Dynamics of a Strongly Coupled Polaron

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Fröhlich Hamiltonian: we consider

$$\widetilde{H}_\alpha = -\Delta \otimes 1 + 1 \otimes \int dk\, a_k^* a_k + \sqrt{\alpha} \int \frac{dk}{|k|} \left[e^{-ik\cdot x} \otimes a_k^* + e^{ik\cdot x} \otimes a_k \right]$$

acting on Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathcal{F}$.

Here

$$\mathcal{F} = \bigoplus_{n \geq 0} L^2(\mathbb{R}^3; dk)^{\otimes_s n}$$

is bosonic **Fock space**, with canonical commutation relations

$$\left[a_k, a_{k'}^* \right] = \delta(k - k'), \qquad \left[a_k, a_{k'} \right] = \left[a_k^*, a_{k'}^* \right] = 0$$

Remark: $\widetilde{H}_\alpha$ bounded below, because **[Lieb-Yamazaki, 58]**:

$$\pm \left[a(e^{-ik\cdot x} f) + a^*(e^{-ik\cdot x} f) \right] \leq -\delta \Delta + 4\delta^{-1} \left\| |.|^{-1} f \right\|_2^2 (\mathcal{N} + 1)$$

with number of phonon operator

$$\mathcal{N} = \int dk\, a_k^* a_k$$

Strong coupling units: introducing **new variables**

$$x \to \alpha x, \qquad k \to k/\alpha, \qquad a_k \to \sqrt{\alpha}\, a_{\alpha k},$$

we find $\widetilde{H}_\alpha = \alpha^2 H_\alpha$, with

$$\begin{aligned} H_\alpha &= -\Delta \otimes 1 + 1 \otimes \int dk\, a_k^* a_k + \int \frac{dk}{|k|} \left[e^{-ik\cdot x} \otimes a_k^* + e^{ik\cdot x} \otimes a_k \right] \\ &= -\Delta \otimes 1 + 1 \otimes \mathcal{N} + \phi(G_x) \end{aligned}$$

where we denote $G_x(k) = |k|^{-1} e^{-ik\cdot x}$ and

$$\phi(G_x) = a^*(G_x) + a(G_x) = \int dk \left[G_x(k) \otimes a_k^* + \overline{G_x(k)} \otimes a_k \right]$$

New creation and annihilation operators satisfy **rescaled CCR**

$$[a_k, a_{k'}^*] = \frac{1}{\alpha^2}\, \delta(k - k'), \qquad [a_k, a_{k'}] = [a_k^*, a_{k'}^*] = 0$$

Strong coupling limit $\alpha \to \infty$ is **classical limit** for phonon field.

Weyl operators: for $\varphi \in L^2(\mathbb{R}^3, dk)$, let

$$W(\varphi) = \exp(a^*(\varphi) - a(\varphi)) = \exp\left[\int dk\, (\varphi(k)a_k^* - \overline{\varphi}(k)a_k)\right]$$

Then

$$W^*(\varphi)a_k W(\varphi) = a_k + \alpha^{-2}\varphi(k), \qquad W^*(\varphi)a_k^* W(\varphi) = a_k^* + \alpha^{-2}\varphi(k)$$

Coherent states: let $\Omega = \{1, 0, 0, \ldots\}$ denote **vacuum** in $\mathcal{F}$.
For $\varphi \in L^2(\mathbb{R}^3)$, the coherent state

$$\begin{aligned} W(\alpha^2\varphi)\Omega &= \exp\left(\alpha^2 a^*(\varphi) - \alpha^2 a(\varphi)\right)\Omega \\ &= e^{-\alpha^2\|\varphi\|_2^2/2}\left\{1, \alpha^2\varphi, \ldots, \frac{(\alpha^2\varphi)^{\otimes j}}{\sqrt{j!}}, \ldots\right\} \end{aligned}$$

is **eigenvector** of all annihilation operators, with

$$a_k W(\alpha^2\varphi)\Omega = \varphi(k)W(\alpha^2\varphi)\Omega$$

Ground state energy: consider **product trial states**

$$\Psi = \psi \otimes W(\alpha^2 \varphi)\Omega$$

We find

$$\langle \Psi, H_\alpha \Psi \rangle = \int dx \, |\nabla \psi(x)|^2 + \int dk \, |\varphi(k)|^2 + \int \frac{dk}{|k|} \left[\langle \psi, e^{-ik\cdot x} \psi \rangle \varphi(k) + \langle \psi, e^{ik\cdot x} \psi \rangle \, \overline{\varphi}(k) \right]$$

Completing the square, we obtain

$$\langle \Psi, H_\alpha \Psi \rangle = \mathcal{E}_{\text{pekar}}(\psi) + \int dk \, \left| \varphi(k) + \frac{1}{|k|} \widehat{|\psi|^2}(k) \right|^2$$

with **Pekar functional**

$$\mathcal{E}_{\text{pekar}}(\psi) = \int |\nabla \psi(x)|^2 dx - \int dx dy \, \frac{|\psi(x)|^2 |\psi(y)|^2}{|x-y|}$$

[Donsker-Varadhan, 83] and **[Lieb-Thomas, 97]** showed that

$$\inf \sigma(H_\alpha) = \inf_{\psi \in L^2(\mathbb{R}^3) : \|\psi\|_2 = 1} \mathcal{E}_{\text{pekar}}(\psi) + o(1), \qquad \text{as } \alpha \to \infty$$

Dynamics: it is natural to ask whether

$$e^{-iH_\alpha t}\left[\psi \otimes W(\alpha^2\varphi)\Omega\right] \simeq \psi_t \otimes W(\alpha^2\varphi_t)\Omega \text{ ?}$$

We have

$$i\partial_t\left[\psi_t \otimes W(\alpha^2\varphi_t)\Omega\right] = (i\partial_t\psi_t)\otimes W(\alpha^2\varphi_t)\Omega + \psi_t \otimes W(\alpha^2\varphi_t)a^*(i\alpha^2\partial_t\varphi_t)\Omega$$

and

$$\begin{aligned}
&H_\alpha\left[\psi_t \otimes W(\alpha^2\varphi_t)\Omega\right] \\
&= (-\Delta\psi_t)\otimes W(\alpha^2\varphi_t)\Omega + \psi_t \otimes W(\alpha^2\varphi_t)a^*(\varphi_t)\Omega \\
&\qquad + 2\mathrm{Re}\int \frac{dk}{|k|}e^{-ik\cdot x}\varphi_t(k)\psi_t \otimes W(\alpha^2\varphi_t)\Omega + \int \frac{dk}{|k|}e^{-ik\cdot x}\psi_t \otimes W(\alpha^2\varphi_t)a_k^*\Omega
\end{aligned}$$

With

$$\int \frac{dk}{|k|}e^{-ik\cdot x}\psi_t \otimes W(\alpha^2\varphi_t)a_k^*\Omega \;\to\; \int \frac{dk}{|k|}\langle\psi_t, e^{-ik\cdot x}\psi_t\rangle\psi_t \otimes W(\alpha^2\varphi_t)a_k^*\Omega$$

we obtain **Landau-Pekar equations**

$$\begin{cases} i\partial_t\psi_t(x) & = \left[-\Delta + 2\,\mathrm{Re}\;\widehat{|.|^{-1}\varphi_t}(x)\right]\psi_t(x) \\ i\alpha^2\partial_t\varphi_t(k) & = \varphi_t(k) + |k|^{-1}\widehat{|\psi_t|^2}(k) \end{cases}$$

Some rigorous results:

[Frank-S., 14], **[Frank-Zhou, 17]**: convergence for $|t| \ll \alpha$, ie.

$$\left\| e^{-iH_\alpha t}(\psi \otimes W(\alpha^2\varphi)\Omega) - \psi_t \otimes W(\alpha^2\varphi_t)\Omega \right\| \leq C|t|/\alpha$$

[Griesemer, 17]: considered data $\psi_0 \otimes W(\alpha^2\varphi_0)\Omega$ with (ψ_0, φ_0) minimizing Pekar energy. He proved

$$\left\| e^{-iH_\alpha t}(\psi_0 \otimes W(\alpha^2\varphi_0)\Omega) - \psi_0 \otimes W(\alpha^2\varphi_0)\Omega \right\| \leq C|t|/\alpha^2$$

[Leopold-Rademacher-S.-Seiringer, 19]: let $\varphi \in L^2(\mathbb{R}^3, dk)$ such that

$$h_\varphi = -\Delta + 2\text{Re}\ \widehat{|.|^{-1}\varphi}$$

has ground state energy $e(\varphi) < 0$ with eigenvector ψ_φ. Then

$$\left\| e^{-iH_\alpha t}(\psi_\varphi \otimes W(\alpha^2\varphi)\Omega) - \psi_t \otimes W(\alpha^2\varphi_t)\Omega \right\| \leq C|t|/\alpha^2$$

where (ψ_t, φ_t) solves **Landau-Pekar** with initial data (ψ_φ, φ).

Adiabatic theorem: let $\varphi \in L^2(\mathbb{R}^3, dk)$ so that $e(\varphi) < 0$. Let (ψ_t, φ_t) be solution of Landau-Pekar with data (ψ_φ, φ). Then **[Leopold-Rademacher-S.-Seiringer, 19]**

$$\|\psi_t - \psi_{\varphi_t}\|_2 \leq C\alpha^{-2}$$

for all $|t| \leq C\alpha^2$.

An adiabatic theorem for one-dimensional version of Landau-Pekar was also proved by **[Frank-Zhou, 19]**.

Bogoliubov dynamics: consider evolution $\mathcal{S}(t;s)$ defined by

$$i\partial_t \mathcal{S}(t;s) = (\mathcal{N} - \mathcal{A}_t)\mathcal{S}(t;s), \qquad \text{with } \mathcal{S}(s;s) = 1$$

and

$$\begin{aligned} \mathcal{A}_t &= \langle \psi_{\varphi_t}, \phi(G_x) R_t \phi(G_x) \psi_{\varphi_t} \rangle_{L^2(\mathbb{R}^3)} \\ &= \int \frac{dk}{|k|} \frac{dk'}{|k'|} \langle \psi_{\varphi_t}, e^{-ik\cdot x} R_t e^{ik'\cdot x} \psi_{\varphi_t} \rangle_{L^2(\mathbb{R}^3)} (a_k^* + a_{-k})(a_{-k'}^* + a_{k'}) \end{aligned}$$

with $R_t = q_t (h_{\varphi_t} - e(\varphi_t))^{-1} q_t$ and $q_t = 1 - |\psi_{\varphi_t}\rangle\langle\psi_{\varphi_t}|$.

Main theorem: let $\varphi_0 \in L^2(\mathbb{R}^3)$ with $e(\varphi_0) < 0$. Then

$$\left\| e^{-iH_\alpha t}(\psi_{\varphi_0} \otimes W(\alpha^2\varphi_0)\Omega) - \psi_t \otimes W(\alpha^2\varphi_t)\mathcal{S}(t;0)\Omega \right\| \leq C\alpha^{-1}$$

for all $|t| \leq C\alpha^2$.

Remark: restriction to $|t| \leq C\alpha^2$ ensures **persistence of gap**

$$\Lambda(t) = \inf\{|\lambda - e(\varphi_t)| > 0 : \lambda \in \sigma(h_{\varphi_t}) \backslash \{e(\varphi_t)\}\}$$

Corollary: define electron **reduced density matrix**

$$\gamma_t^{\text{el}} = \text{Tr}_{\mathcal{F}} \, |e^{-iH_\alpha t}(\psi_{\varphi_0} \otimes W(\alpha^2\varphi_0)\Omega)\rangle\langle e^{-iH_\alpha t}(\psi_{\varphi_0} \otimes W(\alpha^2\varphi_0)\Omega)|$$

Then

$$\|\gamma_t^{\text{el}} - |\psi_t\rangle\langle\psi_t|\|_{\text{tr}} \leq C\alpha^{-1}, \qquad \text{for all } |t| \leq C\alpha^2$$

Assuming additionally that $\varphi_0 \in L^2(\mathbb{R}^3, |k|^{1/2}dk)$, we also find

$$\left\|\gamma_t^{\text{ph}} - |\varphi_t\rangle\langle\varphi_t|\right\|_{\text{tr}} \leq C\alpha^{-1/4}, \qquad \text{for all } |t| \leq C\alpha^2$$

where

$$\gamma_t^{\text{ph}}(k;k') = \langle e^{-iH_\alpha t}(\psi_{\varphi_0} \otimes W(\alpha^2\varphi_0)\Omega), a_{k'}^* a_k e^{-iH_\alpha t}(\psi_{\varphi_0} \otimes W(\alpha^2\varphi_0)\Omega)\rangle$$

Remark: corollary shows validity of Landau-Pekar equations for $t \simeq \alpha^2$, at level of reduced densities.

Bogoliubov dynamics captures **quantum fluctuations** around classical Landau-Pekar equations.

It is crucial to establish a **norm-approximation**.

In fact, for $\delta > 0$ small, there is $C_\delta > 0$ such that, for $t = \delta\alpha^2$,

$$\|e^{-iH_\alpha t}(\psi_{\varphi_0} \otimes W(\alpha^2\varphi_0)\Omega) - (\psi_t \otimes W(\alpha^2\varphi_t)\Omega)\| \geq C_\delta, \quad \text{for all } \alpha$$

for all α large.

Remark: also for ground state energy, Bogoliubov theory is expected to describe corrections to classical Pekar energy.

For polarons on bounded domains, this was recently proved by **[Frank-Seiringer, 19]**.

Remark: for data (ψ_0, φ_0) minimizing Pekar energy, result was previously obtained by **[Mitrouskas, 20]**.

Fluctuation dynamics: observe that

$$\left\| e^{-iH_\alpha t}(\psi_{\varphi_0} \otimes W(\alpha^2 \varphi_0)\Omega) - \psi_t \otimes W(\alpha^2 \varphi_t)\mathcal{S}(t;0)\Omega \right\| = \| [\mathcal{G}(t) - \mathcal{U}(t;0) \otimes \mathcal{S}(t;0)] \, (\psi_{\varphi_0} \otimes \Omega) \|$$

where

$$i\partial_t \mathcal{U}(t;s) = h_{\varphi_t} \mathcal{U}(t;s), \qquad \mathcal{U}(s;s) = 1$$

and

$$\mathcal{G}(t) = W^*(\alpha^2 \varphi_t) e^{-iH_\alpha t} W(\alpha^2 \varphi_0)$$

Generators: we have

$$i\partial_t \, [\mathcal{U}(t;0) \otimes \mathcal{S}(t;0)] = (h_{\varphi_t} + \mathcal{N} - \mathcal{A}_t) \, [\mathcal{U}(t;0) \otimes \mathcal{S}(t;0)]$$

On the other hand,

$$i\partial_t \mathcal{G}(t) = \mathcal{L}_t \mathcal{G}(t)$$

with **generator**

$$\mathcal{L}_t = \left[i\partial_t W^*(\alpha^2 \varphi_t) \right] W(\alpha^2 \varphi_t) + W^*(\alpha^2 \varphi_t) H_\alpha W(\alpha \varphi_t)$$

Computation of $\mathcal{L}_t$: we have

$$
\begin{aligned}
&W^*(\alpha^2\varphi_t)H_\alpha W(\alpha\varphi_t)\\
&\qquad = -\Delta + \int (a_k^* + \overline{\varphi}_t(k))(a_k + \varphi_t(k))dk\\
&\qquad\qquad + \int \frac{dk}{|k|}\left[e^{-ik\cdot x}(a_k^* + \overline{\varphi}_t(k)) + e^{ik\cdot x}(a_k + \varphi_t(k))\right]\\
&\qquad = -\Delta + \mathcal{N} + \phi(\varphi_t) + 2\mathrm{Re}\ \widehat{|.|^{-1}\varphi}(x) + \phi(G_x)
\end{aligned}
$$

and

$$
\left[i\partial_t W^*(\alpha^2\varphi_t)\right] W(\alpha^2\varphi_t) = -\phi(i\alpha^2\partial_t\varphi_t) = -\phi(\varphi_t) - \phi(\widehat{|\psi_t|^2}/|.|)
$$

Thus

$$
\mathcal{L}_t = h_{\varphi_t} + \mathcal{N} + \phi(\delta_t G_x)
$$

with

$$
\phi(\delta_t G_x) = \phi(G_x) - \phi(\widehat{|\psi_t|^2}/|.|) = \int \frac{dk}{|k|}\left[e^{-ik\cdot x} - \langle \psi_t, e^{-ik\cdot x}\psi_t\rangle\right] a_k^* + \text{h.c.}
$$

Sketch of proof: we have

$$\left\| e^{-iH_\alpha t}(\psi_{\varphi_0} \otimes W(\alpha^2\varphi_0)\Omega) - \psi_t \otimes W(\alpha^2\varphi_t)\mathcal{S}(t;0)\Omega \right\|^2$$

$$= \|[\mathcal{G}(t) - \mathcal{U}(t;0) \otimes \mathcal{S}(t;0)]\,(\psi_{\varphi_0} \otimes \Omega)\|^2$$

$$= 2\,\mathrm{Im} \int_0^t ds\ \langle \mathcal{G}(s)(\psi_{\varphi_0} \otimes \Omega), [\phi(\delta_s G_x) - \mathcal{A}_s]$$

$$\times (\mathcal{U}(s;0) \otimes \mathcal{S}(s;0))(\psi_{\varphi_0} \otimes \Omega)\rangle$$

With **adiabatic theorem**

$$\left\| e^{-iH_\alpha t}(\psi_{\varphi_0} \otimes W(\alpha^2\varphi_0)\Omega) - \psi_t \otimes W(\alpha^2\varphi_t)\mathcal{S}(t;0)\Omega \right\|^2$$

$$\simeq 2\,\mathrm{Im} \int_0^t ds\ \langle \mathcal{G}(s)(\psi_{\varphi_0} \otimes \Omega), [\phi(\delta_s G_x) - \mathcal{A}_s]\,(\psi_{\varphi_s} \otimes \mathcal{S}(s;0)\Omega)\rangle$$

$$=: \mathrm{I} + \mathrm{II}$$

Consider **term**

$$\mathrm{I} = 2\,\mathrm{Im}\ \int_0^t ds \langle \mathcal{G}(s)(\psi_{\varphi_0} \otimes \Omega), \phi(\delta_s G_x)(\psi_{\varphi_s} \otimes \mathcal{S}(s;0)\Omega)\rangle$$

Since $p_s \phi(\delta_s G_x) p_s = 0$, we arrive at

$$\mathrm{Im}\ \int_0^t ds \langle \mathcal{G}(s)(\psi_{\varphi_0} \otimes \Omega), q_s \phi(G_x)(\psi_{\varphi_s} \otimes \mathcal{S}(s;0)\Omega)\rangle$$

Now, write

$$-\mathcal{U}(s;0)\left[i\partial_s \mathcal{U}^*(s;0)\right] = h_{\varphi_s} - e(\varphi_s)$$

We obtain

$$\mathrm{I} = \ -2\,\mathrm{Re}\ \int_0^t ds \langle \mathcal{U}^*(s;0)\mathcal{G}(s)(\psi_{\varphi_0} \otimes \Omega), \left[\partial_s \mathcal{U}^*(s;0)\right] \times R_s \phi(G_x)(\psi_{\varphi_s} \otimes \mathcal{S}(s;0)\Omega)\rangle$$

with **resolvent** $R_s = q_s(h_{\varphi_s} - e(\varphi_s))^{-1} q_s$.

To bound

$$\mathrm{I} = \, -2\,\mathrm{Re} \int_0^t ds \langle \mathcal{U}^*(s;0)\mathcal{G}(s)(\psi_{\varphi_0} \otimes \Omega), [\partial_s \mathcal{U}^*(s;0)] \times R_s \phi(G_x)(\psi_{\varphi_s} \otimes \mathcal{S}(s;0)\Omega)\rangle$$

we **integrate by parts**:

$$\mathrm{I} \simeq 2\,\mathrm{Re} \int_0^t ds \langle \mathcal{U}^*(s;0)(\mathcal{N} + \phi(\delta_s G_x))\mathcal{G}(s)(\psi_{\varphi_0} \otimes \Omega), \times \mathcal{U}^*(s;0) R_s \phi(G_x)(\psi_{\varphi_s} \otimes \mathcal{S}(s;0)\Omega)\rangle$$

$$\simeq 2\,\mathrm{Re} \int_0^t ds \langle \mathcal{G}(s)(\psi_{\varphi_0} \otimes \Omega), \phi(\delta_s G_x) R_s \phi(G_x)(\psi_{\varphi_s} \otimes \mathcal{S}(s;0)\Omega)\rangle$$

Inserting $p_s + q_s = 1$, we conclude that

$$\mathrm{I} \simeq 2\,\mathrm{Re} \int_0^t ds \langle \mathcal{G}(s)(\psi_{\varphi_0} \otimes \Omega), p_s \phi(G_x) R_s \phi(G_x)(\psi_{\varphi_s} \otimes \mathcal{S}(s;0)\Omega)\rangle$$
$$+ 2\mathrm{Re} \int_0^t ds \langle \mathcal{G}(s)(\psi_{\varphi_0} \otimes \Omega), q_s \phi(\delta_s G_x) R_s \phi(G_x)(\psi_{\varphi_s} \otimes \mathcal{S}(s;0)\Omega)\rangle$$

First term **cancels** precisely with term II! For second term, we repeat procedure integrating by parts once again.

Conclusions:

- In **strong coupling** regime $\alpha \to \infty$, quantized phonon field approaches **classical limit**.

- To leading order, the energy determined by **Pekar** functional, dynamics by the **Landau-Pekar** equations.

- Next order corrections depend on **quantum fluctuations**, described by **Bogoliubov theory**.

• Many similarities with **mean field** bosons, with

$$\mathcal{H}_N = \int \nabla_x a_x^* \nabla a_x + \frac{1}{2N} \int dxdyV(x-y) a_x^* a_y^* a_y a_x$$

Setting $b_x = N^{-1/2} a_x$, we find

$$\frac{1}{N}\mathcal{H}_N = \int \nabla_x b_x^* \nabla_x b_x + \frac{1}{2} \int dxdyV(x-y) b_x^* b_y^* b_x b_y$$

where b_x, b_y satisfy rescaled CCR

$$\left[b_x, b_y^*\right] = \frac{1}{N}\delta(x-y), \qquad \left[b_x, b_y\right] = \left[b_x^*, b_y^*\right] = 0$$

As $N \to \infty$, energy approaches **classical Hartree functional**

$$\mathcal{E}_{\text{hartree}}(\varphi) = \int |\nabla\varphi|^2 + \frac{1}{2} \int dxdyV(x-y)|\varphi(x)|^2|\varphi(y)|^2$$

Fluctuations around Hartree are described by **Bogoliubov** theory.

For **dynamics**, this approach goes back to **[Hepp, 74]**.