Derivation of an effective evolution equation for a strongly coupled polaron

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Talk based on:

R.L.F., B. Schlein: Dynamics of a strongly coupled polaron.


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The Polaron Model

Introduced by Fröhlich in 1937, as a model of an electron interacting with the quantized optical modes of a polar crystal. It is described by the Hamiltonian

\[ H = -\Delta + \sqrt{\alpha} \int_{\mathbb{R}^3} \frac{dk}{|k|} \left( e^{-ik \cdot x} a(k) + e^{ik \cdot x} a^\dagger(k) \right) + \int_{\mathbb{R}^3} dk \: a^\dagger(k) a(k) \]

acting on \( L^2(\mathbb{R}^3) \otimes \mathcal{F} \), with \( \mathcal{F} \) the bosonic Fock space on \( \mathbb{R}^3 \).

Although \( |k|^{-1} e^{ik \cdot x} \notin L^2_k(\mathbb{R}^3) \), \( H \) can be defined as self-adjoint, lower bounded operator.

We are interested in the large coupling (semi-classical) limit \( \alpha \to \infty \).

Classical Hamiltonian on phase space \( H^1(\mathbb{R}^3, \mathbb{C}) \oplus L^2(\mathbb{R}^3, \mathbb{C}) \),

\[ \mathcal{H}(\psi, \phi) = \int_{\mathbb{R}^3} dx \: |\nabla \psi(x)|^2 + \sqrt{\alpha} \int_{\mathbb{R}^3 \times \mathbb{R}^3} dx \: dk \: \frac{|\psi(x)|^2}{|k|} \left( e^{-ik \cdot x} \phi(k) + e^{ik \cdot x} \overline{\phi(k)} \right) + \int_{\mathbb{R}^3} dk \: |\phi(k)|^2 \]

**Question:** Can one quantify the relation between \( H \) and \( \mathcal{H} \) as \( \alpha \to \infty \)?

Result about ground state energy (Donsker–Varadhan, 1983, Lieb–Thomas, 1997):

\[ \inf \text{spec} H \sim \inf_{\|\psi\|=1, \phi} \mathcal{H}(\psi, \phi) \quad \text{as} \quad \alpha \to \infty. \]
DYNAMICS

\[ H = -\Delta + \sqrt{\alpha} \int_{\mathbb{R}^3} \frac{dk}{|k|} \left( e^{-ik \cdot x} a(k) + e^{ik \cdot x} a^\dagger(k) \right) + \int_{\mathbb{R}^3} dk \, a^\dagger(k) a(k) \]

\[ \mathcal{H}(\psi, \phi) = \int_{\mathbb{R}^3} dx \, |\nabla \psi(x)|^2 + \sqrt{\alpha} \int_{\mathbb{R}^3} dx dk \, \frac{|\psi(x)|^2}{|k|} \left( e^{-ik \cdot x} \phi(k) + e^{ik \cdot x} \bar{\phi}(k) \right) + \int_{\mathbb{R}^3} dk \, |\phi(k)|^2 \]

Today: Compare dynamics generated by \( H \) and by \( \mathcal{H} \).

\[ i\partial_t \Psi_t = H \Psi_t \]

Landau–Pekar equations (1948) (phenomenologically derived)

\[ i\partial_t \psi_t = \left( -\Delta + \sqrt{\alpha} \int_{\mathbb{R}^3} \frac{dk}{|k|} \left( e^{ik \cdot x} \phi_t(k) + e^{-ik \cdot x} \bar{\phi}_t(k) \right) \right) \psi_t \]

\[ i\partial_t \phi_t = \phi_t + \frac{\sqrt{\alpha}}{|k|} \int_{\mathbb{R}^3} dx \, e^{ik \cdot x} |\psi_t(x)|^2 \]

Equivalent form of LP equations, usually in physics literature:

\[ i\partial_t \psi_t = \left( -\Delta + \sqrt{\alpha} |x|^{-1} * P_t \right) \psi_t , \quad \partial_t^2 P_t = -P_t - \sqrt{\alpha}(2\pi)^2 |\psi_t|^2 . \]

(Write \( P + iQ = (2\pi)^{-1} \int e^{-ik \cdot x} |k| \phi_t(k) \), so \( \partial_t P_t = Q_t \), \( \partial_t Q_t = -P_t - \sqrt{\alpha}(2\pi)^2 |\psi_t|^2 \).)

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# 3
Rescaling

How to choose initial conditions and time scale?
Rescale $x \mapsto \alpha^{-1} x$, $k \mapsto \alpha k$ and $a_k \mapsto \sqrt{\alpha} a_{\alpha k} =: b_k$, then $H \mapsto \alpha^2 \tilde{H}$ with

$$
\tilde{H} = -\Delta + \int_{\mathbb{R}^3} \frac{dk}{|k|} \left( e^{-ik \cdot x} b(k) + e^{ik \cdot x} b^\dagger(k) \right) + \int_{\mathbb{R}^3} dk \ b^\dagger(k) b(k)
$$

where $[b(k), b^\dagger(k')] = \alpha^{-2} \delta(k - k')$, $[b(k), b(k')] = 0$, $[b^\dagger(k), b^\dagger(k')] = 0$.

We are dealing with a partially classical limit. (Ginibre, Nironi, Velo, 2006)
Consider coherent states $W(f)\Omega$ defined with Weyl operator $W(f) = e^{b^\dagger(f) - b(f)}$.

$$
\langle \psi \otimes W(\alpha^2 \phi)\Omega | \tilde{H} | \psi \otimes W(\alpha^2 \phi)\Omega \rangle = \tilde{H}(\psi, \phi),
$$

$$
\tilde{H}(\psi, \phi) = \int_{\mathbb{R}^3} dx \ |\nabla \psi(x)|^2 + \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{dx \, dk \ |\psi(x)|^2}{|k|} \left( e^{-ik \cdot x} \phi(k) + e^{ik \cdot x} \phi(k) \right) + \int_{\mathbb{R}^3} dk \ |\phi(k)|^2
$$

This yields immediately the upper bound $\inf \text{spec} \tilde{H} \leq \inf \tilde{H}$ on ground state energy.

**Advantage:** For ground state problem, all quantities are now order one.
How to choose initial conditions and time scale?

\[ \tilde{H} = -\Delta + \int_{\mathbb{R}^3} \frac{dk}{|k|} \left( e^{-ik \cdot x} b(k) + e^{ik \cdot x} b^\dagger(k) \right) + \int_{\mathbb{R}^3} dk \, b^\dagger(k) b(k) \]

where \([b(k), b^\dagger(k')] = \alpha^{-2} \delta(k - k'), \quad [b(k), b(k')] = 0, \quad [b^\dagger(k), b^\dagger(k')] = 0.\]

This motivates to choose initial conditions of the form \(\psi \otimes W(\alpha^2 \phi) \Omega\) and to consider time scales \(\alpha^{-2}\) for \(H\) (so times of order one for \(\tilde{H}\)).

Disadvantage: After rescaling (of \(x, k, a\) and \(t\)) the LP equations become

\[ i\partial_t \psi_t = \left( -\Delta + \int_{\mathbb{R}^3} \frac{dk}{|k|} \left( e^{ik \cdot x} \phi_t(k) + e^{-ik \cdot x} \phi_t(k) \right) \right) \psi_t \]

\[ i\alpha^2 \partial_t \phi_t = \phi_t + \frac{1}{|k|} \int_{\mathbb{R}^3} dx \, e^{ik \cdot x} |\psi_t(x)|^2 \]

So there are two different time scales for the particle and the field.
**AN INITIAL RESULT**

**Theorem 1** (F., Schlein, 2014 + careful referee). If \( \psi_0 \in H^1(\mathbb{R}^3) \), \( \phi_0 \in L^2(\mathbb{R}^3) \), then

\[
\left\| e^{-it\tilde{H}} \psi_0 \otimes W(\alpha^2 \phi_0) \Omega - e^{-it\| \phi_0 \|^2} e^{-ith\phi_0} \psi_0 \otimes W(\alpha^2 \phi_0) \Omega \right\|
\leq C \min \left\{ \left( e^{C|t|/\alpha} - 1 \right)^{1/2}, \alpha^{-1} \left( e^{C|t|} - 1 \right)^{1/2} \right\}
\]

with

\[
h_\phi = -\Delta + \int_{\mathbb{R}^3} \frac{dk}{|k|} \left( e^{-ik \cdot x} \phi(k) + e^{ik \cdot x} \overline{\phi(k)} \right) \quad \text{in} \; L^2(\mathbb{R}^3).
\]

**Remarks.** (1) Non-trivial since \( \psi \) moves; disappointing since \( \phi \) does not move. But not surprising in view of rescaled LP equations.
(2) Proof would be straightforward if \( |k|^{-1} \) was in \( L^2 \), but it is not.
(3) **Where to go from here?** Either longer time scales or more precise asymptotics on same time scale. We choose second possibility, but first possibility would also be interesting.
**Main result. EZ Version**

**Theorem 2** (F., Gang, 2015). If $\psi_0 \in H^4(\mathbb{R}^3)$, $\phi_0 \in L^2(\mathbb{R}^3, (1 + k^2)^3 \, dk)$, then for all $\alpha \geq 1$ and $|t| \leq \alpha$,

$$
\text{tr}_{L^2(\mathbb{R}^3)} \left| \gamma_t^{\text{particle}} - |\psi_t\rangle \langle \psi_t| \right| \leq C \alpha^{-2}(1 + t^2),
$$

$$
\text{tr}_\mathcal{F} \left| \gamma_t^{\text{field}} - \left| W(\alpha^2 \phi_t)\Omega \right\rangle \langle W(\alpha^2 \phi_t)\Omega \right| \leq C \alpha^{-2}(1 + t^2).
$$

where

$$
\gamma_t^{\text{particle}} := \text{tr}_\mathcal{F} \left| e^{-i\tilde{H}t} \psi_0 \otimes W(\alpha^2 \phi_0)\Omega \right\rangle \langle e^{-i\tilde{H}t} \psi_0 \otimes W(\alpha^2 \phi_0)\Omega \right|, \quad \gamma_t^{\text{field}} := \text{tr}_{L^2(\mathbb{R}^3)} ... 
$$

Here $(\psi_t, \phi_t)$ satisfy the (rescaled) **LP equations** with initial conditions $(\psi_0, \phi_0)$.

**Remarks.** (1) **Better** approximation at the expense of **more regularity** of initial data and approximation only for **reduced density matrices**.

(2) Crucial that $\phi_t$ does move, see next slide.

(3) Maximal times $o(\alpha)$ are natural for our proof, but unclear whether also for the problem.

(4)Technical difficulties due to $|k|^{-1} \not\in L^2(\mathbb{R}^3)$ become even more severe as one moves away from energy space.
Our main result says, in particular, that
\[
\text{tr}_\mathcal{F} |\gamma_t^\text{field} - |W(\alpha^2 \phi_t)\Omega\rangle\langle W(\alpha^2 \phi_t)\Omega| | \leq C\alpha^{-2}(1 + t^2).
\]

This would not be true if \(\phi_0\) would not move:

**Lemma 3.** If \(\psi_0 \in H^4(\mathbb{R}^3), \phi_0 \in L^2(\mathbb{R}^3, (1 + k^2)^3 dk)\) such that
\[
\phi_0(k) + \frac{1}{|k|} \int_{\mathbb{R}^3} dx e^{ik \cdot x} |\psi_0(x)|^2 \neq 0.
\]

Then there are \(\epsilon > 0, C > 0\) and \(c > 0\) such that for all \(|t| \in [C\alpha^{-1}, \epsilon]\) and \(\alpha \geq C/\epsilon\),
\[
\text{tr}_\mathcal{F} |\gamma_t^\text{field} - |W(\alpha^2 \phi_0)\Omega\rangle\langle W(\alpha^2 \phi_0)\Omega| | \geq c\alpha^{-1}|t|.
\]
**Main result. Full version**

**Theorem 4** (F., Gang, 2015). If $\psi_0 \in H^4(\mathbb{R}^3)$, $\phi_0 \in L^2(\mathbb{R}^3, (1 + k^2)^3 \, dk)$, then for all $\alpha \geq 1$ and $|t| \leq \alpha$,

$$\left\| e^{-it\tilde{H}} \psi_0 \otimes W(\alpha^2 \phi_0) \Omega - e^{-i\int_0^t ds \, \omega(s) \psi_t \otimes W(\alpha^2 \phi_t) \Omega - R(t)} \right\| \leq C\alpha^{-2} |t|(1 + |t|),$$

where $(\psi_t, \phi_t)$ satisfy the (rescaled) **LP equations** with initial conditions $(\psi_0, \phi_0)$, 

$$\omega(s) = \alpha^2 \text{Im}(\phi_s, \partial_s \phi_s) + \|\phi_s\|^2$$

and

$$R(t) = -iW(\alpha^2 \phi_t) \int_0^t \left[ e^{-i\phi_t(t-s) - i\int_s^0 \omega(s_1) \, ds_1} \right] ds$$

Moreover,

$$\left\| \langle \Omega, W^* (\alpha^2 \phi_t) R(t) \rangle \right\|_{L^2(\mathbb{R}^3)} \leq C\alpha^{-2} t^2,$$

and

$$\left\| R(t) \right\|_{L^2(\mathbb{R}^3)} \leq C\alpha^{-1} (1 + |t|).$$
Remarks on main result

\[ \left\| e^{-it\hat{H}}\psi_0 \otimes W(\alpha^2\phi_0)\Omega - e^{-i\int_0^t ds \omega(s)}\psi_t \otimes W(\alpha^2\phi_t)\Omega - R(t) \right\| \leq C\alpha^{-2}|t|(1 + |t|), \]

**Message:** An approximation to \( O(\alpha^{-2}) \) (for times of order one) is **not** possible by **product states**. One needs to include **correlations** which are of order \( \alpha^{-1} \). However, due to orthogonality conditions, they **do not contribute** to the reduced density matrices.

Full version of main result implies simplified version due to the following **abstract lemma**.

**Lemma 5.** Let \( \Psi, \Phi \in \mathcal{H}_1 \otimes \mathcal{H}_2 \) and \( f \in \mathcal{H}_1 \) and \( g \in \mathcal{H}_2 \) such that

\[ \Psi = f \otimes g + \Phi \]

and, for some \( C > 0 \) and \( \epsilon > 0 \),

\[ \|f\|_{\mathcal{H}_1} \leq C, \quad \|g\|_{\mathcal{H}_2} \leq C, \quad \|\Phi\|_{\mathcal{H}_1 \otimes \mathcal{H}_2} \leq C\epsilon, \quad \|\langle g, \Phi\rangle_{\mathcal{H}_2}\|_{\mathcal{H}_1} \leq C\epsilon^2, \quad \|\langle f, \Phi\rangle_{\mathcal{H}_1}\|_{\mathcal{H}_2} \leq C\epsilon^2. \]

Then \( \gamma_1 = \text{tr}_{\mathcal{H}_2} |\Psi\rangle\langle \Psi| \) and \( \gamma_2 = \text{tr}_{\mathcal{H}_1} |\Psi\rangle\langle \Psi| \) satisfy

\[ \text{tr}_{\mathcal{H}_1} |\gamma_1 - \|g\|_{\mathcal{H}_2}^2 |f\rangle\langle f|\| \leq 3C^2\epsilon^2, \quad \text{tr}_{\mathcal{H}_2} |\gamma_2 - \|f\|_{\mathcal{H}_1}^2 |g\rangle\langle g|\| \leq 3C^2\epsilon^2. \]
Ingredients in the proof

- **Second-order Duhamel expansion.** Each term in the expansion has at least one $b$ or $b^\dagger$, which is of size $\alpha^{-1}$ (when close to $\Omega$). There are time integrals of length $t$, which leads to the restriction $|t| = o(\alpha)$.

- The statement ‘$b$ or $b^\dagger$ is of size $\alpha^{-1}$’ would be correct if $|k|^{-1}$ was in $L^2(\mathbb{R}^3)$. It is not and this leads to significant technical difficulties, in particular, in the second order Duhamel terms, since the operator domain of $\tilde{H}$ is not explicit. Moreover, it is not clear whether the Lieb–Yamazaki-technique works even for first order terms.

- **Study of the LP equations.** $H^4 \oplus L^2((1+k^2)^3)$-regularity is preserved up to $O(\alpha^2)$. 
THANK YOU FOR YOUR ATTENTION!