

STABILITY OF CHARGE DENSITY WAVES IN ELECTRON-PHONON SYSTEMS

HIMEJI CONFERENCE ON PARTIAL DIFFERENTIAL EQUATIONS
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Based on:

[T.M.](#) “Stability of charge density waves in electron-phonon systems”, To appear in Jour. Stat. Phys., arXiv:2303.05667

Part 1: Background

MOTIVATION

- ▶ Various phases are anticipated to emerge in many-electron systems.
Eg. ferromagnetic phase, antiferromagnetic phase, charge density wave phase, Mott insulator, Luttinger liquid, Fermi liquid, etc..
- ▶ The mathematical justification of phase diagrams has only been partially achieved.
- ▶ Systems with electron-phonon interactions are typically more challenging to handle than ordinary many-electron systems, and there is little mathematical proof of phase diagrams for low-temperature phases.

HISTORY

- ▶ The original meaning of **CDW** refers to the periodic structure of charge with a period of $2a$ (where a is the lattice spacing) in **one-dimensional** electron systems. In 1954, **H. Fröhlich**¹ proposed this mechanism to theoretically explain superconductivity (which was incorrect as a theory of superconductivity).
- ▶ In the 1970s, CDWs were discovered in several one-dimensional conductors, and their behavior was experimentally and theoretically elucidated.²
- ▶ In present times, the term “charge density wave” is commonly used to describe the type of order depicted in the figure, even in **multi-dimensional** electron systems.

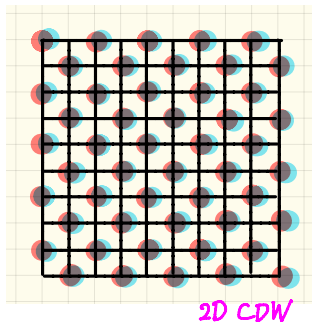
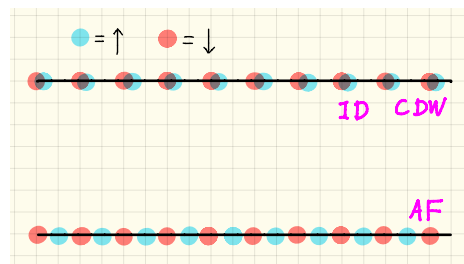
¹**H. Fröhlich**. On the Theory of Superconductivity: The One-Dimensional Case. Proceedings of the Royal Society A 223 (1154): 296–305.

²**G. Grüner**, Density Waves in Solids. Addison-Wesley, 1994.

MATHEMATICAL INVESTIGATIONS OF CHARGE DENSITY WAVES

WAVES

- ▶ $D = 1$: Lieb–Nachtergaele³, T.M.⁴, Gontier–Kouande–Sere⁵
- ▶ $D \geq 2$: Macris–Piguet⁶, Borgs–Jedrzejewski–Kotecky⁷, Borgs–Kotecky⁸, T.M.⁹



³E. H. Lieb and B. Nachtergaele, Phys. Rev. B 51, 4777, 1995

⁴T. M., Rev. Math. Phys. Vol. 23, No. 07, pp. 749-822 (2011)

⁵D. Gontier, A. E. K. Kouande and E. Sere, A. H. Poincare, Vol. 24, pages 3945–3966, (2023)

⁶N. Macris and C.-A. Piguet, Phys. Rev. B 60, 13484 (1999)

⁷C Borgs, J Jedrzejewski, R Kotecky, J. Phys. A: Math. Gen. 29 733 (1999)

⁸C. Borgs, R. Kotecky, Comm. Math. Phys., Vol. 208, pages 575–604, (2000)

⁹T.M., J. Stat. Phys., Vol. 165, pages 225–245, (2016)

Part 2: The Existence of Charge Density Waves as Long-Range Order

MATHEMATICAL DESCRIPTION OF ELECTRONS

- ▶ Here I give a mathematical framework for describing electrons on finite lattice $\Lambda = \mathbb{Z}^d \cap [-L, L]^d$. A state of a **single electron** is represented by a unit vector in the Hilbert space

$$\ell^2(\Lambda \times \{\uparrow, \downarrow\}).$$

- ▶ Since **electrons are fermions**, states of N electrons are expressed as vectors in the **antisymmetric** tensor product Hilbert space:

$$\mathfrak{F}_{e,N}(\Lambda) = \bigwedge^N \ell^2(\Lambda \times \{\uparrow, \downarrow\}).$$

- ▶ It is more convenient to employ the **fermionic Fock space** to describe states with various numbers of electrons:

$$\mathfrak{F}_e(\Lambda) = \bigoplus_{N=0}^{2|\Lambda|} \mathfrak{F}_{e,N}(\Lambda).$$

- The **creation and annihilation operators** $\{c_{x,\sigma}, c_{x,\sigma}^* : x \in \Lambda, \sigma = \{\uparrow, \downarrow\}\}$ acting on $\mathfrak{F}_e(\Lambda)$ will be needed to define various operators:¹⁰

$$\begin{aligned}\{c_{x\sigma}, c_{y\tau}\} &= 0 = \{c_{x\sigma}^*, c_{y\tau}^*\}, \\ \{c_{x\sigma}, c_{y\tau}^*\} &= \delta_{xy}\delta_{\sigma\tau}.\end{aligned}$$

- **Number operator** of electrons:

$$\hat{n}_{x\sigma} = c_{x\sigma}^* c_{x\sigma}, \quad \hat{n}_x = \hat{n}_{x\uparrow} + \hat{n}_{x\downarrow}.$$

¹⁰A. Arai. Analysis on Fock Spaces and Mathematical Theory of Quantum Fields. WORLD SCIENTIFIC, Dec. 2016.

O. Bratteli and D. W. Robinson. Operator Algebras and Quantum Statistical Mechanics 2: Equilibrium States. Models in Quantum Statistical Mechanics. Springer Berlin Heidelberg, 1997.

PHASE DIAGRAM IN CLASSICAL SYSTEMS

Toy model:

$$H_{C,\Lambda} = U \sum_{x \in \Lambda} \hat{n}_{x,\uparrow} \hat{n}_{x,\downarrow} + W \sum_{\langle x,y \rangle \in E_\Lambda} \hat{n}_x \hat{n}_y - \left(\mu + 2dW + \frac{U}{2} \right) \sum_{x \in \Lambda} \hat{n}_x.$$

- ▶ U, W, μ : real parameters.
- ▶ The family of number operators $\{\hat{n}_{x\sigma}\}$ consists of **commuting** operators, thus $H_{C,\Lambda}$ is a **classical** Hamiltonian.
- ▶ The ground state of $H_{C,\Lambda}$ varies depending on the values of the parameters.
↪ **Phase diagram**

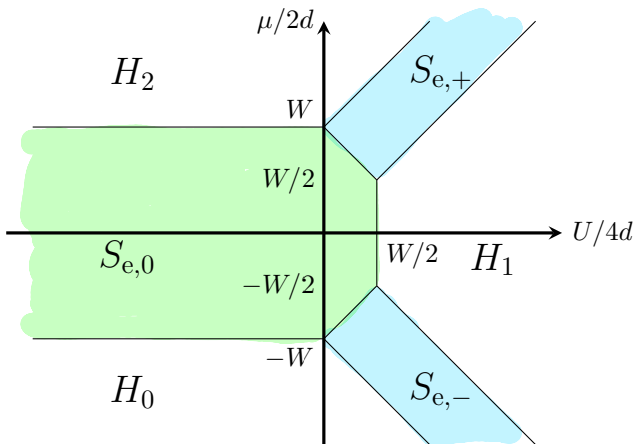


FIGURE: Phase diagram of the ground states for $H_{C,\Lambda}$.

ORDER PARAMETER AND PHASE DIAGRAM

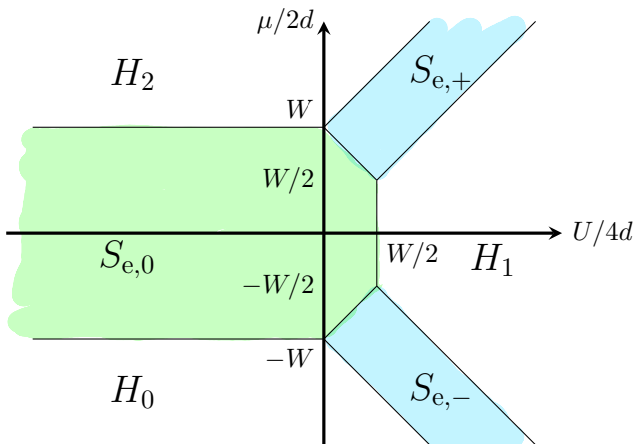
- ▶ Let $H_{C,\Lambda}^{(P)}$ be the Hamiltonian with the **periodic boundary conditions** imposed.
- ▶ \mathfrak{A}_e is the $*$ -algebra generated by $\{c_{x,\sigma} : x \in \mathbb{Z}^d, \sigma \in \{\uparrow, \downarrow\}\}$.
- ▶ Given an observable $\Psi \in \mathfrak{A}_e$, the **thermal expectation value** of Ψ with respect to $H_{C,\Lambda}^{(P)}$ is defined as

$$\langle \Psi \rangle_{\beta, C, \Lambda}^{(P)} = \frac{\text{Tr} \left[\Psi e^{-\beta H_{C,\Lambda}^{(P)}} \right]}{Z_{C,\Lambda}^{(P)}}, \quad Z_{C,\Lambda}^{(P)} = \text{Tr} \left[e^{-\beta H_{C,\Lambda}^{(P)}} \right].$$

- ▶ For any state $\langle \cdot \rangle$ on \mathfrak{A}_e , we define the **staggered density** as

$$\Delta_C = \lim_{L \rightarrow \infty} \frac{1}{|\Lambda|} \sum_{x \in \Lambda} (-1)^x \langle \hat{n}_x \rangle.$$

When $\Delta_C \neq 0$, a CDW emerges.



- ▶ $\Delta_C = 1$ ($S_{e,0}$), $\Delta_C = 1/2$ ($S_{e,\pm}$)
- ▶ $\Delta_C = 0$ ($H_i, i = 0, 1, 2$)

CDW IN ITINERANT ELECTRON SYSTEMS

The extended Hubbard model:

$$H_{H,\Lambda} = T_{\Lambda} + H_{C,\Lambda}.$$

Here,

$$T_{\Lambda} = -t \sum_{\langle x,y \rangle \in E_{\Lambda}} \sum_{\sigma=\uparrow,\downarrow} (c_{x,\sigma}^* c_{y,\sigma} + c_{y,\sigma}^* c_{x,\sigma}).$$

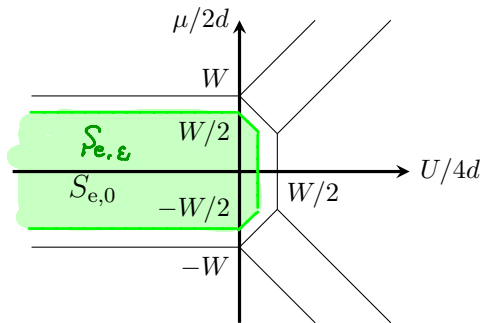
- ▶ Consider the electron hopping term as a **quantum perturbation**.
- ▶ It is logical to ask **whether charge density waves are stable in the case $t \neq 0$** .

THEOREM 2.1 (BORGS AND KOTECKY(2000))

The charge density waves are **stable**, i.e., $\Delta_C \neq 0$ in the parameter region:

$$S_{e,\varepsilon} = \left\{ (U, \mu) \in \mathbb{R}^2 : U < 2d(W - \varepsilon), |\mu| < 2d \min \left\{ W - \varepsilon, W - \varepsilon - \frac{U}{4d} \right\} \right\},$$

if the temperature is low enough and $\varepsilon > 0$ and $|t|$ are sufficiently small.



- ▶ The proof is based on the **Pirogov–Sinai theory**.
Remark: The method of **reflection positivity** can cover the case where $\mu = 0$ (**half-filling system**) only.
- ▶ The Pirogov–Sinai theory has emerged as a potent approach in **classical** statistical mechanics for delineating first-order phase transitions and coexistence of phases at low temperatures.¹¹
- ▶ Noteworthy research works that utilize the Pirogov–Sinai theory to many-electron systems include **Borgs-Kotecký-Ueltschi(1996)**, **Datta-Fernández-Fröhlich(1996)**, **Borgs-Kotecký(2000)**.¹²

¹¹S. A. Pirogov and Y. G. Sinai, Theoretical and Mathematical Physics, 25(3):1185–1192, Dec. 1975.

¹²Borgs, C.; Kotecký, R.; Ueltschi, D. Comm. Math. Phys. 181 (1996), 409–446,

Borgs, C.; Kotecký, R. Comm. Math. Phys. 208 (2000), 575–604,

Datta, Nilanjana; Fernández, Roberto; Fröhlich, Jürg, J. Statist. Phys. 84 (1996), 455–534.

Part 3: Enhancement of Charge Density Waves by Electron-Phonon Interaction

THE HOLSTEIN–HUBBARD MODEL

The Holstein–Hubbard model:

$$H_{\Lambda} = H_{\text{H},\Lambda} + g \sum_{x \in \Lambda} \hat{n}_x (b_x + b_x^*) + \omega_0 \sum_{x \in \Lambda} b_x^* b_x.$$

- ▶ H_{Λ} acts on the following Hilbert space:

$$\mathfrak{H}_{\Lambda} = \mathfrak{F}_e(\Lambda) \otimes \mathfrak{F}_p(\Lambda),$$

where $\mathfrak{F}_p(\Lambda)$ is the **bosonic Fock space** over $\ell^2(\Lambda)$:

$$\mathfrak{F}_p(\Lambda) = \bigoplus_{n=0}^{\infty} \otimes_s^n \ell^2(\Lambda);$$

$\otimes_s^n \ell^2(\Lambda)$ stands for the n -fold **symmetric tensor product** of $\ell^2(\Lambda)$, with $\otimes_s^0 \ell^2(\Lambda) = \mathbb{C}$.

- ▶ The **annihilation- and creation operators** of phonons are denoted by b_x and b_x^* , respectively.

$$[b_x, b_y^*] = \delta_{x,y}, \quad [b_x, b_y] = 0.$$

- ▶ The phonons are assumed to be dispersionless with energy $\omega_0 > 0$.
- ▶ The parameter g is the strength of the electron-phonon interaction.
- ▶ Given $\Psi \in \mathfrak{A}_e$, the thermal expectation value of Ψ with respect to $H_\Lambda^{(P)}$ is defined as

$$\langle \Psi \rangle_{\beta, \Lambda}^{(P)} = \frac{\text{Tr} \left[\Psi e^{-\beta H_\Lambda^{(P)}} \right]}{Z_\Lambda^{(P)}}, \quad Z_\Lambda^{(P)} = \text{Tr} \left[e^{-\beta H_\Lambda^{(P)}} \right].$$

- ▶ As before, we define the staggered density as

$$\Delta = \lim_{L \rightarrow \infty} \frac{1}{|\Lambda|} \sum_{x \in \Lambda} (-1)^x \langle \hat{n}_x \rangle. \quad (\text{I})$$

- ▶ We can prove the existence of charge density waves in the following region:

$$S_{\text{ep},\varepsilon} = \left\{ (U, \mu) \in \mathbb{R}^2 : U < 2d(W - \varepsilon) + \frac{2g^2}{\omega_0}, \right. \\ \left. |\mu| < 2d \min \left\{ W - \varepsilon, W - \varepsilon - \frac{U}{4d} + \frac{g^2}{2d\omega_0} \right\} \right\},$$

provided that $|t|$ is small enough, ω_0 is large enough and at sufficiently low temperatures.

- ▶ $S_{\text{e},\varepsilon} \subset S_{\text{ep},\varepsilon} \rightsquigarrow$ The electron-phonon interaction has a significant stabilizing effect on the charge density waves.
- ▶ Such effects have been anticipated in theoretical physics based on numerical computations and discussions relying on certain approximation theories.

The **spin operators**, $(S_x^{(1)}, S_x^{(2)}, S_x^{(3)})$, at site x are defined to be

$$S_x^{(i)} = \frac{1}{2} \sum_{\sigma, \sigma' = \uparrow, \downarrow} c_{x, \sigma}^* (s^{(i)})_{\sigma, \sigma'} c_{x, \sigma}, \quad i = 1, 2, 3,$$

where $s^{(i)}$ ($i = 1, 2, 3$) are the **Pauli matrices**:

$$s^{(1)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad s^{(2)} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad s^{(3)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

$(s^{(i)})_{\sigma, \sigma'}$ represents the matrix elements of $s^{(i)}$, with the correspondence $\uparrow = 1, \downarrow = 2$ ¹³.

¹³Under this convention, for example, $(s^{(1)})_{\uparrow, \uparrow} = (s^{(1)})_{1,1} = 0$ and $(s^{(1)})_{\uparrow, \downarrow} = (s^{(1)})_{1,2} = 1$.

THEOREM 3.1 (T.M., 2023)

Suppose that $0 < \varepsilon < W$ and $(U, \mu) \in S_{ep, \varepsilon}$. There exist certain constants $0 < \beta_0 < \infty, 0 < \omega_* < \infty$ and $0 < t_0 < \infty$, such that, if $\beta \geq \beta_0, \omega_0 \geq \omega_*$ and $|t| \leq t_0$, then the following (i)-(iii) hold:

(i) Given an arbitrary local observable $\Psi \in \mathfrak{A}_e$, the infinite volume limit:

$$\langle \Psi \rangle_{\beta}^{(P)} = \lim_{L \rightarrow \infty} \langle \Psi \rangle_{\beta, \Lambda}^{(P)}$$

converges. The state $\langle \cdot \rangle_{\beta}^{(P)}$ on \mathfrak{A}_e defined in this way can be represented by the convex combination of two pure states:

$$\langle \Psi \rangle_{\beta}^{(P)} = \frac{1}{2} \langle \Psi \rangle_{\beta}^{(+)} + \frac{1}{2} \langle \Psi \rangle_{\beta}^{(-)}.$$

The states $\langle \cdot \rangle_{\beta}^{(\pm)}$ describe charge density waves:

$$\langle \hat{n}_x \rangle_{\beta}^{(+)} = \rho + (-1)^x \Delta, \quad \langle \hat{n}_x \rangle_{\beta}^{(-)} = \rho - (-1)^x \Delta.$$

Here, $\Delta^{(+)} = -\Delta^{(-)} = \Delta > 0$, where $\Delta^{(+)}$ and $\Delta^{(-)}$ are staggered densities defined with respect to states $\langle \cdot \rangle_{\beta}^{(\pm)}$ in equation (1). Additionally, ρ is given as

$$\rho = \lim_{L \rightarrow \infty} \frac{1}{|\Lambda|} \sum_{x \in \Lambda} \langle \hat{n}_x \rangle_{\beta}^{(+)}$$

and coincides with the density associated with $\langle \cdot \rangle_{\beta}^{(-)}$.

THEOREM 3.2 (CONT'D)

- (ii) *No magnetic order exists.* Namely, $\langle S_x^{(i)} \rangle_\beta^{(\pm)} = 0$ ($i = 1, 2, 3$) holds for every $x \in \mathbb{Z}^d$.
- (iii) *The two-point correlation function concerning arbitrary local observables $\Psi, \Phi \in \mathfrak{A}_e$ decays exponentially.* Namely, there are constants $C_{\Psi, \Phi} > 0$ and $\xi_\ell > 0$ such that

$$\left| \langle \Psi \Phi \rangle_\beta^{(\pm)} - \langle \Psi \rangle_\beta^{(\pm)} \langle \Phi \rangle_\beta^{(\pm)} \right| \leq C_{\Psi, \Phi} \exp \left\{ - \frac{\text{dist}(\text{supp } \Psi, \text{supp } \Phi)}{\xi_\ell} \right\},$$

where, for any two finite subsets A and B of \mathbb{Z}^d , the distance between A and B is defined as $\text{dist}(A, B) = \min\{\|x - y\| : x \in A, y \in B\}$.

OUTLINE OF THE PROOF

► HH Hamiltonian:

$$H_{\Lambda} = -t \sum_{\sigma} \sum_{\langle x;y \rangle} c_{x,\sigma}^* c_{y,\sigma} + H_{C,\Lambda} + g \sum_{x \in \Lambda} \hat{n}_x (b_x + b_x^*) + \omega_0 N_{p,\Lambda}$$

↪ Lang–Firsov transformation:

$$H_{\Lambda} = -t \sum_{\sigma} \sum_{\langle x;y \rangle} e^{i\Phi_{x,y}} c_{x,\sigma}^* c_{y,\sigma} + H_{C,\Lambda}^{(\text{eff})} + \omega_0 N_{p,\Lambda}$$

where

$$\Phi_{x,y} = -\frac{\sqrt{2}g}{\omega_0} (q_x - q_y), \quad q_x = \frac{1}{\sqrt{2}} \overline{(b_x + b_x^*)},$$

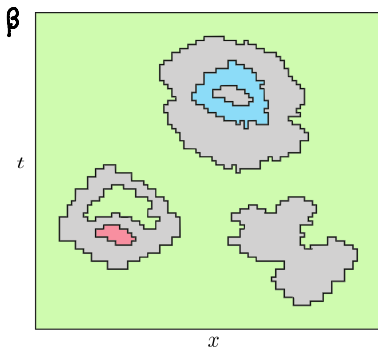
$$H_{C,\Lambda}^{(\text{eff})} = U_{\text{eff}} \sum_{x \in \Lambda} n_{x,\uparrow} n_{x,\downarrow} + W \sum_{\langle x,y \rangle} n_x n_y - \left(\mu + 2dW + \frac{U_{\text{eff}}}{2} \right) \sum_{x \in \Lambda} n_x,$$

$$U_{\text{eff}} = U - \frac{2g^2}{\omega_0}.$$

↪ The partition function can be represented as a **contour model** on the $(d + 1)$ -dimensional spacetime $\mathbb{T}_\Lambda := [-L, L - 1]^d \times [0, \beta]$:¹⁴

$$Z_{\ell, \Lambda} = \sum_{\{Y_1, \dots, Y_n\}} e^{-\tilde{\beta} \sum_{\ell} e_{\ell} |V_{\ell}|} \prod_{i=1}^n \rho(Y_i)$$

↪ The **Pirogov–Sinai theory** can be applied.



¹⁴In the case of classical systems such as the Ising model, the partition function can be represented by a contour model in d -dimensional space.

Difficulties:

- ▶ The construction of the contour model is complex.
- ▶ Existing methods cannot be applied due to the non-conservation of the boson particle number.
 - ↪ It is challenging to control $\rho(Y)$.
 - ↪ By utilizing **explicit formulas for correlation functions in quantum field theory**, it becomes possible to evaluate $\rho(Y)$.

THEOREM 3.3 (T.M. (2023))

Suppose that $0 < \varepsilon < W$ and $(U, \mu) \in S_{\text{ep}, \varepsilon}$. There exist certain constants $0 < \beta_0 < \infty, 0 < \omega_* < \infty$ and $0 < t_0 < \infty$, such that, if $\beta \geq \beta_0, \omega_0 \geq \omega_*$ and $|t| \leq t_0$, then the following holds:

$$|\rho(Y)| \leq e^{-(\tilde{\beta}e_e + \tilde{\beta}c + \gamma)|\text{supp } Y|},$$
$$\left| \frac{\partial}{\partial \underline{v}_i} \rho(Y) \right| \leq \left(2\tilde{\beta}C_0 + \frac{e}{e-1} + \frac{5}{\alpha e^{1/2}} \right) |\text{supp } Y| e^{-(\tilde{\beta}e_e + \tilde{\beta}c + \gamma_+)|\text{supp } Y|},$$

where, γ, γ_+ and c are some positive numbers, and the symbols \underline{v}_i represent the parameters U, μ, W, g .

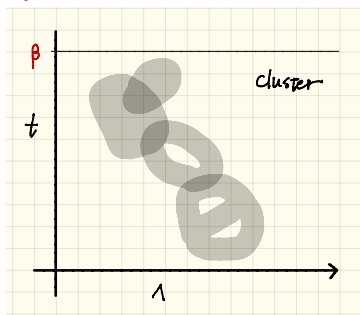
- Define the **weight** of the contour Y as follows:

$$W_\ell(Y) = \rho(Y) e^{\tilde{\beta} e_\ell |Y|} \prod_{m=1}^r \frac{Z_{m, \text{Int}_m Y}}{Z_{\ell, \text{Int}_m Y}}.$$

- The partition function can be expressed as follows:

$$Z_{\ell, \Lambda} = e^{-\tilde{\beta} e_\ell |\Lambda|} \sum_{\{Y_1, \dots, Y_n\} \subset \mathbb{T}_\Lambda^n} \prod_{i=1}^n W_\ell(Y_i).$$

- The set $X = \{Y_1, \dots, Y_n\}$ is called a **cluster**, if Y_1, \dots, Y_n are “connected”.



► For each cluster $X = \{Y_1, \dots, Y_n\}$, set

$$\Psi(X) = \left\{ \prod_{Y \in X} \frac{1}{n(Y)!} \right\} \varphi(Y_1, \dots, Y_n) \prod_{i=1}^n W_\ell(Y_i).$$

↪ Cluster expansion:

$$\log Z_{\ell, \Lambda} = \sum_{X: \text{supp } X \subset \Lambda} \Psi(X).$$

PROPOSITION 3.4

$$f_\ell = - \lim_{L \rightarrow \infty} \frac{1}{|\Lambda|} \log Z_{\ell, \Lambda} = e_\ell - \frac{1}{\beta} \sum_{X: o \in \text{supp } X} \frac{1}{|\text{supp } X|} \Psi(X).$$

PROPOSITION 3.5

The limit $\langle \Psi \rangle_\ell = \lim_{L \rightarrow \infty} \langle \Psi \rangle_{\ell, \Lambda}$ exists, and the following holds:

$$\langle \Psi \rangle_\ell = \sum_{\mathcal{Y}_\Psi} W_{\ell, \Psi}(\mathcal{Y}_\Psi) \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{\{Y_1, \dots, Y_n\}} \left[\prod_{i=1}^n W_\ell(Y_i) \right] \varphi(\mathcal{Y}_\Psi, Y_1, \dots, Y_n).$$

PROPOSITION 3.6

$$\begin{aligned} & \langle \Psi \Phi \rangle_\ell - \langle \Psi \rangle_\ell \langle \Phi \rangle_\ell \\ &= \sum_{\mathcal{Y}_\Psi, \mathcal{Y}_\Phi} W_{\ell, \Psi}(\mathcal{Y}_\Psi) W_{\ell, \Phi}(\mathcal{Y}_\Phi) \sum_{n=2}^{\infty} \frac{1}{(n-2)!} \sum_{\{Y_3, \dots, Y_n\}} \left[\prod_{i=3}^n W_\ell(Y_i) \right] \varphi(\mathcal{Y}_\Psi, \mathcal{Y}_\Phi, Y_3, \dots, Y_n). \end{aligned}$$

From this, it follows that :

$$|\langle \Psi \Phi \rangle_\ell - \langle \Psi \rangle_\ell \langle \Phi \rangle_\ell| \leq C_{\Psi, \Phi} \exp \left\{ -\frac{\text{dist}(\text{supp } \Psi, \text{supp } \Phi)}{\xi_\ell} \right\}.$$

SUMMARY

- ▶ We provided a mathematical justification for the physicists' prediction that CDW stabilizes due to the electron-phonon interaction.
- ▶ The proof relied on the quantum Pirogov–Sinai theory.
- ▶ Consideration was limited to on-site electron-phonon interactions, but extension to finite range is possible (though the proof becomes more complex).
- ▶ There are many aspects of magnetic ordering that are not yet fully understood mathematically.

Thank you!