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. Lett. Math. Phys. 104 (2014), no. 8, 911 - 929.*
R.L.F., **Z. Gang***: Derivation of an effective evolution equation for a strongly coupled polaron. Preprint:* `arXiv:1505.03059`

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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 $H^1(\mathbb{R}^3, \mathbb{C}) \oplus L^2(\mathbb{R}^3, \mathbb{C})$,

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

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**):

$$\inf \operatorname{spec} H \sim \inf_{\|\psi\|=1,\, \phi} \mathcal{H}(\psi, \phi) \qquad \text{as } \alpha \to \infty\,.$$

Dynamics

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

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

Today: Compare **dynamics** generated by H and by $\mathcal{H}$.

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

Landau–Pekar equations (1948) (phenomenologically derived)

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

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

Equivalent form of LP equations, usually in physics literature:

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

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

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

We are dealing with a **partially classical limit**. (**Ginibre, Nironi, Velo, 2006**)

Consider **coherent states** $W(f)\Omega$ defined with **Weyl operator** $W(f) = e^{b^\dagger(f) - b(f)}$.

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

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

This yields immediately the **upper bound** $\inf \mathrm{spec} \tilde{H} \le \inf \tilde{\mathcal{H}}$ on ground state energy.

Advantage: For ground state problem, all quantities are now order one.

Rescaling, cont'd

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

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

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

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

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

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

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

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

Remarks. (1) Non-trivial since ψ **moves**; disappointing since ϕ 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* $|t| \leq \alpha$,

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

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

where

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

Here (ψ_t, ϕ_t) *satisfy the (rescaled)* **LP equations** *with initial conditions* (ψ_0, ϕ_0).

Remarks. (1) **Better** approximation at the expense of **more regularity** of initial data and approximation only for **reduced density matrices**.
(2) Crucial that ϕ_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 $|k|^{-1} \notin L^2(\mathbb{R}^3)$ become even more severe as one moves away from energy space.

And yet it moves...

Our main result says, in particular, that

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

This would not be true if ϕ_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*

$$\phi_0(k) + \frac{1}{|k|} \int_{\mathbb{R}^3} dx e^{ik\cdot x} |\psi_0(x)|^2 \not\equiv 0\,.$$

Then there are $\epsilon > 0$, $C > 0$ and $c > 0$ such that for all $|t| \in [C\alpha^{-1}, \epsilon]$ and $\alpha \geq C/\epsilon$,

$$\operatorname{tr}_{\mathcal{F}} \left| \gamma_t^{\text{field}} - |W(\alpha^2 \phi_0)\Omega\rangle\langle W(\alpha^2\phi_0)\Omega| \right| \geq c\alpha^{-1}|t|\,.$$

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 (ψ_t, ϕ_t) *satisfy the (rescaled)* **LP equations** *with initial conditions* (ψ_0, ϕ_0), $\omega(s) = \alpha^2\,\mathrm{Im}(\phi_s, \partial_s\phi_s) + \|\phi_s\|^2$ *and*

$$R(t) = -\, iW(\alpha^2\phi_t) \int_0^t \Big[e^{-iH_{\phi_t}(t-s) - i\int_0^s \omega(s_1)\, ds_1} \times P_{\psi_s}^{\perp} \int_{\mathbb{R}^3} \Big(e^{ik\cdot x} W^\dagger(\alpha^2\phi_t) W(\alpha^2\phi_s) b_k^\dagger\ \psi_s \otimes \Omega \Big) \frac{dk}{|k|} \Big]\, ds\,.$$

Moreover,

$$\left\| \big\langle \Omega,\ W^*(\alpha^2\phi_t) R(t) \big\rangle_{\mathcal{F}} \right\|_{L^2(\mathbb{R}^3)} \leq C\alpha^{-2} t^2, \quad \left\| \big\langle \psi_t,\ W^*(\alpha^2\phi_t) R(t) \big\rangle_{L^2(\mathbb{R}^3)} \right\|_{\mathcal{F}} \leq C\alpha^{-2} t^2$$

and

$$\|R(t)\|_{L^2(\mathbb{R}^3)\otimes\mathcal{F}} \leq C\alpha^{-1}\,(1+|t|)\,.$$

Remarks on main result

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

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 α^{-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 $\epsilon > 0$,

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

Then $\gamma_1 = \mathrm{tr}_{\mathcal{H}_2} |\Psi\rangle\langle\Psi|$ and $\gamma_2 = \mathrm{tr}_{\mathcal{H}_1} |\Psi\rangle\langle\Psi|$ satisfy

$$\mathrm{tr}_{\mathcal{H}_1} \left|\gamma_1 - \|g\|^2_{\mathcal{H}_2} |f\rangle\langle f|\right| \leq 3C^2\epsilon^2\,, \quad \mathrm{tr}_{\mathcal{H}_2} \left|\gamma_2 - \|f\|^2_{\mathcal{H}_1} |g\rangle\langle g|\right| \leq 3C^2\epsilon^2\,.$$

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 α^{-1} (when close to Ω). There are time integrals of length t, which leads to the restriction $|t| = o(\alpha)$.

• The statement 'b or $b^\dagger$ is of size α^{-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!