangle = \frac{\beta^{-2}}{Z} \int dq_1 \cdots dq_N \, e^{\beta\phi_\Lambda} \Sigma_{i,j} \partial_i (\varphi_i e^{-\beta\phi_\Lambda}) \cdot \partial_j (\bar{\varphi}_j e^{-\beta\phi_\Lambda})$

$$= -\frac{\beta^{-1}}{Z} \int dq_1 \cdots dq_N \sum_{i,j} \Big(\sum_{k\neq i} \partial_i v_{ik} + \varepsilon \, \partial_i w_i \Big) \varphi_i \, \partial_j (\bar{\varphi}_j e^{-\beta\phi_\Lambda})$$

$$- \frac{\beta^{-2}}{Z} \int dq_1 \cdots dq_N \, \Sigma_{i,j} \varphi_i \, \partial \partial_j (\bar{\varphi}_j e^{-\beta\phi_\Lambda})$$

$$= \beta^{-1} \Sigma_{i,j} \sum_{k\neq i} \langle \partial_i \partial_j v_{ik}^{\,(1)} \varphi_i \bar{\varphi}_j \rangle + \varepsilon\beta^{-1} \sum_i \langle \Delta w_i |\varphi_i|^2 \rangle$$

$$+ \beta^{-1} \Sigma_i \Sigma_{k\neq i} \cancel{\langle \partial_i v_{ik}} \, \partial_i \varphi_i \, \bar{\varphi}_i \rangle + \varepsilon \beta^{-1} \Sigma_i \cancel{\langle \partial w_i} \, \partial_i \varphi_i \bar{\varphi}_i \rangle +$$

$$+ \beta^{-2} \Sigma_i \langle |\partial_i \varphi_i|^2 \rangle$$

$$- \beta^{-1} \Sigma_i \langle \partial \varphi_i \bar{\varphi}_i \Big(\cancel{\sum_{k\neq i} \partial_i v_{ik}} + \varepsilon \cancel{\partial_i w_i} \Big) \rangle$$

Now: $(1) = \beta^{-1} \sum_i \sum_{k\neq i} \langle \partial_i^2 v_{ik} \left(|\varphi_i|^2 - \varphi_i \bar{\varphi}_k \right) \rangle$

$$= \frac{\beta^{-1}}{2} \sum_i \sum_{k\neq i} \langle \Delta v_{ik} |\varphi_i - \varphi_k|^2 \rangle,$$

from which, putting things together, the desired inequality follows.]

Tomorrow we will show that, choosing

$\psi(\underline{q}) = e^{-i(\underline{k}+\underline{G})\cdot \underline{q}}$ and $\varphi(\underline{q}) = \sin(\underline{k}\cdot\underline{q})$

(here $\underline{G} \in \Lambda^*_\infty$ and, at finite volume,

$\underline{k} = \frac{n_1 \underline{G}_1}{L} + \frac{n_2}{L}\underline{G}_2$ for some integers $0 \le n_1, n_2 < L$)

Bogoliubov's inequality implies an INFRARED (lower) BOUND of the form:

$$\frac{1}{N} \langle |\Sigma_i e^{-i(\underline{k}+\underline{G})\underline{q}_i}|^2 \rangle \ge |\hat{\rho}_\epsilon(\underline{G})|^2 \int_B d\underline{k} \, \frac{C_0}{|\underline{k}|^2 + C_1\epsilon}$$

which, in turn, implies that

$$\lim_{\epsilon \to 0^+} |\hat{\rho}_\epsilon(\underline{G})|^2 = 0 .$$