RESEARCH REPORT:
THE POLARON AT STRONG COUPLING AND THE PEKAR FUNCTIONAL

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1. THE POLARON MODEL

The Polaron is a quasi-particle used to describe the behaviour of an electron moving through a solid material. The picture to bear in mind is that of a negatively charged particle moving through a sea of neutral particles, arranged in a lattice configuration. The electron polarizes the neutral charges and displace them from their equilibrium position, thus triggering vibrations of the lattice. The polarized charges, in turn, generate a potential on the electron, decreasing its mobility and increasing its effective mass. This two phenomena couple the electron with phonons, which are quasi-particles used to describe the vibrations of a lattice, thus making the system rather complicated to analyze.

The model has one dimensionless coupling constant, α, which was very early understood to heavily influence the structure of ground states. In particular, there is difference between the two regimes of weak and strong coupling.

We consider **Fröhlich's Hamiltonian**, which, in appropriate units, reads:

$$H = -\Delta + \int_{\mathbb{R}^3} a_k^* a_k dk + (4\pi\alpha)^{1/2} \int_{\mathbb{R}^3} \left(\frac{e^{ik\cdot x}}{k} a_k + \frac{e^{-ik\cdot x}}{k} a_k^* \right) dk. \tag{1.1}$$

The minimization of this Hamiltonian over pure tensors (which is equivalent to assume that the phonon field behaves classically) reduces to a minimization problem only involving the electronic state function ϕ and the so-called called **Pekar functional**:

$$\mathcal{E}(\phi) = \int_{\mathbb{R}^3} |\nabla\phi|^2 dx - \alpha \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|\phi(x)|^2 |\phi(y)|^2}{|x-y|} dxdy. \tag{1.2}$$

We denote by $e_P(\alpha)$ the g.s. energy of the Pekar functional (which, trivially scales as $e_P(\alpha) = \alpha^2 e_p(1)$) and by $E(\alpha)$ the g.s. energy of the Fröhlich's Hamiltonian. It was long conjectured that $e_P(\alpha)$ and $E(\alpha)$ coincide to leading order as $\alpha \to \infty$, i.e. that:

$$E(\alpha) = \alpha^2 e_P(1) + \text{lower order terms}.$$

This was proven rigorously in [1] and [5]. The natural succesive step, which is also the main goal of my research, is to try to investigate the lower order terms appearing in this asymptotic.

The first results in this direction were obtained in [2]. In this work, the two authors are able to show that, for some explicit C, it holds:

$$E(\alpha) = \alpha^2 e_P(1) + C + o(1). \tag{1.3}$$

This result is obtained at the price of considering an easier situation than the full problem on $\mathbb{R}^3$: the polaron confined to a bounded domain. The Hamiltonian is modified and the resulting Pekar functional, confined to some open bounded $\Omega \subset \mathbb{R}^3$, reads as follow:

$$\mathcal{E}_\Omega(\phi) = \int_\Omega |\nabla\phi|^2 dx - \int_\Omega \int_\Omega -\Delta_\Omega^{-1}(x,y) |\phi(x)|^2 |\phi(y)|^2 dxdy. \tag{1.4}$$

Here $-\Delta_\Omega^{-1}(x,y)$ denotes the integral kernel of the inverse Laplacian with Dirichlet boundary conditions on Ω and the factor α in front of the second term that was appearing in the Pekar functional defined on $\mathbb{R}^3$ has been scaled out by considering Ω of size α^{-1}.

To obtain the results in [2], the authors need to assume some properties on $\mathcal{E}_\Omega$, in particular that it admits a unique minimizer, up to phase, and that the Hessian of $\mathcal{E}_\Omega$ is strictly positive at the unique minimizer (up to the trivial zero-modes given by uniqueness up to phase). This is the problem on which I first focused during my PhD: in collaboration Robert Seiringer we managed to show that, at least when Ω is a ball in $\mathbb{R}^3$, these assumptions are satisfied (see Abstract of Talk below).

It is now an ongoing challenge to generalize and extend the techniques introduced and exploited in [2] to analyze the full space problem. I am currently working with Robert Seiringer to extend the results to the case of a torus, which would serve as a stepping stone to better understand the structure of the problem and then maybe the tackle the $\mathbb{R}^3$ case. Of course, we consider on the torus the Laplacian with periodic boundary conditions.

Again, the problem splits in two parts: one aimed at analyzing the properties of the Pekar functional (i.e.existence and uniqueness of minimizers and positivity properties of the Hessian of the functional at its minima) and one focusing on computing explictly the lower order corrections to the Fröhlich Hamiltonian g.s. energy.

2. Abstract of Talk: Uniqueness and Non-Degeneracy of Minimizers of the Pekar Functional on a Ball

In this talk, we review some properties of the Pekar functional confined to balls. In particular, some recent results, obtained in collaboration with Robert Seiringer and concerning existence, uniqueness and non-degeneracy of minimizers, are presented. These properties were already known to hold on the full space (thanks to works of Lieb [4] and Lenzmann [3]). The study of the confined case is motivated by a recent paper by Rupert Frank and Robert Seiringer [2], in which the validity of the aforementioned results is conjectured and taken as a working assumption.

References

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