Ground state properties of bipolaron systems

Rupert Frank
Department of Mathematics
Princeton University

Joint work with E. Lieb and R. Seiringer

Binding of polarons and atoms at thresholds, Comm. Math. Phys.(2012), to appear
Symmetry of bipolaron bound states for small Coulomb repulsion, `arXiv:1201.3954`

Spectral Days, Munich, April 10, 2012

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 to be symmetric decreasing. It is unique up to translations and a phase. The Hessian of the energy functional at the minimizer is non-degenerate (Lenzmann 2009). 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 Bipolaron Problem

For two electrons, the functional becomes

$$\mathcal{E}_U^{(2)}[\psi] = \sum_{j=1}^{2} \int_{\mathbb{R}^6} dx |\nabla_j \psi|^2 + U \int_{\mathbb{R}^6} dx \frac{|\psi(x)|^2}{|x_1 - x_2|} - \frac{\alpha}{2} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} dx dx' \frac{\rho_\psi(x) \rho_\psi(x')}{|x - x'|}$$

with the density

$$\rho_\psi(x) = \int_{\mathbb{R}^3} dx' \left(|\psi(x, x')|^2 + |\psi(x', x)|^2 \right) .$$

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

We are interested in the ground state energy

$$E^{(2)}(U) = \inf \left\{ \mathcal{E}_U^{(2)}[\psi] : \ \psi \in H^1(\mathbb{R}^6), \ \|\psi\|_2 = 1 \right\} .$$

The minimizer will automatically be permutation symmetric, i.e., $\psi(x_1, x_2) = \psi(x_2, x_1)$.

The Bipolaron Ground State Energy

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 $E^{(2)}(U) < 2E$, then the infimum $E^{(2)}(U)$ is attained (Lewin 2011). The two electrons will form a bound pair, a **bipolaron**. This happens for small U.

Conversely, (FLS and Thomas 2010): There is a $U_c > \alpha$ such that $E^{(2)}(U) = 2E$ for $U \geq U_c$. In particular, for $U > U_c$ there is no minimizer. **No bipolaron formation**

Explicit bound $U_c < 14.7\alpha$ (but $U_c \geq 1.15\alpha$ by Verbist et al.; results by Benguria–Bley)
We also have results for **N-polaron systems** and thermodynamic stability.

Today's topic: What happens for $0 \leq U \leq U_c$, in particular as $U \nearrow U_c$?
• How does the **disassociation** occur? • Is the ground state density **radial**?

Main Results: Ground States of Bipolarons

Theorem 1 (**Finite bipolaron radius**). *The infimum $E^{(2)}(U_c)$ is attained. In particular, $E^{(2)}(U)$ is not differentiable at $U = U_c$.*

Key idea: If ψ_U is optimizer for $E^{(2)}(U)$ and $\alpha(1+\delta) \le U < U_c$, then **lower bound**

$$\langle \psi_U, |x_1 - x_2|^{-1} \psi_U \rangle \ge C_\delta > 0 \,.$$

Existence of optimizer follows from this by compactness arguments.
A similar lower bound holds for N polarons and also (for approximate ground states) in the case of quantized fields provided $U_c(\alpha) > \alpha$.

Theorem 2 (**Symmetry for small U**). *For all sufficiently small $U \ge 0$ the ground state is unique (up to translations and a constant phase). In particular, it has angular momentum zero.*

Perturbative argument based on Lenzmann's result for the single polaron. No control on 'sufficiently small'. *Is this true up to $U = U_c$? There is something to be understood!*

Model Problem: The Helium Problem

Instead of the bipolaron functional, consider the **linear** Hamiltonian

$$H_U = -\Delta_1 - |x_1|^{-1} - \Delta_2 - |x_2|^{-1} + U|x_1 - x_2|^{-1}$$

in $L^2(\mathbb{R}^6)$. **Ground state energy** E_U is increasing and concave wrt U.
There is a **critical repulsion** $U_c > 1$ such that

$$E_U < -\frac{1}{4} = \inf \operatorname{spec}(-\Delta_1 - |x_1|^{-1}) \text{ if } U < U_c \quad \text{and } E_U = -\frac{1}{4} \text{ if } U \geq U_c \,.$$

Theorem 3 (HO^2–Simon (1983)). *$-1/4$ is an eigenvalue of H_{U_c} at $U = U_c$.*

New proof based on

Lemma 4. *If ψ_U is the eigenfunction for E_U and $1+\delta \leq U < U_c$, then*

$$\langle \psi_U, |x|_\infty^{-1} \psi_U \rangle \geq C_\delta > 0 \quad \textit{where } |x|_\infty = \max\{|x_1|, |x_2|\} \,.$$

We do **not** need positivity of ψ_U. Our proof works, e.g., for **magnetic fields**.

Ideas of the Proof

Lemma 5. $\langle \psi_U, |x|_\infty^{-1} \psi_U \rangle \geq C_\delta > 0$ *if* $1 + \delta \leq U < U_c$ *and* $|x|_\infty = \max\{|x_1|, |x_2|\}$.

Key inequality - potential barrier:

$$H_U - E_U \geq -\frac{C}{\ell^2} \chi_{\{|x|_\infty \leq \ell\}} + \left(-\frac{1}{4} - E_U + \frac{c}{|x|_\infty} \right) \chi_{\{|x|_\infty > \ell\}}$$

for some C, c and all $\ell \geq \ell_0$. Thus,

$$\frac{C}{\ell^2} \int_{\{|x|_\infty \leq \ell\}} \psi_U^2 \, dx \geq c \int_{\{|x|_\infty > \ell\}} \frac{\psi_U^2}{|x|_\infty} \, dx \, .$$

This, together with a **calculus lemma**, implies Lemma 5.

Proof of key inequality via **localization** into four regions (ϵ, ℓ parameters). (1) $|x|_\infty \leq 2\ell$,
(2) $|x|_\infty \geq \ell$, $|x|_\infty \leq (1-\epsilon)|x_1 - x_2|$, — **here nuclear attraction is small**
(3) $|x|_\infty \geq \ell$, $|x|_\infty \geq (1-2\epsilon)|x_1 - x_2|$, $|x_1| \leq (1+\epsilon)|x_2|$ — **use $U \geq 1 + \delta$**
(4) similarly. □

Lesson learned: Discont. binding if net repulsion larger than r^{-2} at infinity

THANK YOU FOR YOUR ATTENTION!