

Landau-Pekar equations and quantum fluctuations for the dynamics of a strongly coupled polaron

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Joint work with David Mitrouskas, Simone Rademacher, Benjamin Schlein
and Robert Seiringer

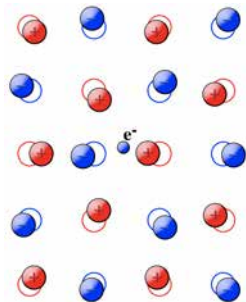
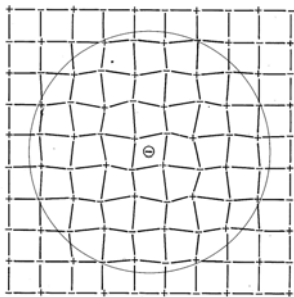
SwissMAP General Meeting
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Outline of the talk

- ▶ Fröhlich Polaron model
- ▶ Landau-Pekar equations
- ▶ Main results
- ▶ Sketch of the proof

The Polaron

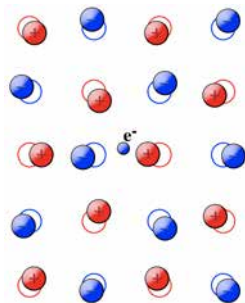
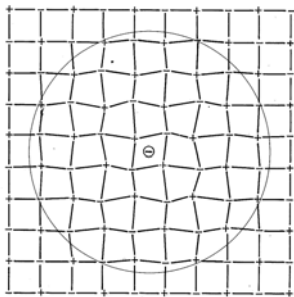
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Figures: Madelung Festkörpertheorie II, Wikipedia

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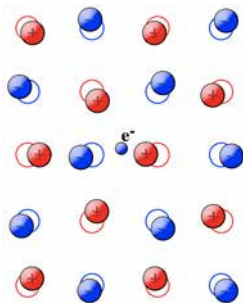
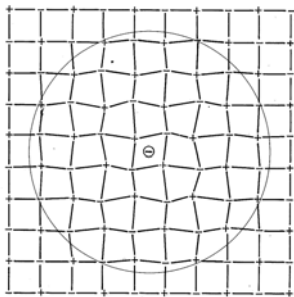


Figures: Madelung Festkörpertheorie II, Wikipedia

► 1937: The Fröhlich Model,

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- ▶ 1937: The Fröhlich Model,
- ▶ 1948: The Landau-Pekar equations.

The Fröhlich Model

$$i\partial_t \Psi_t = H \Psi_t,$$

$$H = -\Delta + \sqrt{\alpha} \int d^3k \left(G_x(k) a_k^* + \overline{G_x(k)} a_k \right) + \int d^3k a_k^* a_k,$$

$$[a_k, a_l^*] = \delta(k - l) \quad \text{and} \quad [a_k, a_l] = [a_k^*, a_l^*] = 0.$$

Remarks:

- ▶ $\mathcal{H} = L^2(\mathbb{R}^3) \otimes \left[\bigoplus_{n \geq 0} L^2(\mathbb{R}^3)^{\otimes n} \right]$
- ▶ $G_x(k) = |k|^{-1} e^{-ik \cdot x} \notin L^2(\mathbb{R}^3)$ but e^{-iHt} can be defined via the associated quadratic form,

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- ▶ **strong coupling units:** $x \rightarrow \alpha^{-1}x$, $\alpha_k \rightarrow \alpha^{-1/2} a_{\alpha^{-1}k}$, $t \rightarrow \alpha^2 t$
- ▶ classical behavior of the phonon field for large α .

Pekar product states

Weyl operator: $W(\varphi) = e^{a^*(\varphi) - a(\varphi)}$

$$W^*(\varphi)a_k W(\varphi) = a_k + \alpha^{-2}\varphi(k) \quad \text{and} \quad W^*(\varphi)a_k^* W(\varphi) = a_k^* + \alpha^{-2}\overline{\varphi(k)}.$$

Pekar product state: For $\Psi = \psi \otimes W(\alpha^2\varphi)\Omega$ we have

$$a_k\Psi = \varphi(k)\Psi \quad \text{and} \quad a_k^*\Psi = (\overline{\varphi(k)} + \mathcal{O}(\alpha^{-1}))\Psi.$$

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Ground state energy:

$$\begin{aligned} \langle \Psi, H \Psi \rangle &= \int d^3x |\nabla \psi(x)|^2 + 2\text{Re} \int d^3k |k|^{-1} \langle \psi, e^{ik \cdot x} \psi \rangle \varphi(k) + \|\varphi\|_2^2 \\ &=: \mathcal{E}(\psi, \varphi). \end{aligned}$$

Rigorous results:

$$\inf \sigma(H) = \inf_{\psi, \varphi \in L^2(\mathbb{R}^3): \|\psi\|_2=1} \mathcal{E}(\psi, \varphi) + c\alpha^{-2} + o(\alpha^{-2}).$$

[Donsker, Varadhan '83], [Lieb, Thomas '97], [Frank, Seiringer '19].

The Landau-Pekar equations

Let $(\psi_t, \varphi_t) \in H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$ satisfy

$$\begin{cases} i\partial_t \psi_t(x) &= h_{\varphi_t} \psi_t(x) \\ i\alpha^2 \partial_t \varphi_t(k) &= \varphi_t(k) + \sigma_{\psi_t} \end{cases} \quad (\text{LP})$$

with $(\psi_0, \varphi_0) \in H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$. Here, $h_\varphi = -\Delta + V_\varphi$ and

$$V_\varphi = 2\text{Re} \int d^3k |k|^{-1} e^{ik \cdot x} \varphi(k), \quad \sigma_\psi(k) = (2\pi)^{3/2} |k|^{-1} \widehat{|\psi|^2}(k).$$

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- ▶ nonlinear equations,
- ▶ well-posedness was shown by [Frank, Gang '15],
- ▶ large $\alpha \Rightarrow$ separation of scales.

Main results

$$\text{Goal: } e^{iHt}\psi_0 \otimes W(\alpha^2\varphi_0)\Omega \approx \psi_t \otimes W(\alpha^2\varphi_t)\Omega$$

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Let (ψ_t, φ_t) be the solution of (LP) with initial value $(\psi_{\varphi_0}, \varphi_0)$.

[L., Mitrouskas, Rademacher, Schlein, Seiringer (2020)]: Let $\Psi_0 = \psi_{\varphi_0} \otimes W(\alpha^2\varphi_0)\Omega$, $\gamma_t^{\text{el}} = \text{Tr}_{\mathcal{F}} |e^{-iHt}\Psi_0\rangle\langle e^{-iHt}\Psi_0|$ and $\gamma_t^{\text{ph}}(k, l) = \langle e^{-iHt}\Psi_0, a_l^* a_k e^{-iHt}\Psi_0 \rangle_{\mathcal{H}}$. Then, there exist $C, T > 0$ such that for all $|t| \leq T\alpha^2$

$$\left\| \gamma_t^{\text{el}} - |\psi_t\rangle\langle\psi_t| \right\|_{\text{tr}} \leq C\alpha^{-1} \quad \text{and} \quad \left\| \gamma_t^{\text{ph}} - |\varphi_t\rangle\langle\varphi_t| \right\|_{\text{tr}} \leq C(\alpha^{-1/4} + \alpha^{-2}).$$

Main results

Let $\varphi_0 \in L^2(\mathbb{R}^3)$ such that $e(\varphi_0) < 0$, ψ_{φ_0} be the ground state of h_{φ_0} and (ψ_t, φ_t) be the solution of (LP) with initial value $(\psi_{\varphi_0}, \varphi_0)$.

Bogoliubov dynamics: For $\Upsilon \in \mathcal{F}$ and $t \leq T\alpha^2$, we define

$$i\partial_t \Upsilon_t = (\mathcal{N} - \mathcal{A}_t) \Upsilon_t, \quad \Upsilon_0 = \Upsilon$$

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$$\left\| e^{-iHt} (\psi_{\varphi_0} \otimes W(\alpha^2 \varphi_0) \Upsilon) - e^{-i \int_0^t du \omega(u)} \psi_t \otimes W(\alpha^2 \varphi_t) \Upsilon_t \right\| \leq C\alpha^{-1}.$$

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Note: $\mathcal{A}_t = \langle \psi_{\varphi_t}, \phi(G.) R_{\varphi_t} \phi(G.) \psi_{\varphi_t} \rangle_{L^2(\mathbb{R}^3)}$ with $q_{\varphi_t} = 1 - |\psi_{\varphi_t}\rangle\langle\psi_{\varphi_t}|$ and $R_t = q_{\varphi_t} (h_{\varphi_t} - e(\varphi_t)) q_{\varphi_t}$.

Remarks:

For $\Upsilon_0 = \Omega$ and $\delta > 0$ sufficiently small $\exists C_\delta > 0$ s.t for $t = \delta\alpha^2$

$$\left\| e^{-iHt} (\psi_{\varphi_0} \otimes W(\alpha^2\varphi_0)\Omega) - e^{-i\int_0^t du \omega(u)} \psi_t \otimes W(\alpha^2\varphi_t)\Omega \right\| \geq C_\delta.$$

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Summary:

- ▶ The L.P.-equations approximate well the time evolution of the one-particle reduced density matrices.
- ▶ For a norm approximation quantum fluctuations has to be taken into account.
- ▶ Non-trivial variations of the phonon field happen over times of order α^2 .
- ▶ The condition that the initial electron wave function is a ground state of h_{φ_0} is crucial.

Comparison with the literature

$$\Psi_0 = \psi_0 \otimes W(\alpha^2 \varphi_0) \Omega, \quad i\partial \tilde{\psi}_t = h_{\varphi_0} \tilde{\psi}_t:$$

$$\left. \begin{array}{l} \text{[Frank, Schlein '13] :} \\ \text{[Frank, Gang '15] :} \end{array} \right\} \begin{array}{l} e^{-iHt} \Psi_0 \approx \tilde{\psi}_t \otimes W(\alpha^2 \varphi_0) \Omega \\ e^{-iHt} \Psi_0 \approx \psi_t \otimes W(\alpha^2 \varphi_t) \Omega \end{array} \quad \text{for } |t| \ll \alpha,$$

$\Psi_{\varphi^P} = \psi^P \otimes W(\alpha^2 \varphi^P) \Omega$ with (ψ^P, φ^P) minimizing the Pekar energy;

$\Psi_{\varphi_0} = \psi_{\varphi_0} \otimes W(\alpha^2 \varphi_0) \Omega$ with $(\psi_{\varphi_0}, \varphi_0)$ as in the previous theorem:

$$\left. \begin{array}{l} \text{[Griesemer '16] :} \\ \text{[L., R., S., S. '19] :} \end{array} \right\} \begin{array}{l} e^{-iHt} \Psi_{\varphi^P} \approx e^{-iE_P t} \Psi_{\varphi^P} \\ e^{-iHt} \Psi_{\varphi_0} \approx \psi_t \otimes W(\alpha^2 \varphi_t) \Omega \end{array} \quad \text{for } |t| \ll \alpha^2,$$

$$\text{[Mitrouskas '20] :} \quad e^{-iHt} \Psi_{\varphi^P} \approx e^{-i\tilde{H}t} \Psi_{\varphi^P} \quad \text{for } |t| \sim \alpha^2,$$

$$\text{[L., M., R., S., S. '20] :} \quad e^{-iHt} \Psi_{\varphi_0} \approx \psi_t \otimes W(\alpha^2 \varphi_t) \Upsilon_t \quad \text{for } |t| \leq T\alpha^2.$$

Sketch of the proof

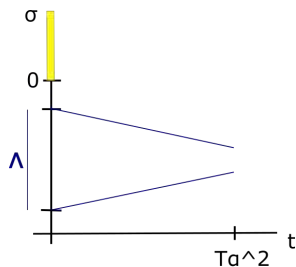
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- ▶ Existence of a spectral gap,
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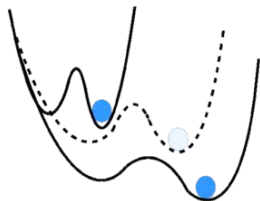


$$h_{\varphi_t} = h_{\varphi_0} - \alpha^{-2} \int_0^t ds V_{i\varphi_s}.$$

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$$\left\| \psi_t - e^{-i \int_0^t du e(\varphi_u)} \psi_{\varphi_t} \right\|_2^2 \leq C \alpha^{-4} (1 + \alpha^{-4} |t|^2) \quad \text{for all } |t| \leq T \alpha^2.$$

Figure: <https://medium.com>

Sketch of the proof

$$\begin{aligned} & \left\| e^{-iHt} (\psi_{\varphi_0} \otimes W(\alpha^2 \varphi_0) \Upsilon) - e^{-i \int_0^t ds \omega(s)} \psi_t \otimes W(\alpha^2 \varphi_t) \Upsilon_t \right\| \\ & \leq C\alpha^{-2} + \left\| e^{-iHt} (\psi_{\varphi_0} \otimes W(\alpha^2 \varphi_0) \Upsilon) - e^{-i \int_0^t ds \omega(s) + e(\varphi_s)} \psi_{\varphi_t} \otimes W(\alpha^2 \varphi_t) \Upsilon_t \right\| \\ & \leq C\alpha^{-2} + \|\xi_t - \psi_{\varphi_t} \otimes \Upsilon_t\|, \quad \text{where} \end{aligned}$$

$$\xi_t = e^{i \int_0^t ds \omega(s) + e(\varphi_s)} W^*(\alpha^2 \varphi_t) e^{-iHt} (\psi_{\varphi_0} \otimes W(\alpha^2 \varphi_0) \Upsilon)$$

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- ▶ $q_{\varphi_s} i\partial_s \xi_s = q_{\varphi_s} (h_{\varphi_s} - e(\varphi_s) + \phi(\delta_s G_x) + \mathcal{N}) \xi_s \sim 1 + \alpha^{-1} + \alpha^{-2}$

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 & \leq C \alpha^{-2} + \|\xi_t - \psi_{\varphi_t} \otimes \Upsilon_t\|, \quad \text{where}
 \end{aligned}$$

$$\xi_t = e^{i \int_0^t ds \omega(s) + e(\varphi_s)} W^*(\alpha^2 \varphi_t) e^{-iHt} (\psi_{\varphi_0} \otimes W(\alpha^2 \varphi_0) \Upsilon)$$

Duhamel's formula: $\|\xi_t - \psi_{\varphi_t} \otimes \Upsilon_t\|^2 = -2\text{Re} \int_0^t ds \frac{d}{ds} \langle \xi_s, \psi_{\varphi_s} \otimes \Upsilon_s \rangle.$

- ▶ $i\partial_s \xi_s = (h_{\varphi_s} - e(\varphi_s) + \underbrace{\phi(G_x) - \langle \psi_s, \phi(G_x) \psi_s \rangle}_{\phi(\delta_s G_x)} + \mathcal{N}) \xi_s$
- ▶ $q_{\varphi_s} i\partial_s \xi_s = q_{\varphi_s} (h_{\varphi_s} - e(\varphi_s) + \phi(\delta_s G_x) + \mathcal{N}) \xi_s \sim 1 + \alpha^{-1} + \alpha^{-2}$
- ▶ The time derivatives of all other quantities are of order α^{-2} .
- ▶ $q_{\varphi_s} \xi_s = R_s (i\partial_s - \phi(\delta_s G_x) - \mathcal{N}) \xi_s$ with $R_s = q_{\varphi_s} (h_{\varphi_s} - e(\varphi_s))^{-1} q_{\varphi_s}$.

Related results

Adiabatic theorem:

[Frank '17], [Frank, Gang '19].

Classical limit of quantum fields:

[Davies '79], [Ginibre, Velo '79] [Hiroshima '98], [Teufel '02],
[Ginibre, Nironi, Velo '06], [Falconi '12], [Ammari, Falconi '16], [L., Pickl '16],
[Correggi, Falconi '17], [Correggi, Falconi, Olivieri '18], [L., Pickl '18], [L., Petrat
'18], [Carlone, Correggi, Falconi, Olivieri '19], [L., Mitrouskas, Seiringer '20].

Effective mass ($m \sim \alpha^4$):

[Landau, Pekar '48], [Feynman '54], [Lieb, Seiringer '14], [Lieb, Seiringer '19],
[Dybalski, Spohn '19].

Thank you for your attention!

Simple example

Let $f \in C^1(\mathbb{R}, \mathbb{R})$, $c, d, e \in \mathbb{R}$ with $c > 0$ and $\omega = c + \alpha^{-1}d + \alpha^{-2}e$.

$$\begin{aligned} & \int_0^t ds f(\alpha^{-2}s) e^{-i\omega s} \\ &= c^{-1} \int_0^t ds f(\alpha^{-2}s) \left(i \frac{d}{ds} - \alpha^{-1}d - \alpha^{-2}e \right) e^{-i\omega s} \\ &= \text{b.t.} + \mathcal{O}(\alpha^{-2}t) - \alpha^{-1}c^{-1}d \int_0^t ds f(\alpha^{-2}s) e^{-i\omega s} \\ &= \text{b.t.} + \mathcal{O}(\alpha^{-2}t) - \alpha^{-1}c^{-2}d \int_0^t ds f(\alpha^{-2}s) \left(i \frac{d}{ds} - \alpha^{-1}d - \alpha^{-2}e \right) e^{-i\omega s} \\ &= \text{b.t.} + \mathcal{O}(\alpha^{-2}t). \end{aligned}$$