Phase Transition in the Peierls model for polyacetylene

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Joint work with David Gontier and Eric Séré

CEREMADE, Université Paris-Dauphine

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Hideki Shirakawa.

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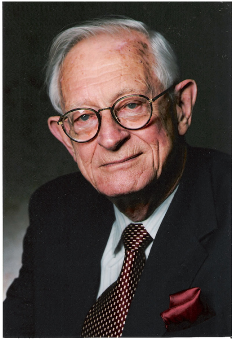

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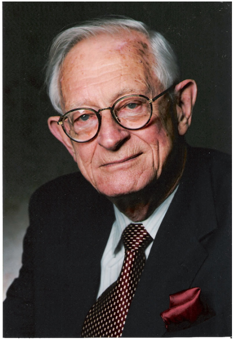

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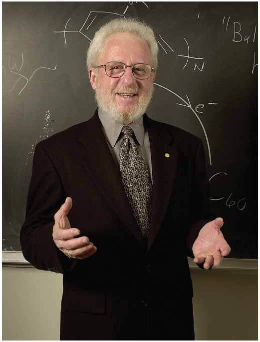

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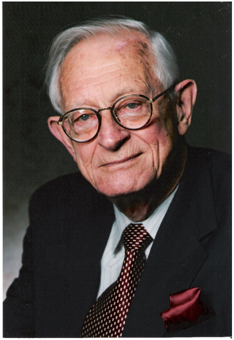

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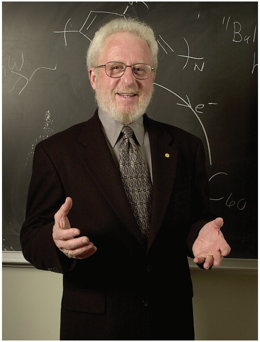

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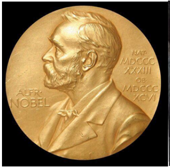

For the discovery and development of conductive polymers

Outline

1. Description of the model, scope and aim
2. The Peierls model at zero temperature
3. The Peierls model with temperature
4. Statement of our results

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Description of the model, scope and aim

- What is Polyacetylene ?

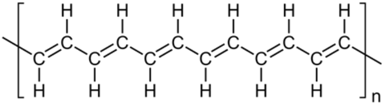

Figure: Dimerized Polyacetylene.

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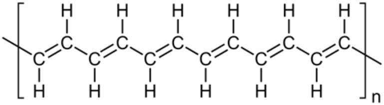

Figure: Dimerized Polyacetylene.

- Practical and technological applications: Rechargeable batteries, Biomedical, OLED bulbs...

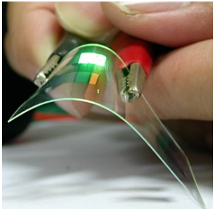

Figure: Light-emitting plastic film

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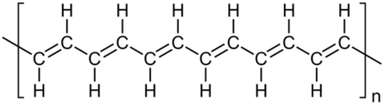

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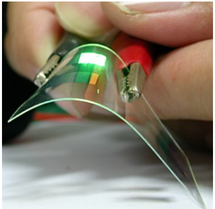

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- Aim: understand how conductivity changes with temperature.

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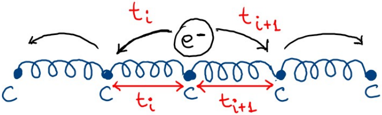
The Peierls model



- Consider a linear chain of L carbon atoms linked by springs of strength $\mu > 0$ with a length at rest $\ell = 1$.
- Denote by t_i the distance between the i-th and $(i+1)$-th atoms, and set $\mathbf{t} = \{t_1, \cdots, t_L\}$ with periodicity L, which means $i \in \mathbb{Z}/L\mathbb{Z}$.
- To any $\mathbf{t} = \{t_1, \cdots, t_L\}$ we associate a matrix T defined by

$$T = T(\mathbf{t}) := \begin{pmatrix} 0 & t_1 & 0 & 0 & \cdots & t_L \\ t_1 & 0 & t_2 & \cdots & 0 & 0 \\ 0 & t_2 & 0 & t_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & t_{L-2} & 0 & t_{L-1} \\ t_L & 0 & \cdots & 0 & t_{L-1} & 0 \end{pmatrix} \quad (1)$$

- The Peierls energy 1930. At the half filled band, the Peierls energy of the system is given by

$$\mathcal{E}^{(L)}(\mathbf{t}, \gamma) := \frac{\mu}{2} \sum_{i=1}^{L} (t_i - 1)^2 + 2\mathrm{Tr}\,(T\gamma), \quad \gamma \in \mathcal{S}_L(\mathbb{C}); 0 \le \gamma \le 1 \quad (2)$$

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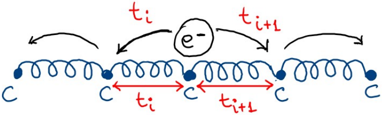

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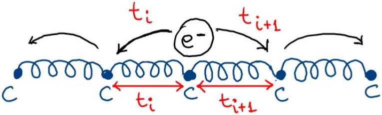

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Ground state of the Peierls energy

$$\mathcal{E}^{(L)}(\mathbf{t}, \gamma) := \frac{\mu}{2}\sum_{i=1}^{L}(t_i - 1)^2 + 2\mathrm{Tr}\,(T\gamma)$$

$$\inf\left\{\mathcal{E}^{(L)}, \mathbf{t} \in (\mathbb{R}_+)^L, \quad \gamma \in \mathcal{S}_L(\mathbb{C}), 0 \leq \gamma \leq 1\right\}.$$

Lemma

For any $T \in \mathcal{S}_L(\mathbb{C})$,

$$\inf_{\substack{\gamma \in \mathcal{S}_L(\mathbb{C}) \\ 0 \leq \gamma \leq 1}} \{2\mathrm{Tr}\,(T\gamma)\} = -\mathrm{Tr}\left(\sqrt{T^2}\right) = -\mathrm{Tr}\,(|T|)\,.$$

New minimization problem

$$E^{(L)} := \inf\left\{\mathcal{E}^{(L)}, \quad \mathbf{t} \in (\mathbb{R}_+)^L\right\}$$

with

$$\mathcal{E}^{(L)}(\mathbf{t}) := \frac{\mu}{2}\sum_{i=1}^{L}(t_i - 1)^2 - \mathrm{Tr}\,(|T|). \tag{3}$$

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Remarks and even case ($L = 2N$)

$$\mathcal{E}^{(2N)}(\mathbf{t}) := \frac{\mu}{2}\sum_{i=1}^{2N}(t_i - 1)^2 - \mathrm{Tr}\,(|T|)$$

- $\mathcal{U}^\dagger T \mathcal{U} = -T \quad$ with $\quad \mathcal{U}_{ij} = (-1)^i \delta_{ij}, \quad .$
- If $L = 2N + 1$, then $0 \in \sigma(T)$.
- This model is translation invariant, in the sense

$$\mathcal{E}^{(L)}(\mathbf{t}) = \mathcal{E}^{(L)}(\tau_k \mathbf{t}), \tau_k \mathbf{t} := \{t_{k+1}, \cdots, t_{k+L}\}, k = 1, \ldots, L.$$

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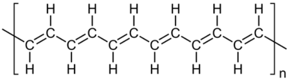
Theorem (Even case: Kennedy and Lieb 1987)

For $L = 2N$, and $\mu > 0$, there are exactly two minimizing configurations for $E^{(2N)}$, of the form

$$t_i = W + (-1)^i \delta \text{ or } t_i = W - (-1)^i \delta, \quad \text{with } \delta \geq 0 \text{ (2-periodic)}. \tag{4}$$



- The electrons are blocked, hence low conductivity of these configurations.

Odd case ($L = 2N + 1$)

Theorem (Odd case: Garcia Arroyo and Séré 2011)

For odd L ($L = 2N + 1$) the minimizers of the Peierls energy look like "kinks". Let $\mathbf{t}(2N+1) = (t_i)_{i \in \mathbb{Z}/(2N+1)\mathbb{Z}}$ be a global minimizer of $E^{(2N+1)}$. Up to translation and subsequence, $\lim_{N \to +\infty} t_i(2N+1) =: t_i^\infty$ exists and satisfies

$$\left| t_i^\infty - \left(W \pm (-1)^i \delta\right) \right| \xrightarrow[i \to -\infty]{} 0, \text{ and } \left| t_i^\infty - \left(W \mp (-1)^i \delta\right) \right| \xrightarrow[i \to \infty]{} 0.$$

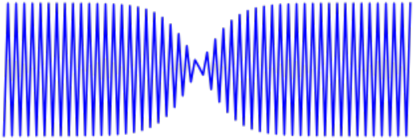


Figure: $L = 101$, we observe a localized kink.

- Kinks can move, low conductivity of these configurations too.

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The Energy with temperature

In presence of positive temperature θ, the energy is given by

$$\mathcal{F}_\theta^{(L)}(\mathbf{t}, \gamma) := \frac{\mu}{2} \sum_{i=1}^{L} (t_i - 1)^2 + 2 \left(\mathrm{Tr}\,(T\gamma) + \theta \mathrm{Tr}\,[S(\gamma)] \right),$$

$\gamma \in \mathcal{S}_L(\mathbb{C}), 0 \leq \gamma \leq 1$ and $S(\gamma) = (1-\gamma)\log(1-\gamma) + \gamma \log(\gamma).$

Study the minimizers of the energy

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attained at $\gamma_* = (1 + e^{T/\theta})^{-1}$, with $h_\theta(x) := 2\theta \log\left(2\cosh\left(\frac{\sqrt{x}}{2\theta}\right)\right)$ concave on $\mathbb{R}_+$.

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$$\min \left\{ \mathcal{F}_\theta^{(L)}(\mathbf{t}),\ \mathbf{t} \in \mathbb{R}_+^L \right\}$$

with

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Goal: study the phase diagram in the (μ, θ) plane.

Define the energy $\mathcal{G}_\theta^{(L)}$ by

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$$\langle T^2 \rangle = \frac{1}{L} \sum_{k=1}^{L} \Theta_k T^2 \Theta_k^{-1}, \text{ with } \Theta_k = \Theta_1^k \text{ and } \Theta_1 := \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \end{pmatrix}.$$

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General lower bound

Theorem (GLB)

- *$\mathcal{H}$ be a separable Hilbert space (real or complex),*
- *I an interval of $\mathbb{R}$ containing 0,*
- *$\varphi : I \to \mathbb{R}$ a convex function,*
- *$\mathcal{S}_{\mathcal{H}}$, the space of linear bounded self-adjoint trace class operators $A : \mathcal{H} \to \mathcal{H}$* i.e. *compact and $\sum_{\lambda \in \sigma(A)} |\lambda| < \infty$,*
- *$\mathcal{M}_I := \{A \in \mathcal{S}_{\mathcal{H}}, \quad \sigma(A) \subset I\}$.*

Then the function $f : A \in \mathcal{M}_I \mapsto \mathrm{Tr}\,(\varphi(A))$ is well defined and convex.

Applying this theorem with
$\mathcal{H} = \mathbb{R}^L, \quad I = \mathbb{R}_+, \quad \varphi(x) = -h_\theta(x), \quad \mathcal{S}_{\mathcal{H}} = \mathcal{S}_L(\mathbb{R}), \quad A = T^2, \mathcal{M}_I = \mathcal{S}_L^+(\mathbb{R}),$
we get

$$\mathrm{Tr}\,(h_\theta(T^2)) \le \mathrm{Tr}\,(h_\theta(\langle T^2 \rangle)) \Longrightarrow \boxed{\mathcal{F}_\theta^{(L)}(\mathbf{t}) \ge \mathcal{G}_\theta^{(L)}(\mathbf{t})},$$

with equality for 2-periodic configurations $\mathbf{t}_2 = \{t_i\}_i$ with $t_i = W \pm (-1)^i \delta$
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First Result

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$$\mathcal{F}_\theta^{(L)}(\mathbf{t}) \geq \mathcal{G}_\theta^{(L)}(\mathbf{t})$$

Theorem (Gontier, K, Séré 2022)

For any $L = 2N$, with N an integer and $N \geq 2$, there exists a critical temperature $\theta_c^{(L)} := \theta_c^{(L)}(\mu) \geq 0$ such that:

- *for $\theta \geq \theta_c^{(L)}$, the minimizer of $\mathcal{F}_\theta^{(L)}$ is unique and 1-periodic;*
- *for $\theta \in (0, \theta_c^{(L)})$ (this set is empty if $\theta_c^{(L)} = 0$), there are exactly two minimizers, which are 2-periodic, of the form $t_i = W \pm (-1)^i\delta$, with $\delta \geq 0$.*

In addition,

1. *If $L \equiv 0 \mod 4$, this critical temperature is positive ($\theta_c^{(L)}(\mu) > 0$ for all $\mu > 0$).*
2. *If $L \equiv 2 \mod 4$, there is $\mu_c := \mu_c(L) > 0$ such that for $\mu \leq \mu_c$, $\theta_c^{(L)}$ is positive ($\theta_c^{(L)} > 0$), whereas for $\mu > \mu_c$, $\theta_c^{(L)} = 0$. Moreover as a function of L we have $\mu_c(L) \sim \frac{2}{\pi}\ln(L)$ at $+\infty$.*

By the above general lower

$$\inf_{\mathbf{t}} \mathcal{G}_\theta^{(2N)}(\mathbf{t}) \geq \mathcal{F}_\theta^{(2N)}(\mathbf{t}_2) = \mathcal{G}_\theta^{(2N)}(\mathbf{t}_2) \geq \inf_{\mathbf{t}} \mathcal{G}_\theta^{(2N)}(\mathbf{t})$$

Then as in the null temperature case, the minimizers are always 2-periodic

First Result

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Then as in the null temperature case, the minimizers are always 2-periodic.

The minimization problem is reduced to a minimization over the two variables W and δ. Actually, we have

$$F_\theta^{(2N)} = (2N) \min \left\{ g_\theta^{(2N)}(W, \delta), \quad W \geq 0,\ \delta \geq 0 \right\},$$

with the energy *per unit atom*

$$g_\theta^{(2N)}(W,\delta) = \frac{\mu}{2}\left[(W-1)^2 + \delta^2\right] - \frac{1}{2N}\sum_{k=1}^{2N} h_\theta\left(4W^2\cos^2\left(\frac{2k\pi}{2N}\right) + 4\delta^2\sin^2\left(\frac{2k\pi}{2N}\right)\right)$$

We recognize a Riemann sum in the last expression. We can take the thermodynamic limit free energy (per unit atom) as $L \to +\infty$, and we get

$$\boxed{f_\theta := \liminf_{N\to+\infty} \frac{1}{2N} F_\theta^{(2N)}}. \tag{7}$$

Lemma

We have $f_\theta = \min\{g_\theta(W,\delta), \quad W \geq 0,\ \delta \geq 0\}$ *with*

$$g_\theta(W,\delta) := \frac{\mu}{2}\left[(W-1)^2+\delta^2\right] - \frac{1}{2\pi}\int_0^{2\pi} h_\theta\left(4W^2\cos^2(s) + 4\delta^2\sin^2(s)\right) ds.$$

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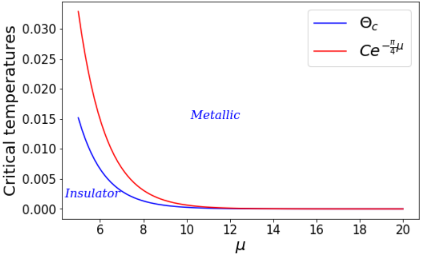
Second result

Theorem (Gontier, K, Séré 2022)

There is a critical (thermodynamic) temperature $\theta_c = \theta_c(\mu) > 0$, which is always positive, and so that for all $\theta \geq \theta_c$, the minimizer of g_θ satisfies $\delta = 0$, whereas for all $\theta < \theta_c$, it satisfies $\delta > 0$.
In the large μ limit, we have

$$\theta_c(\mu) \sim C \exp\left(-\frac{\pi}{4}\mu + o(1)\right), \quad \textit{with} \quad C \approx 1.6686.$$

Then in an infinite chain, there is a transition between the dimerized states ($\delta > 0$), which is insulating, to the 1-periodic state ($\delta = 0$), which is metallic.



Third result

Finally, we study the nature of the transition. It is not difficult to see that $\delta \to 0$ as $\theta \to \theta_c$. There is a bifurcation around this critical temperature,

Theorem (Gontier, K, Séré 2022)

There is $C > 0$, *such that* $\delta(\theta) = C\sqrt{(\theta_c - \theta)_+} + o\left(\sqrt{(\theta_c - \theta)_+}\right)$.

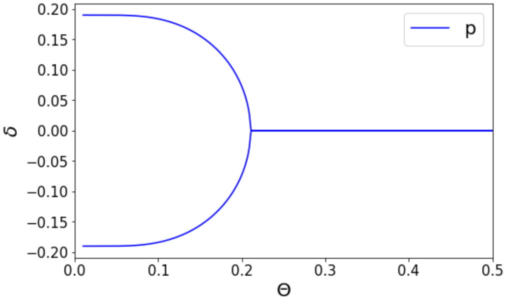


Figure: Phase profile of δ in thermodynamic limit case.

What to keep in mind ?

In presence of positive temperature θ:

- Existence of a nonnegative critical temperature for all L such that,the closed even polyacetylene chain behaves like metal above and insulator below.
- For $L = 0 \mod 4$, and thermodynamic limit cases, uniqueness and positivity while for $L = 2 \mod 4$, there is a critical value of μ noted $\mu_c(L)$ which behaves like $\frac{2}{\pi}\ln(L)$ at $+\infty$, such for all $\mu > \mu_c$, there is no phase transition.
- In thermodynamic limit case, for $\mu > 0$ large enough $\theta_c \sim Ce^{-\frac{\pi}{4}\mu}$,
- Bifurcation study gives behaviour of the phase profile below θ_c.

Thank you...