Spectral Theory and Dynamics of Quantum Systems
GRADUIERTENKOLLEG 1838

On the Dynamics of the Polaron in the Strong Coupling Limit

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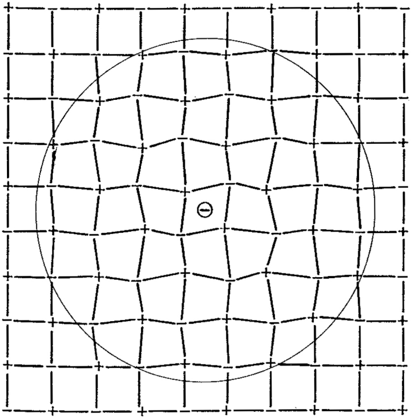
- Jochen Schmid
- Andreas Wünsch

What are Polarons?



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Electron and lattice polarization (deformation) together constitute a quasi-particle (polaron).

Quelle: Madelung, Festkörpertheorie

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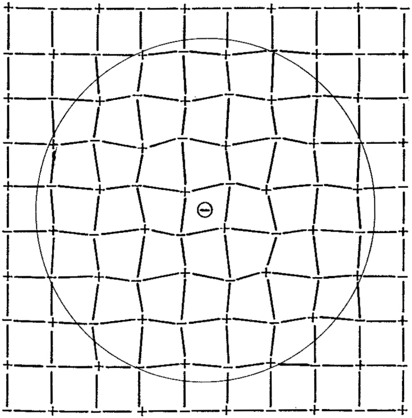

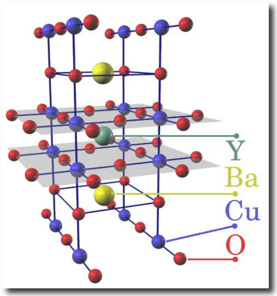

www.physics.ubc.ca/research/condensed.php

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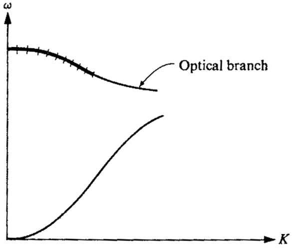

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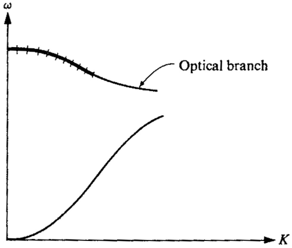

Dispersion in a crystal.

- The band electron has a parabolic dispersion relation.

The Large Polaron Model of H. Fröhlich

The Hilbert space is

$$\mathscr{H} = L^2(\mathbb{R}^3) \otimes \mathcal{F}$$
$$\mathcal{F} = \oplus_{n\geq 0} \otimes_s^n L^2(\mathbb{R}^3) \quad \text{symmetric Fock space.}$$

We choose units where $m = 1/2, \hbar = 1, \omega_0 = 1$, so that

$$\boxed{H_\alpha = -\Delta + N_{\mathrm{ph}} + \sqrt{\alpha} W}$$

where N_{ph} is the number operator on $\mathcal{F}$,

$$W = \frac{1}{2\pi} \int \frac{dk}{|k|} \left(e^{ik\cdot x} a(k) + e^{-ik\cdot x} a^*(k) \right)$$

One parameter: $\sqrt{\alpha}$ is a dimensionless coupling constant. Often $\alpha \gg 1$, therefore one is interested in the limit

$$\boxed{\alpha \to \infty.}$$

Self-adjointness

The Hamiltonian

$$H = -\Delta + N_{\mathrm{ph}} + \sqrt{\alpha} W$$

- is NOT a sum of operators but a sum of forms. Use the KLMN theorem to define a self-adjoint hamiltonian.
- $H_\Lambda \to H$ in the norm resolvent sense as $\Lambda \to \infty$. Hence

$$e^{-iH_\Lambda t} \to e^{-iHt} \qquad (\Lambda \to \infty)$$

in the strong operator topology.

Properties of the domain

There is an explicitly known dressing transform U such that UHU^* is self-adjoint on $D(H_0)$. Exploiting mapping properties of U we obtain:

Theorem (A. Wünsch, M.G.)

$$D(H) \subset \Big(\bigcap_{0<s<3/4} D((-\Delta)^s) \Big) \cap D(N),$$

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- In particular $D(H) \cap D(H_0) \subset D(H) \cap D(-\Delta) = \{0\}$.
- Since $D(H_\Lambda) = D(H_0)$ there is no vector $\psi \neq 0$ such that $H\psi = \lim_{\Lambda\to\infty} H_\Lambda \psi$ is true.

Ingredient of the proof

Lemma (Frank, Schlein 2014)

If $f \in L^2(\mathbb{R}^n)$ *and* $f_x(k) = e^{-ikx} f(k)$, *the for all* $\psi \in D(H_0)$

$$\|a(f_x)\psi\| \leq C(f) \left\| \sqrt{N}(1-\Delta_x)^{1/2}\psi \right\|$$

where

$$C(f) := \sup_{p \in \mathbb{R}^n} \left(\int \frac{|f(k)|^2}{1+(p-k)^2}\, dk \right)^{1/2}$$

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Application: $C(f_\Lambda)$ and hence $\|a(f_\Lambda)\psi\|$ is bounded uniformly in Λ for

$$f_\Lambda(k) = \frac{1}{|k|} \chi(|k| < \Lambda).$$

Minimal Energy and the Pekar Functional

Let

$$E_\alpha = \inf_{\|\psi\|=1} \langle \psi, H_\alpha \psi \rangle.$$

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Minimizing w.r.to product states only

$$\psi = \varphi \otimes \eta \in L^2 \otimes \mathcal{F}, \qquad \|\varphi\| = 1 = \|\eta\|$$

gives an upper bound

$$\begin{aligned} E_\alpha &\leq \inf \langle \varphi \otimes \eta, H_\alpha \varphi \otimes \eta \rangle \\ &= \inf_{\|\varphi\|=1} \left(\int |\nabla \varphi|^2 \, dx - \frac{\alpha}{2} \int \frac{|\varphi(x)|^2 |\varphi(y)|^2}{|x-y|} \, dxdy \right) \\ &= \alpha^2 E_{\text{Pekar}} \end{aligned}$$

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Theorem (Donsker, Varadhan 1983 and Lieb, Thomas 1997)

$$E_\alpha = \alpha^2 E_{\text{Pekar}} + O(\alpha^{9/5}) \qquad (\alpha \to \infty)$$

Euler-Lagrange and Landau-Pekar equations......

Theorem (Schmid, Schneider, M.G.)

Let $u \in C([0, T_0], H^4(\mathbb{R}^3))$ *be a solution of the Choquard equation and* $C_1 > 0$*, then there exits a constant* C_2 *and* $\varepsilon_0 > 0$ *such the following holds: every solution* $(\varphi_\varepsilon, V_\varepsilon)$ *of the LP-system with* $\varepsilon \leq \varepsilon_0$ *and initial data satisfying*

$$\varphi_\varepsilon = u, \qquad V_\varepsilon = -|\cdot|^{-1} * |u|^2 \qquad (t = 0)$$

and

$$\|\partial_t V_\varepsilon\|_\infty + \|\Delta \partial_t V_\varepsilon\|_{L^2 \cap L^1} \leq C_1 \qquad (t = 0)$$

exists on $[0, T_0]$ *and for all* $t \in [0, T_0]$*:*

$$\|\varphi_\varepsilon - u\|_{H^2} + \|V + |\cdot|^{-1} * |u|^2\|_\infty < C_2 \varepsilon.$$

The Dirac-Frenkel variational principle

Let $\mathcal{M} \subset \mathscr{H}$ be the manifold

$$\mathcal{M} = \{u = a\varphi \otimes \eta \neq 0 \mid a \in \mathbb{C},\ \varphi \in L^2,\ \eta \in \mathcal{F}\}$$

Given $u_0 \in \mathcal{M}$ we determine the orbit $u_t = a_t\varphi_t \otimes \eta_t \in \mathcal{M}$ by the conditions that the velocity $\partial_t u \in T_u\mathcal{M}$ is the **best approximation** to $-iHu \notin T_u\mathcal{M}$.

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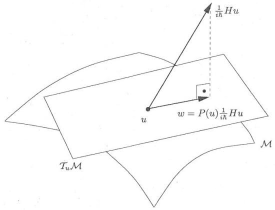
This means that

$$\boxed{i\partial_t u = P(u)Hu}$$

Dirac-Frenkel-equation

$P(u) =$ orthogonal projection onto $T_u\mathcal{M}$.



Orthogonal projection to the tangent space.

Rescaling of Space and Time

Since $E_\alpha = O(\alpha^2)$ as $\alpha \to \infty$ it is convenient to scale out α^2: Let $x_{\rm lab}, k_{\rm lab}$ be the old (laboratory) variables for electron position and phonon momentum. Implementing

$$x = \alpha x_{\rm lab}, \qquad k = \frac{1}{\alpha} k_{\rm lab}$$

unitarily (in terms of U) we find

$$U H_{F,\alpha} U^* = \alpha^2 (-\Delta + \alpha^{-2} N_{\rm ph} + \alpha^{-1} W).$$

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unitarily (in terms of U) we find

$$UH_{F,\alpha}U^* = \alpha^2(-\Delta + \alpha^{-2} N_{\rm ph} + \alpha^{-1} W).$$

The factor α^2 is removed by the rescaling of time

$$t = \alpha^2 t_{\rm lab}.$$

We arrive at

$$\boxed{i\partial_t \psi = H\psi, \qquad H = -\Delta + \alpha^{-2} N_{\rm ph} + \alpha^{-1} W.}$$

For each annihilation/creation operator a factor of α^{-1}.

The Dirac-Frenkel approximation

If $\|\varphi\| = \|\eta\| = 1$ and $u = a\varphi \otimes \eta$ we find $P(u)Hu = \tilde{H}(u)u$

$$\tilde{H}(u) = (-\Delta + \alpha^{-1} V_\eta) \otimes 1 + 1 \otimes (\alpha^{-2} N + \alpha^{-1}\phi(f)) - \alpha^{-1}\langle W \rangle_{\varphi\otimes\eta}$$

where

$$V_\eta(x) = \frac{1}{2\pi}\int \frac{dk}{|k|}\left(e^{ikx}\langle \eta, a(k)\eta\rangle + h.c.\right)$$

$$\phi(f) = a(f) + a^*(f), \qquad f(k) = \frac{1}{2\pi}\frac{\hat{\rho}(k)}{|k|} \quad \rho = |\varphi|^2$$

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The Dirac-Frenkel equation $i\partial u = \tilde{H}(u)u$ becomes the system

$$\begin{cases} i\dot{\varphi} = (-\Delta + V_\eta)\varphi \\ i\dot{\eta} = (\alpha^{-2} N_{\mathrm{ph}} + \alpha^{-1} \phi(f))\eta. \end{cases}$$

and

$$a(t) = \exp\left(i\alpha^{-1} \int_0^t \langle W \rangle_{\varphi \otimes \eta} \, ds \right)$$

The phonon potential

The equation for η can be solved explicitly and one finds $V_\eta = V_{0,t} + V_{\varphi,t}$ with

$$V_{0,t}(x) = \frac{1}{2\pi\alpha} \int \frac{dk}{|k|} \left(e^{ikx - it/\alpha^2} \langle \eta_0, a(k)\eta_0 \rangle + \text{h.c.} \right)$$

$$V_{\varphi,t}(x) = \frac{1}{\alpha^2} \int_0^t \left(\sin((s-t)\alpha^{-2}) \int \frac{|\varphi_s(y)|^2}{|x-y|}\, dy \right) ds$$

- $V_{0,t}$ is due to the freely evolved initial state η_0 of the phonons, it solves the homogeneous equation $(\partial_t^2 + \alpha^{-4}) V_{0,t} = 0$.

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- $V_{0,t}$ is due to the freely evolved initial state η_0 of the phonons, it solves the homogeneous equation $(\partial_t^2 + \alpha^{-4}) V_{0,t} = 0$.
- $V_{\varphi,t}$ is due to the phonons generated by the electron, the retarded self-interaction. It solves

$$(\partial_t^2 + \alpha^{-4}) V_{\varphi,t} = -\alpha^{-4} |\cdot|^{-1} * |\varphi|^2.$$

with vanishing initial data: $V_{\varphi,0} = \partial_t V_{\varphi,0} = 0$.

Let $\varphi_0 \in H^2(\mathbb{R}^3)$, $\eta_0 \in W(\alpha g)^*\Omega$, where $g \in L^2(\mathbb{R}^3, (1+k^2)\,dk)$. Let φ_t, η_t be the corresponding solution to the DF-equations and

$$u_t := a(t)\varphi_t \otimes \eta_t, \qquad t \in \mathbb{R}.$$

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There exists a constant $C \in \mathbb{R}$ such that for all $\alpha \geq 1$ and all $t \in \mathbb{R}$,

$$\|e^{-iHt}(\varphi_0 \otimes \eta_0) - u_t\|^2 \leq C \left| \frac{t}{\alpha} \right|.$$

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- There are similar results due to Frank/Schlein (2014) and Frank/Gang (2015).
- The time scale is too short to uniquely characterise the effective dynamics. (Mitrouskas)

Initial data $\varphi_0 \otimes \eta_0 \in \mathcal{M}$ minimizing the energy

- If φ_0 is the minimizer of the Pekar functional then

$$\varphi_t = e^{-i\lambda t}\varphi_0, \qquad V = -|\varphi_0|^2 * |\cdot|^{-1}$$

solves the Landau-Pekar system, which reduces to the EL equation

$$(-\Delta - |\varphi_0|^2 * |\cdot|^{-1})\varphi_0 = \lambda\varphi_0$$

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  of the Pekar-functional.

- The phonon state η_0 which is associated to the potential V is the coherent state

$$\eta_0 = e^{-i\pi(\alpha f)}\Omega, \qquad f(k) = \frac{\hat{\rho}(k)}{2\pi|k|}$$

  where $\rho = |\varphi_0|^2$. It is the ground state of $\alpha^{-2}N_{\rm ph} + \alpha^{-1}\phi(f)$ and if $u_0 := \varphi_0 \otimes \eta_0$ then $\tilde{H}(u_0)u_0 = E_{\rm P}u_0$. Hence the Dirac-Frenkel-Eq. is solved by

$$u = e^{-iE_{\rm P}t}u_0.$$

Theorem (2016)

Let φ_0 be the minimiser of the Pekar functional and $\eta_0 \in \mathcal{F}$ be the corresponding phonon state, then

$$\|e^{-iHt}(\varphi_0 \otimes \eta_0) - e^{-iE_{\mathrm{P}}t}(\varphi_0 \otimes \eta_0)\|^2 \leq C\frac{|t|}{\alpha^2}$$

for all $t \in \mathbb{R}$ and some $C \in \mathbb{R}$.

Elements of the Proof

We need to compare

$$e^{-iHt}u_0 = \lim_{\Lambda\to\infty} e^{-iH_\Lambda t}u_0$$

with

$$e^{-iE_{\mathrm{P}}t}u_0 = e^{-i\tilde{H}t}u_0$$

where $\tilde{H}$ is the effective (Dirac-Frenkel) Hamiltonian $\tilde{H} = \tilde{H}(u_0)$.

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where $\tilde{H}$ is the effective (Dirac-Frenkel) Hamiltonian $\tilde{H} = \tilde{H}(u_0)$.
The difference $\delta H := H - \tilde{H}$ is not small, but $(H - \tilde{H})u_0$ is, because $u_0 = \varphi_0 \otimes \eta_0$ where $\eta_0 = \exp(-i\pi(\alpha f))\Omega$ and

$$e^{i\pi(\alpha f)}(H - \tilde{H})e^{-i\pi(\alpha f)} = \frac{1}{\alpha}(W - \phi(f))$$

where

$$(H_0 + 1)^{-1/2}(W - \phi(f))(H_0 + 1)^{-1/2}$$

is a bounded operator.

the Proof continued

Let $\psi_t = e^{-iHt}u_0$. Using that $u_t = e^{-iE_{\mathrm{P}}t}u_0$ solves the Dirac-Frenkel equation we get

$$\|\psi_t - u_t\|^2 = 2\,\mathrm{Im}\int_0^t \langle \psi_s - u_s, P(u)^{\perp}\delta H u_s\rangle\, ds$$

which formally is of size $O(t/\alpha)$.

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$$\psi_s - u_s = e^{-i\tilde{H}s}\int_0^s e^{i\tilde{H}\tau}\delta H e^{-iHt}u_0\, d\tau$$

$$e^{i(\tilde{H}-E_{\mathrm{P}})s}P(u)^{\perp} = \frac{d}{ds}e^{i(\tilde{H}-E_{\mathrm{P}})s}(\tilde{H}-E_{\mathrm{P}})^{-1}P(u)^{\perp}$$

and integrate by parts.

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and integrate by parts. This works because

$$\tilde{H} - E_{\mathrm{P}} \restriction P(u)^{\perp}\mathscr{H}$$

has a gap in the spectrum above $E = \inf \sigma(\tilde{H})$ which is independent of α.

Extension to N Polarons

The (rescaled) N-polaron Hamiltonian

$$H_N = \sum_{j=1}^{N} \left(-\Delta_{x_j} + \alpha^{-1} W_j\right) + \sum_{i<j} \frac{U}{|x_i - x_j|} + \alpha^{-2} N_{\mathrm{ph}}$$

can be defined as a norm-resolvent limit of $H_{N,\Lambda}$ as $\Lambda \to \infty$. $U > 1$.
The **Pekar-Tomasevich** functional

$$\begin{aligned}\mathcal{E}_N(\varphi) &:= \inf_{\eta \in \mathcal{F}} \langle \varphi \otimes \eta, H_N(\varphi \otimes \eta)\rangle \\ &= \langle \varphi, \left(\sum_{j=1}^{N} (-\Delta_{x_j}) + \sum_{i<j} \frac{U}{|x_i - x_j|} \right) \varphi \rangle - \frac{1}{2} \int \frac{\rho(x)\rho(y)}{|x-y|}\, dxdy\end{aligned}$$

(constrained by $\|\varphi\| = 1$) where ρ is the electron density of φ.

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(constrained by $\|\varphi\| = 1$) where ρ is the electron density of φ.
$\mathcal{E}_N$ has a minimizer for $U < 1 + \varepsilon_N$ and for any type of statistics (Lewin / Anapolitanos, Griesemer).

Initial data

$$\varphi_0 = \text{minimizer of } \mathcal{E}_N$$

$$\eta_0 = e^{-i\pi(\alpha f)}\Omega, \qquad f(k) = \frac{\hat{\rho}(k)}{2\pi|k|}$$

$$\rho = \text{density of } \varphi_0.$$

Theorem

Let $u_0 = \varphi_0 \otimes \eta_0$ *be as above and* $E_N^{(\mathrm{PT})} = \mathcal{E}_N(\varphi_0) = \langle u_0, H_N u_0 \rangle$*, then*

$$\| e^{-iH_N t} u_0 - e^{-iE_N^{(\mathrm{PT})} t} u_0 \|^2 \leq C_N \frac{|t|}{\alpha^2}$$

for all $t \in \mathbb{R}$ *and some* $C_N \in \mathbb{R}$*.*

Conclusion

There is no self-trapping of the polaron (i.e. no ground state), but for large α any minimizer $\varphi_0 \otimes \eta_0$ of the energy among all product states is a long-lived metastable state – self-trapping!

Happy birthday, Herbert !