Stability and Absence of Binding for Multi-Polaron Systems

Rupert Frank
Department of Mathematics
Princeton University

Joint work with E. Lieb, R. Seiringer and L. Thomas

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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**

$$H = -\Delta + \frac{\sqrt{\alpha}}{2\pi} \int_{\mathbb{R}^3} \frac{dk}{|k|} \left(e^{ikx} a(k) + e^{-ikx} a^\dagger(k) \right) + \int_{\mathbb{R}^3} dk\, a^\dagger(k) a(k)$$

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

In the **large coupling limit** $\alpha \to \infty$ its ground state energy behaves asymptotically like the minimum of the **Pekar functional**

$$E = \inf \left\{ \mathcal{E}[\psi] : \ \psi \in H^1(\mathbb{R}^3),\ \|\psi\|_2 = 1 \right\}$$

where

$$\mathcal{E}[\psi] = \int_{\mathbb{R}^3} dx\, |\nabla \psi(x)|^2 - \frac{\alpha}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} dx\, dx' \, \frac{|\psi(x)|^2 |\psi(x')|^2}{|x - x'|}$$

(Donsker/Varadhan 1983, Lieb/Thomas 1997)

The non-linear eigenvalue problem

Some known results (Lieb 1976) about

$$E = \inf_{\|\psi\|_2=1} \left\{ \int_{\mathbb{R}^3} dx\, |\nabla\psi(x)|^2 - \frac{\alpha}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} dx\, dx' \, \frac{|\psi(x)|^2 |\psi(x')|^2}{|x-x'|} \right\} .$$

The infimum is attained and the optimizer can be chosen as a symmetric decreasing function. It is unique up to translations and a phase. The **Euler-Lagrange equation** reads

$$\left(-\Delta - \alpha\psi^2 * |x|^{-1}\right) \psi = -e\psi \, .$$

Should be compared with **linear** Schrödinger equations, e.g., for the hydrogen atom

$$\left(-\Delta - \alpha|x|^{-1}\right) \psi = -\tfrac{\alpha^2}{4}\psi$$

or for a mean-field model with charge density ρ

$$\left(-\Delta - \alpha\rho * |x|^{-1}\right) \psi = \lambda\psi \, .$$

The Multi-Polaron Problem

For N electrons, the functional becomes

$$\mathcal{E}_U^{(N)}[\psi] = \sum_{j=1}^{N} \int_{\mathbb{R}^{3N}} dx |\nabla_j \psi|^2 + U \sum_{j<k} \int_{\mathbb{R}^{3N}} dx \frac{|\psi(x)|^2}{|x_j - x_k|} - \frac{\alpha}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} dx dx' \frac{\rho_\psi(x) \rho_\psi(x')}{|x - x'|}$$

with the density

$$\rho_\psi(x) = \sum_{j=1}^{N} \int_{\mathbb{R}^{3(N-1)}} \widehat{dx_j} \, |\psi(\hat{x}_j)|^2 \, .$$

The parameter U is the **Coulomb repulsion strength**. In the physical regime one has $U > \alpha$.

We are interested in the ground state energy

$$E^{(N)}(U) = \inf \left\{ \mathcal{E}_U^{(N)}[\psi] : \ \psi \in H^1(\mathbb{R}^{3N}), \ \|\psi\|_2 = 1 \right\} .$$

We do not impose symmetry restrictions.

Two possible scenarios for $N = 2$

(1) The two electrons will form a bound pair, a **bipolaron**. This happens for small U.

(2) The two electrons will move away from each other (**two polarons**). **Does this happen** for large U**???**

Properties of $E^{(2)}(U)$:

- $E^{(2)}(U)$ is a concave, increasing function of U
- $E^{(2)}(U) \leq 2E$ for all U
- $E^{(2)}(0) = 8E < 2E$ for $U = 0$

If scenario (2) occurs, then $E^{(2)}(U) = 2E$.
Conversely, if $E^{(2)}(U) < 2E$, then one can prove existence of a minimizer, that is, scenario (1) occurs.
Hence the question, whether scenario (2) occurs, is the same as **whether $E^{(2)}(U) = 2E$ for large U**.

Absence of Binding

Theorem 1 (**Absence of binding for N polarons**). *There is a finite constant ν_c such that for $U \geq \nu_c \alpha$ one has*

$$\boxed{E^{(N)}(U) = NE \quad \textit{for all } N \geq 2.}$$

Our proof gives the **explicit bound** $\nu_c < 14.7$. By computations with trial functions Verbist et al. (1992) showed that $\nu_c > 1.15$ (in particular, $\nu_c > 1$). *There is room for improvement!*

It costs energy to bring two or more particles together!

$$\mathcal{E}_U^{(N)}[\psi] \geq NE + (U - \nu_c \alpha) \sum_{j<k} \int_{\mathbb{R}^{3N}} dx \frac{|\psi(x)|^2}{|x_j - x_k|}$$

In particular, for $U > \nu_c \alpha$ there is **no minimizer**. *Is there one for $U = \nu_c \alpha$?*
Related result in linear case by Hoffmann-Ostenhof^2 and Simon.

Thermodynamic Stability

Theorem 2 (**Stability for $U > \alpha$**). *For any $\nu > 1$, there is a constant $C(\nu)$ such that for all $U \geq \nu\alpha$*

$$\boxed{E^{(N)}(U) \geq -C(\nu)\alpha^2 N \quad \textit{for all } N \geq 2.}$$

Since $E^{(N)}(U)$ is also **subadditive**, i.e., $E^{(N+M)}(U) \leq E^{(N)}(U) + E^{(M)}(U)$, we get

Corollary 3 (**Existence of the thermodynamic limit**). *For $U > \alpha$ the limit*

$$\lim_{N\to\infty} \frac{1}{N} E^{(N)}(U) \qquad \textit{exists.}$$

The restriction $U > \alpha$ is (almost) sharp. In the non-physical regime $U < \alpha$, Griesemer and Schach Møller (2010) have shown that $E^{(N)}(U) \approx -N^2$. *What happens at $U = \alpha$?*

For fermions (anti-symmetric ψ's) they have shown that $E^{(N)}(U) \approx -N^{7/3}$ for $U < \alpha$ and $E^{(N)}(\alpha) \approx -N$ for $U = \alpha$.

Ideas of the proofs: Absence of binding for $N = 2$

Step 0. Linearizing the problem

$$E^{(2)}(U) = \inf \{\langle \psi, H_{U,\sigma}\psi\rangle : \ \|\psi\|_2 = 1, \, \sigma \geq 0\}$$

with the Hamiltonian

$$H_{U,\sigma} = \sum_{j=1}^{2} \left(-\Delta_j - \alpha\sigma * |x_j|^{-1}\right) + \frac{U}{|x_1 - x_2|} + \frac{\alpha}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} dx\, dx' \, \frac{\sigma(x)\sigma(x')}{|x - x'|} \, .$$

Follows from Schwarz, since $D[\rho_\psi, \rho_\psi] = \sup_\sigma \left(2D[\sigma, \rho_\psi] - D[\sigma,\sigma]\right)$.

Step 1. Localization according to particle distance

For $\ell > 0$, divide configuration space into shells

$$2^{k-1}\ell \leq |x_1 - x_2| \leq 2^k \ell \qquad , \quad k \geq 1 \, .$$

The localization cost is $\sim \ell^{-2}4^{-k}$, which is dominated by part of the Coulomb repulsion, $U/|x_1 - x_2| \geq U2^{-k}/\ell$.

Ideas of the proofs: Absence of binding for $N = 2$

Step 2. Further localization for well-separated particles

For $k \geq 1$, we further localize each particle into its own box, of side length $c\ell 2^k$, with c small so that the boxes do not overlap.

Key idea: Each particle is localized to a box the size of which is comparable to the distance between the two boxes.

We delinearize and find the same minimization problem as before but now for ψ's with support in $Q_1 \times Q_2$. For $\rho_\psi = \rho_1 + \rho_2$ with $\mathrm{supp}\rho_j \subset Q_j$,

$$D[\rho_\psi, \rho_\psi] \leq D[\rho_1, \rho_1] + D[\rho_2, \rho_2] + \frac{\alpha}{2\,\mathrm{dist}(Q_1, Q_2)} \,.$$

Each of the terms $D[\rho_j, \rho_j]$, $j = 1, 2$ contributes to one single-polaron energy.

Since $\mathrm{dist}(Q_1, Q_2) \approx 2^k \ell$, the contribution to the total energy from $k \geq 1$ is

$$\geq \underbrace{2E}_{\textbf{wanted}} + \underbrace{U 2^{-k} \ell^{-1}}_{\text{Coulomb repulsion}} - \underbrace{c_1 \alpha 2^{-k} \ell^{-1}}_{\text{attraction}} - \underbrace{c_2 \ell^{-2} 4^{-k}}_{\text{localization}} \,.$$

Ideas of the proofs: Absence of binding for $N = 2$

Step 3. Particles without minimal separation

It remains to study $k = 0$, i.e., the region $|x_1 - x_2| \leq \ell$. Here the Coulomb repulsion is huge. To estimate the attraction we use that for $U = 0$

$$E^{(2)}(0) = 8E = 2E - 6 \cdot (0.109)(\alpha/2)^2 \,.$$

Hence the contribution to the total energy from $k = 0$ is

$$\geq \underbrace{2E}_{\textbf{wanted}} + \underbrace{U\ell^{-1}}_{\text{Coulomb repulsion}} \underbrace{- 6 \cdot (0.109)(\alpha/2)^2}_{\text{attraction}} - \underbrace{c_3 \ell^{-2}}_{\text{localization}} \,.$$

Recall from the previous slide the bound for $k \geq 1$,

$$\geq \underbrace{2E}_{\textbf{wanted}} + \underbrace{U 2^{-k} \ell^{-1}}_{\text{Coulomb repulsion}} - \underbrace{c_1 \alpha 2^{-k} \ell^{-1}}_{\text{attraction}} - \underbrace{c_2 \ell^{-2} 4^{-k}}_{\text{localization}} \,.$$

Both bounds are $\geq 2E$, provided we choose $\ell = c_4 \alpha^{-1}$ and assume that $U/\alpha \geq c_5$. $\square$

Ideas of the proofs: Linear lower bound

We want to bound $N^{-1}E^{(N)}(U)$ from below by a constant.

The **Hoffmann-Ostenhof[2] inequality** tells us that

$$\sum_{i=1}^{N} \int_{\mathbb{R}^{3N}} dx\, |\nabla_i \psi|^2 \geq \int_{\mathbb{R}^3} dx\, |\nabla \sqrt{\rho_\psi}|^2 \,,$$

and the **Lieb-Oxford inequality** tells us that

$$\sum_{i<j} \int_{\mathbb{R}^{3N}} dx\, \frac{|\psi(x)|^2}{|x_i - x_j|} \geq \frac{1}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} dx\, dx'\, \frac{\rho_\psi(x)\, \rho_\psi(x')}{|x - x'|} - (1.68) \int_{\mathbb{R}^3} dx\, \rho_\psi(x)^{4/3} \,.$$

Hence, for $U = \alpha + \delta$ and abbreviating $\phi := \sqrt{\rho_\psi / N}$,

$$\frac{1}{N} \mathcal{E}_U^{(N)}[\psi] \geq \int_{\mathbb{R}^3} dx\, \left(|\nabla \phi|^2 - (1.68) U N^{1/3} \phi^{8/3} \right) + \delta N \iint_{\mathbb{R}^3 \times \mathbb{R}^3} dx\, dx'\, \frac{\phi(x)^2\, \phi(x')^2}{|x - x'|} \,.$$

IDEAS OF THE PROOFS: LINEAR LOWER BOUND

To bound the $\phi^{8/3}$ term we use a new **Sobolev-type inequality**. By Schwarz

$$\left(\int dx\, \phi^3\right)^2 = \left\langle (-\Delta)^{-1/2}\phi^2 \,|\, (\Delta)^{1/2}\phi \right\rangle^2$$

$$\leq \frac{1}{4\pi} \iint dx\, dx' \frac{\phi(x)^2\, \phi(x')^2}{|x-y|} \int dx\, |\nabla \phi|^2 \,,$$

and hence by Hölder

$$\int dx\, \phi^{8/3} \leq \left(\int dx\, \phi^3\right)^{2/3} \left(\int dx\, \phi^2\right)^{1/3}$$

$$\leq \frac{1}{(4\pi)^{1/3}} \left(\iint dx\, dx' \frac{\phi(x)^2\, \phi(x')^2}{|x-x'|}\right)^{1/3} \left(\int dx\, |\nabla\phi|^2\right)^{1/3} \left(\int dx\, \phi^2\right)^{1/3} .$$

Linearizing this bound and plugging it into the lower bound on $N^{-1}\mathcal{E}_U^{(N)}[\psi]$ we find

$$E^{(N)}(U) \geq -\left((1.68)^3/54\pi\right) \left(U^3/(U-\alpha)\right) N \,, \quad \text{as claimed} .$$

THANK YOU FOR YOUR ATTENTION!