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The effective mass problem for the Landau–Pekar equations

Dario Feliciangeli, Simone Rademacher* **and Robert Seiringer**

IST Austria, Am Campus 1, 3400 Klosterneuburg, Austria

E-mail: simone.rademacher@ist.ac.at

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Abstract
We provide a definition of the effective mass for the classical polaron described by the Landau–Pekar (LP) equations. It is based on a novel variational principle, minimizing the energy functional over states with given (initial) velocity. The resulting formula for the polaron's effective mass agrees with the prediction by LP (1948 *J. Exp. Theor. Phys.* **18** 419–423).

Keywords: polaron, effective mass, Landau–Pekar equations

1. Introduction

The polaron is a model of an electron interacting with its self-induced polarization field of the underlying crystal. The description of the polarization as a quantum field corresponds to the Fröhlich model [8]. In the classical approximation, on the other hand, the dynamics of a polaron is described by the Landau–Pekar (LP) equations [14, 15, 24]. For $(\psi_t, \varphi_t) \in H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$, where ψ_t is the electron wave function and φ_t denotes the phonon field, these equations read in suitable units (see [8] or [1])

$$\begin{aligned} i\partial_t \psi_t &= h_{\varphi_t} \psi_t, \\ i\alpha^2 \partial_t \varphi_t &= \varphi_t + \sigma_{\psi_t}, \end{aligned} \tag{1.1}$$

where h_φ is the Schrödinger operator

$$h_\varphi = -\Delta + V_\varphi, \tag{1.2}$$

*Author to whom any correspondence should be addressed.

with potential

$$V_\varphi(x) = 2\,\mathrm{Re}\,[(-\Delta)^{-1/2}\varphi](x) = \pi^{-2}|x|^{-2} * \mathrm{Re}\,\varphi, \tag{1.3}$$

and

$$\sigma_\psi(x) = \left[(-\Delta)^{-1/2}|\psi|^2\right](x) = (2\pi^2)^{-1}|x|^{-2} * |\psi|^2, \tag{1.4}$$

where $*$ denotes convolution. The parameter $\alpha > 0$ quantifies the strength of the coupling of the electron's charge to the polarization field.

Despite its long history, the polaron model continues being actively investigated. For recent experimental and numerical work, we refer to [5, 21, 25, 27, 28] and references there.

The LP equations can be derived from the dynamics generated by the (quantum) Fröhlich Hamiltonian for suitable initial states in the strong coupling limit $\alpha \to \infty$ [17] (see also [6, 7, 13, 18, 22] for earlier results on this problem). One of the outstanding open problems concerns the polaron's effective mass [19, 26, 29]: due to the interaction with the polarization field, the electron effectively becomes heavier and behaves like a particle with a larger mass. This mass increases with the coupling α, and is expected to diverge as α^4 as $\alpha \to \infty$. A precise asymptotic formula was obtained by LP [15] based on the classical approximation, and hence it is natural to ask to what extent the derivation of the LP equations in [17] allows to draw conclusions on the effective mass problem.

It is, however, far from obvious how to rigorously obtain the effective mass even on the classical level, i.e. from the LP equation (1.1). A heuristic derivation, reviewed in section 4.1 below, considers traveling wave solutions of (1.1) for non-zero velocity $v \in \mathbb{R}^3$, and expands the corresponding energy for small v. The existence of such solutions remains unclear, however, and we in fact conjecture that no such solutions exist for non-zero v. This is related to the fact the energy functional corresponding to (1.1) (given in equation (2.1) below) does not dominate the total momentum, and a computation of the ground state energy as a function of the (conserved) total momentum would simply yield a constant function (corresponding to an infinite effective mass). Due to the vanishing of the sound velocity in the medium, a moving electron can be expected to be slowed down to zero speed by emitting radiation. (See [2, 9–12] for the study of a similar effect in a model of a classical particle coupled to a field.)

In this paper, we provide a novel definition of the effective mass for the LP equations. We shall argue that all low energy states have a well-defined notion of (initial) velocity, and hence we can minimize the energy functional among states with given velocity. Expanding the resulting energy–velocity relation for small velocity gives a definition of the effective mass, which coincides with the prediction by LP [15].

1.1. Structure of the paper

In section 2, we explain our rigorous approach to derive the energy–velocity relation of the system, allowing for a precise definition and computation of the effective mass. After introducing some notation and recalling fundamental properties of the Pekar energy functional in section 2.1, we identify in section 2.2 a set of initial data for the LP equations for which it is possible to define the position, and consequently the velocity, at any time. We then arrive at an energy–velocity relation by defining $E(v)$ in section 2.3 as the minimal energy among all admissible initial states of fixed initial velocity v. Finally, in section 2.4 we state our main result, an expansion of $E(v)$ for small velocities v, allowing for the computation the effective mass of the system.

Section 3 contains the proof of our main result, theorem 2.1.

In section 4 we discuss the formal approach to the effective mass via traveling waves. Moreover, we investigate an alternative definition of the effective mass, through an alternative notion of velocity of low-energy states.

2. Main results

2.1. Preliminaries

We start by introducing further notation and recalling some known results. The classical energy functional corresponding to the LP equation (1.1) is defined on $H^1(\mathbb{R}^3)\times L^2(\mathbb{R}^3)$ as

$$\mathcal{G}(\psi,\varphi)=\langle\psi,h_\varphi\psi\rangle+\|\varphi\|_2^2\quad\text{for } \|\psi\|_2=1. \tag{2.1}$$

Equipped with the symplectic form $\frac{1}{2i}\int \mathrm{d}\psi\wedge\mathrm{d}\bar{\psi}+\frac{\alpha^2}{2i}\int\mathrm{d}\varphi\wedge\mathrm{d}\bar{\varphi}$, it defines a dynamical system leading to the LP equation (1.1). Moreover, $\mathcal{G}$ is conserved along solutions of (1.1).

Let e_P denote the Pekar ground state energy

$$e_\mathrm{P}:=\min\,\mathcal{G}(\psi,\varphi). \tag{2.2}$$

(For an estimation of its numerical value, see [23].) It was proved in [20] that the minimum in (2.2) is attained for the Pekar minimizers $(\psi_\mathrm{P},\varphi_\mathrm{P})$, which are radial smooth functions in $C^\infty(\mathbb{R}^3)$ satisfying $\psi_\mathrm{P}>0$, $\varphi_\mathrm{P}=-\sigma_{\psi_\mathrm{P}}$ and $\psi_\mathrm{P}=\psi_{\varphi_\mathrm{P}}$, where ψ_φ denotes the ground state of h_φ whenever it exists. Moreover, this minimizer is unique up to the symmetries of the problem, i.e. translation-invariance and multiplication of ψ by a phase. We shall denote

$$H_\mathrm{P}=h_{\varphi_\mathrm{P}}-\mu_\mathrm{P}\quad\text{with } \mu_\mathrm{P}=\inf\operatorname{spec}h_{\varphi_\mathrm{P}}. \tag{2.3}$$

Associated to $\mathcal{G}$, there are the two functionals

$$\mathcal{E}(\psi):=\inf_{\varphi\in L^2(\mathbb{R}^3)}\mathcal{G}(\psi,\varphi)=\int_{\mathbb{R}^3}|\nabla\psi(x)|^2\mathrm{d}x-\frac{1}{4\pi}\int_{\mathbb{R}^6}\frac{|\psi(x)|^2|\psi(y)|^2}{|x-y|}\mathrm{d}x\,\mathrm{d}y, \tag{2.4}$$

and

$$\mathcal{F}(\varphi):=\inf_{\substack{\psi\in H^1(\mathbb{R}^3)\\ \|\psi\|_2=1}}\mathcal{G}(\psi,\varphi)=\inf\operatorname{spec}h_\varphi+\|\varphi\|_2^2, \tag{2.5}$$

and clearly $e_\mathrm{P}=\min\,\mathcal{G}(\psi,\varphi)=\min\,\mathcal{E}(\psi)=\min\,\mathcal{F}(\varphi)$. We also define the manifolds of minimizers

$$\mathcal{M}_\mathcal{G}:=\{(\psi,\varphi)|\mathcal{G}(\psi,\varphi)=e_\mathrm{P}\},\quad \mathcal{M}_\mathcal{E}:=\{\psi|\mathcal{E}(\psi)=e_\mathrm{P}\},\quad \mathcal{M}_\mathcal{F}:=\{\varphi|\mathcal{F}(\varphi)=e_\mathrm{P}\}. \tag{2.6}$$

The results in [20] imply that we can write these in terms of the Pekar minimizers $(\psi_\mathrm{P},\varphi_\mathrm{P})$ as

$$\begin{aligned}\mathcal{M}_\mathcal{G}&=\{(\mathrm{e}^{\mathrm{i}\theta}\,\psi_\mathrm{P}^y,\varphi_\mathrm{P}^y)|\theta\in[0,2\pi),y\in\mathbb{R}^3\},\\ \mathcal{M}_\mathcal{E}&=\{\mathrm{e}^{\mathrm{i}\theta}\,\psi_\mathrm{P}^y|\theta\in[0,2\pi),y\in\mathbb{R}^3\},\\ \mathcal{M}_\mathcal{F}&=\{\varphi_\mathrm{P}^y|y\in\mathbb{R}^3\},\end{aligned} \tag{2.7}$$

where $f^y := f(\cdot - y)$ for any function f. Furthermore, it can be deduced from the results in [16] that the energy functionals $\mathcal{F}$ and $\mathcal{E}$ are both coercive (see [3, lemmas 2.6 and 2.7]), i.e. there exists $C > 0$ such that

$$\mathcal{F}(\varphi) \geqslant e_\mathrm{P} + C\mathrm{dist}^2_{L^2}(\varphi, \mathcal{M}_\mathcal{F}), \qquad \mathcal{E}(\psi) \geqslant e_\mathrm{P} + C\mathrm{dist}^2_{H^1}(\psi, \mathcal{M}_\mathcal{E}). \tag{2.8}$$

The following lemma on properties of the projection onto the manifold $\mathcal{M}_\mathcal{F}$ will be important for our analysis below. Its proof will be given in appendix A.

Lemma 2.1. *There exists $\delta > 0$ such that the L^2-projection onto $\mathcal{M}_\mathcal{F}$, is well-defined (i.e. unique) on*

$$(\mathcal{M}_\mathcal{F})_\delta := \{\varphi \in L^2(\mathbb{R}^3) \mid \mathrm{dist}_{L^2}(\varphi, \mathcal{M}_\mathcal{F}) \leqslant \delta\}. \tag{2.9}$$

For any $\varphi \in (\mathcal{M}_\mathcal{F})_\delta$, we define $z_\varphi \in \mathbb{R}^3$ via

$$P^{\mathcal{M}_\mathcal{F}}_{L^2}(\varphi) = \varphi_\mathrm{P}^{z_\varphi}. \tag{2.10}$$

Then z_φ is a differentiable function from $(\mathcal{M}_\mathcal{F})_\delta$ to $\mathbb{R}^3$ and its partial derivative in the direction $\eta \in L^2(\mathbb{R}^3)$ is given by

$$\partial_t z_{\varphi+t\eta}\restriction_{t=0} = A_\varphi^{-1}\langle \mathrm{Re}\eta|\nabla\varphi_P^{z_\varphi}\rangle, \tag{2.11}$$

where A is the invertible matrix defined for any $\varphi \in (\mathcal{M}_\mathcal{F})_\delta$ by $A_{i,j} := -\mathrm{Re}\langle\varphi|\partial_i\partial_j\varphi_P^{z_\varphi}\rangle$.

Remark 2.1. Likewise, it can be shown that the H^1- (resp. L^2-) projection onto $\mathcal{M}_\mathcal{E}$ have similar properties: there exists $\delta > 0$ such that the H^1- (resp. the L^2-) projection onto $\mathcal{M}_\mathcal{E}$

$$P^{\mathcal{M}_\mathcal{E}}_{H^1}(\psi) = \mathrm{e}^{\mathrm{i}\theta_\psi}\,\psi_\mathrm{P}^{y_\psi}, \qquad \left(\text{resp. } P^{\mathcal{M}_\mathcal{E}}_{L^2}(\psi) = \mathrm{e}^{\mathrm{i}\theta'_\psi}\,\psi_\mathrm{P}^{y'_\psi}\right), \tag{2.12}$$

is well-defined on the set $(\mathcal{M}_\mathcal{E})^{H^1}_\delta := \{\psi \in L^2(\mathbb{R}^3) | \mathrm{dist}_{H^1}(\psi, \mathcal{M}_\mathcal{E}) \leqslant \delta\}$ (resp. $(\mathcal{M}_\mathcal{E})^{L^2}_\delta := \{\psi \in L^2(\mathbb{R}^3) | \mathrm{dist}_{L^2}(\psi, \mathcal{M}_\mathcal{E}) \leqslant \delta\}$) and the functions y_ψ, θ_ψ (resp. y'_ψ, θ'_ψ) defined through (2.12) are differentiable functions from $(\mathcal{M}_\mathcal{E})^{H^1}_\delta$ (resp. $(\mathcal{M}_\mathcal{E})^{L^2}_\delta$) to $\mathbb{R}^3$ and $\mathbb{R}/(2\pi\mathbb{Z})$.

2.2. Position and velocity of solutions

In this section, we give a meaning to the notion of position, and therefore velocity, for solutions of the LP equations (at least for a class of initial data). There is a natural way of defining, given ψ_t, the position of the electron at time t, which is simply given by

$$\mathrm{X}_\mathrm{el}(t) := \langle\psi_t|x|\psi_t\rangle. \tag{2.13}$$

This yields, by straightforward computations using (1.1), that

$$\mathrm{V}_\mathrm{el}(t) := \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X}_\mathrm{el}(t) = 2\langle\psi_t| - i\nabla|\psi_t\rangle. \tag{2.14}$$

Note that (2.14) is always well-defined for $\psi \in H^1(\mathbb{R}^3)$, even although (2.13) not necessarily is.

For the phonon field, the situation is more complicated as φ cannot be interpreted as a probability distribution over positions. This calls for a different approach. By (2.8), lemma 2.1

and the conservation of $\mathcal{G}$ along solutions of (1.1), we know that there exists δ^* such that for any initial condition (ψ_0, φ_0) such that

$$\mathcal{G}(\psi_0, \varphi_0) \leqslant e_{\mathrm{P}} + \delta^*, \tag{2.15}$$

φ_t admits a unique L^2-projection $\varphi_{\mathrm{P}}^{z(t)}$ onto $\mathcal{M}_{\mathcal{F}}$ for all times. We use this to define

$$\mathrm{X}_{\mathrm{ph}}(t) := z(t), \qquad \mathrm{V}_{\mathrm{ph}} := \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{X}_{\mathrm{ph}}(t) = \dot{z}(t). \tag{2.16}$$

Note that $\mathrm{X}_{\mathrm{ph}}(t)$ is indeed differentiable by lemma 2.1 and the differentiability of the LP dynamics. At this point, for any initial data satisfying (2.15), we have a well-defined notion of position and velocity for all times, admittedly in a much less explicit form for the phonon field.

2.3. Initial conditions of velocity v

For any $v \in \mathbb{R}^3$ (or at least for $|v|$ sufficiently small), we are now interested in considering all initial conditions (ψ_0, φ_0) whose solutions have instantaneous velocity v at $t = 0$ (both in the electron and in the phonon coordinate) and to then minimize the functional $\mathcal{G}$ over such states. This will give us an explicit relation between the energy and the velocity of the system, allowing us to define the effective mass of the polaron in the classical setting defined by the LP equations.

Note that by radial symmetry of the problem only the absolute value of the velocity, and not its direction, affects our analysis. Hence, for $v \in \mathbb{R}$, we consider initial conditions (ψ_0, φ_0) such that

(a) $(\psi_0, \varphi_0) \in H^1(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$ with $\|\psi_0\|_2 = 1$ and such that (2.15) is satisfied,
(b) $\mathrm{V}_{\mathrm{el}}(0) = \mathrm{V}_{\mathrm{ph}}(0) = v(1, 0, 0)$.

The set of admissible initial conditions of velocity $v \in \mathbb{R}$ can hence be compactly written as

$$I_v := \{(\psi_0, \varphi_0) | \text{(a), (b) are satisfied}\}. \tag{2.17}$$

We will show below that it is non-empty for small enough v.

2.4. Expansion of the energy

In order to compute the effective mass of the polaron, we now minimize the energy $\mathcal{G}$ over the set I_v. To this end, we define the energy

$$E(v) := \inf_{(\psi_0,\varphi_0)\in I_v} \mathcal{G}(\psi_0, \varphi_0). \tag{2.18}$$

The following theorem gives an expansion of $E(v)$ for sufficiently small velocities v. Its proof will be given in section 3.

Theorem 2.1. *As $v \to 0$ we have*

$$E(v) = e_{\mathrm{P}} + v^2 \left(\frac{1}{4} + \frac{\alpha^4}{3} \|\nabla \varphi_{\mathrm{P}}\|_2^2 \right) + O(v^3). \tag{2.19}$$

Since the kinetic energy of a particle of mass m and velocity v equals $mv^2/2$, (2.19) identifies the effective mass of the system as

$$m_{\text{eff}} = \lim_{v\to 0} \frac{E(v) - e_{\text{P}}}{v^2/2} = \frac{1}{2} + \frac{2\alpha^4}{3}\|\nabla\varphi_{\text{P}}\|_2^2. \tag{2.20}$$

The first term $1/2$ is simply the bare mass of the electron in our units, while the second term $\frac{2\alpha^4}{3}\|\nabla\varphi_{\text{P}}\|_2^2$ corresponds to the additional mass acquired through the interaction with the phonon field. It agrees with the prediction in [15], and is conjectured to coincide with the effective mass in the Fröhlich model in the limit $\alpha \to \infty$. Note that since $(-\Delta)^{1/2}\varphi_{\text{P}} = -|\psi^{\text{P}}|^2$, $\|\nabla\varphi_{\text{P}}\|_2 = \|\psi^{\text{P}}\|_4^2$, which can be evaluated numerically [23].

Remark 2.2 (Traveling waves). The heuristic computations contained in the physics literature concerning m_{eff} [1, 15] all rely, in one way or another, on the existence of traveling wave solutions of the LP equations of velocity v (at least for sufficiently small velocity), i.e. solutions with initial data (ψ_v, φ_v) such that

$$(\psi_t(x), \varphi_t(x)) = (\mathrm{e}^{-\mathrm{i}e_v t}\,\psi_v(x - vt), \varphi_v(x - vt)), \tag{2.21}$$

for suitable $e_v \in \mathbb{R}$. Such solutions would allow to define the energy of the system at velocity v as $E^{\text{TW}}(v) = \mathcal{G}(\psi_v, \varphi_v)$, and a perturbative calculation (discussed in section 4.1 below) yields indeed

$$\lim_{v\to 0} \frac{E^{\text{TW}}(v) - e_{\text{P}}}{v^2/2} = \frac{1}{2} + \frac{2\alpha^4}{3}\|\nabla\varphi_{\text{P}}\|^2, \tag{2.22}$$

in agreement with (2.20). Unfortunately, this approach turns out to be only formal, and we conjecture traveling wave solutions to not exist for any $\alpha > 0$, $v > 0$, as explained in more detail in section 4.1.

Remark 2.3. In section 2.2, we used the standard approach from quantum mechanics to define the electron's position (2.13) and velocity (2.14). We could, instead, use also for the electron a similar approach to the one we use for the phonon field (i.e. (2.16)) through the projection onto the manifold of minimizers $\mathcal{M}_{\mathcal{E}}$. A natural question is whether one obtains the same effective mass using this different notion of position. In section 4.2, we show that, in fact, this alternate definition yields a different effective mass equal to

$$\widetilde{m}_{\text{eff}} = \frac{2\|\nabla\psi_{\text{P}}\|_2^4}{3\|\nabla\varphi_{\text{P}}\|_2^2} + \frac{2\alpha^4}{3}\|\nabla\varphi_{\text{P}}\|_2^2. \tag{2.23}$$

This coincides with (2.20) and (2.22) for large α (hence still confirming the prediction in [15]), but differs in the $O(1)$ term. In fact, as we discuss in section 4.2, one has $\widetilde{m}_{\text{eff}} < m_{\text{eff}}$.

3. Proof of theorem 2.1

Let us denote $\delta_1 = \psi_0 - \psi_{\text{P}}$ and $\delta_2 = \varphi_0 - \varphi_{\text{P}}$. Expanding $\mathcal{G}$ in (2.1) and using that $\varphi_{\text{P}} = -\sigma_{\psi_{\text{P}}}$ we find

$$\begin{aligned}\mathcal{G}(\psi_0, \varphi_0) &= \mathcal{G}(\psi_{\text{P}} + \delta_1, \varphi_{\text{P}} + \delta_2)\\ &= e_{\text{P}} + 2\,\langle\psi_{\text{P}}|\,h_{\varphi_{\text{P}}}\,|\mathrm{Re}\,\delta_1\rangle + \langle\delta_1|h_{\varphi_{\text{P}}}|\delta_1\rangle + 2\,\langle\mathrm{Re}\,\delta_1|\,V_{\delta_2}\,|\psi_{\text{P}}\rangle + \|\delta_2\|_2^2 + \langle\delta_1|V_{\delta_2}|\delta_1\rangle.\end{aligned} \tag{3.1}$$

Since ψ_0 is normalized, we have

$$1 = \|\psi_0\|_2^2 = \|\psi_{\mathrm{P}} + \delta_1\|_2^2 = 1 + \|\delta_1\|_2^2 + 2\langle\psi_{\mathrm{P}}|\mathrm{Re}\,\delta_1\rangle \iff 2\langle\psi_{\mathrm{P}}|\mathrm{Re}\,\delta_1\rangle = -\|\delta_1\|_2^2. \tag{3.2}$$

Hence

$$2\,\langle\psi_{\mathrm{P}}|\,h_{\varphi_{\mathrm{P}}}\,|\mathrm{Re}\,\delta_1\rangle = 2\mu_{\mathrm{P}}\langle\psi_{\mathrm{P}}|\mathrm{Re}\,\delta_1\rangle = -\mu_{\mathrm{P}}\|\delta_1\|_2^2, \tag{3.3}$$

and using $\|V_{\delta_2}\delta_1\|_2 \leqslant C\|\delta_2\|_2\,\|\delta_1\|_{H^1}$ (see, e.g. [18, lemma III.2]) we arrive at

$$\mathcal{G}(\psi_0,\varphi_0) = e_{\mathrm{P}} + \langle\delta_1|H_{\mathrm{P}}|\delta_1\rangle + 2\,\langle\mathrm{Re}\,\delta_1|\,V_{\delta_2}\,|\psi_{\mathrm{P}}\rangle + \|\delta_2\|_2^2 + O(\|\delta_2\|_2\|\delta_1\|_{H^1}^2). \tag{3.4}$$

By completing the square, we have

$$\begin{aligned}\|\mathrm{Re}\,\delta_2\|_2^2 + 2\,\langle\mathrm{Re}\,\delta_1|\,V_{\delta_2}\,|\psi_{\mathrm{P}}\rangle = {}& \|\mathrm{Re}\,\delta_2 + 2(-\Delta)^{-1/2}(\psi_{\mathrm{P}}\,\mathrm{Re}\,\delta_1)\|_2^2\\ &- 4\langle\mathrm{Re}\,\delta_1|\psi_{\mathrm{P}}(-\Delta)^{-1}\psi_{\mathrm{P}}|\mathrm{Re}\,\delta_1\rangle,\end{aligned} \tag{3.5}$$

and therefore

$$\begin{aligned}\mathcal{G}(\psi_0,\varphi_0) = {}& e_{\mathrm{P}} + \langle\mathrm{Im}\,\psi_0|H_{\mathrm{P}}|\mathrm{Im}\,\psi_0\rangle + \|\mathrm{Im}\,\varphi_0\|_2^2\\ &+ \|\mathrm{Re}\,\delta_2 + 2(-\Delta)^{-1/2}(\psi_{\mathrm{P}}\,\mathrm{Re}\,\delta_1)\|_2^2\\ &+ \langle\mathrm{Re}\,\delta_1|H_{\mathrm{P}} - 4X_{\mathrm{P}}|\mathrm{Re}\,\delta_1\rangle + O(\|\delta_2\|_2\|\delta_1\|_{H^1}^2),\end{aligned} \tag{3.6}$$

where X_{P} is the operator with integral kernel $X_P(x,y) := \psi_P(x)(-\Delta)^{-1}(x,y)\psi_{\mathrm{P}}(y)$. Since X_{P} is bounded, and $\|P_{\psi_{\mathrm{P}}}\,\mathrm{Re}\,\delta_1\| = \|\delta_1\|_2^2/2$ by (3.2) (with $P_{\psi_{\mathrm{P}}} = |\psi_{\mathrm{P}}\rangle\langle\psi_{\mathrm{P}}|$ the rank one projection onto ψ_{P}), we also have

$$\begin{aligned}\mathcal{G}(\psi_0,\varphi_0) = {}& e_{\mathrm{P}} + \langle\mathrm{Im}\,\psi_0|H_{\mathrm{P}}|\mathrm{Im}\,\psi_0\rangle + \|\mathrm{Im}\,\varphi_0\|_2^2\\ &+ \|\mathrm{Re}\,\delta_2 + 2(-\Delta)^{-1/2}(\psi_{\mathrm{P}}\,\mathrm{Re}\,\delta_1)\|_2^2\\ &+ \langle\mathrm{Re}\,\delta_1|Q(H_{\mathrm{P}} - 4X)Q|\mathrm{Re}\,\delta_1\rangle + O(\|\delta_2\|_2\|\delta_1\|_{H^1}^2) + O(\|\delta_1\|_{L^2}^3),\end{aligned} \tag{3.7}$$

where $Q = \mathbb{1} - P_{\psi_{\mathrm{P}}}$.

Upper bound: for sufficiently small v, we use as a trial state

$$(\bar{\psi}_0,\bar{\varphi}_0) = \left(f_v\psi_{\mathrm{P}} + ig_vH_{\mathrm{P}}^{-1}\partial_1\psi_{\mathrm{P}},\ \varphi_{\mathrm{P}} + iv\alpha^2\partial_1\varphi_{\mathrm{P}}\right), \tag{3.8}$$

with $f_v, g_v > 0$ given by

$$f_v^2 := \frac{2v^2\|H_{\mathrm{P}}^{-1}\partial_1\psi_{\mathrm{P}}\|_2^2}{1 - \sqrt{1 - 4v^2\|H_{\mathrm{P}}^{-1}\partial_1\psi_{\mathrm{P}}\|_2^2}}, \qquad g_v^2 := \frac{1 - \sqrt{1 - 4v^2\|H_{\mathrm{P}}^{-1}\partial_1\psi_{\mathrm{P}}\|_2^2}}{2\|H_{\mathrm{P}}^{-1}\partial_1\psi_{\mathrm{P}}\|_2^2}. \tag{3.9}$$

Note that $\partial_1\psi_{\mathrm{P}}$ is orthogonal to ψ_{P}, hence $H_{\mathrm{P}}^{-1}\partial_1\psi_{\mathrm{P}}$ is well-defined. We begin by showing that (3.8) is an element of the set of admissible initial data I_v in (2.17). To prove that $(\bar{\psi}_0,\bar{\varphi}_0)$ satisfies (a), we only need to check that $\bar{\psi}_0$ is normalized (which follows easily from (3.9)) as the condition (2.15) will follow *a posteriori* from the energy bound we shall derive. We now proceed to show that $(\bar{\psi}_0,\bar{\varphi}_0)$ satisfies (b). For the electron, using that $H_{\mathrm{P}}^{-1}\partial_j\psi_{\mathrm{P}} = -x_j\psi_{\mathrm{P}}/2$ (which can be checked by applying H_{P} and using that $[H_{\mathrm{P}}, x_1] = -2\partial_1$) and consequently that

$$\langle\partial_i\psi_{\mathrm{P}}|\,H_{\mathrm{P}}^{-1}\,|\partial_j\psi_{\mathrm{P}}\rangle = \delta_{ij}/4, \tag{3.10}$$

since ψ_P is radial, we can conclude that

$$-2\langle\bar{\psi}_0|i\partial_j|\bar{\psi}_0\rangle = 4f_v g_v\langle H_{\mathrm{P}}^{-1}\partial_1\psi_{\mathrm{P}}|\partial_j\psi_{\mathrm{P}}\rangle = v\delta_{j1}, \tag{3.11}$$

i.e. that $\mathrm{V_{el}}(0) = v(1,0,0)$, as required.

For the phonons, we first note that $\mathrm{X_{ph}}(0) = 0$, since $\mathrm{Re}\,\bar{\varphi}_0 = \varphi_{\mathrm{P}}$. Next, we derive a relation for the velocity of the phonons $\mathrm{V_{ph}}(t) = \dot{z}(t)$ in terms of their position $\mathrm{X_{ph}}(t) = z(t)$ for general time t. Since

$$\min_z \|\varphi_t - \varphi_{\mathrm{P}}^z\|_2^2 = \|\varphi_t - \varphi_{\mathrm{P}}^{z(t)}\|_2^2, \tag{3.12}$$

the position $z(t)$ necessarily has to satisfy

$$\mathrm{Re}\langle\varphi_t|(u\cdot\nabla)\varphi_{\mathrm{P}}^{z(t)}\rangle = 0 \quad \text{for all } u\in\mathbb{S}^2 \iff \mathrm{Re}\,\varphi_t \perp \mathrm{span}\{\nabla\varphi_{\mathrm{P}}^{z(t)}\}. \tag{3.13}$$

Differentiating (3.13) w.r.t. time, using (1.1) and evaluating the resulting expression at $t = 0$, we arrive at

$$\begin{aligned} 0 &= \mathrm{Re}\langle -i\alpha^{-2}(u\cdot\nabla)(\bar{\varphi}_0 + \sigma_{\bar{\psi}_0})|\varphi_{\mathrm{P}}\rangle - \mathrm{Re}\langle(\dot{z}(0)\cdot\nabla)\bar{\varphi}_0|(u\cdot\nabla)\varphi_{\mathrm{P}}\rangle \\ &= \langle -\alpha^{-2}\,\mathrm{Im}\,\bar{\varphi}_0|(u\cdot\nabla)\varphi_{\mathrm{P}}\rangle - \langle(\dot{z}(0)\cdot\nabla)\mathrm{Re}\,\bar{\varphi}_0|(u\cdot\nabla)\varphi_{\mathrm{P}}\rangle \\ &= -\langle v\partial_1\varphi_{\mathrm{P}}|(u\cdot\nabla)\varphi_{\mathrm{P}}\rangle - \langle(\dot{z}(0)\cdot\nabla)\varphi_{\mathrm{P}}|(u\cdot\nabla)\varphi_{\mathrm{P}}\rangle, \end{aligned} \tag{3.14}$$

which the velocity $\dot{z}(0)$ has to satisfy for all $u\in\mathbb{S}^2$, given its position $\mathrm{X_{ph}}(0) = z(0) = 0$. By invertibility of the coefficient matrix, (3.14) has the unique solution $\dot{z}(0) = v(1,0,0)$, and we indeed conclude that $\mathrm{V_{ph}}(0) = v(1,0,0)$.

We now evaluate $\mathcal{G}(\bar{\psi}_0,\bar{\varphi}_0)$. Since $f_{v=1+O(v^2),gv=v+O(v^3)}$, using (3.7) and (3.10) we find

$$E(v) \leqslant \mathcal{G}(\bar{\psi}_0,\bar{\varphi}_0) = e_{\mathrm{P}} + v^2\left(\frac{1}{4} + \alpha^4\|\partial_1\varphi_{\mathrm{P}}\|_2^2\right) + O(v^3), \tag{3.15}$$

verifying on the one hand (2.15) for sufficiently small v, and on the other hand the rhs of (2.19) as an upper bound on $E(v)$ (using that φ_{P} is radial).

Lower bound: we first observe that to derive a lower bound on $E(v)$ we can w.l.o.g. restrict to initial conditions (ψ_0,φ_0) satisfying additionally

$$P_{L^2}^{\mathcal{M}_{\mathcal{E}}}(\psi_0) > 0, \tag{3.16}$$

$$\mathrm{X_{ph}}(0) = 0. \tag{3.17}$$

This simply follows from the invariance of $\mathcal{G}$ under translations (of both ψ and φ) and under changes of phase of ψ. Moreover, by the upper bound derived in the first step of this proof and the coercivity of $\mathcal{E}$ and $\mathcal{F}$ in (2.8), we conclude that it is sufficient to minimize over elements of I_v such that $\mathrm{dist}_{H^1}(\psi_0,\mathcal{M}_{\mathcal{E}}) = O(v) = \mathrm{dist}_{L^2}(\varphi_0,\mathcal{M}_{\mathcal{F}})$ for small v. Since the L^2-projection of φ_0 is φ_{P} by (3.17), it immediately follows that $\|\delta_2\|_2 = O(v)$. We now proceed to show that necessarily also $\|\delta_1\|_{H^1} = O(v)$. Let $y', y \in \mathbb{R}^3$ and $\theta \in [0, 2\pi)$ be such that

$$P_{L^2}^{\mathcal{M}_{\mathcal{E}}}(\psi_0) = \psi_{\mathrm{P}}^{y'}, \qquad P_{H^1}^{\mathcal{M}_{\mathcal{E}}}(\psi_0) = \mathrm{e}^{\mathrm{i}\theta}\,\psi_{\mathrm{P}}^{y}, \tag{3.18}$$

where we recall that the L^2-projection is assumed to be positive by (3.16). Combining the upper bound derived in the first step with [3, equation (53)], we get

$$\|\varphi_0 - \varphi_{\mathrm{P}}^{y}\|_2^2 \leqslant C\,(\mathcal{G}(\psi_0, \varphi_0) - e_{\mathrm{P}}) \leqslant Cv^2. \tag{3.19}$$

There exist $\delta, C_1, C_2 > 0$ such that

$$\|\varphi_{\mathrm{P}} - \varphi_{\mathrm{P}}^{y}\|_2 \geqslant \begin{cases} C_1|y|\|\nabla\varphi_{\mathrm{P}}\|_2, & |y| \leqslant \delta \\ C_2 & |y| > \delta \end{cases}, \tag{3.20}$$

and this allows to conclude that $|y| = O(v)$. In other words, assuming centering w.r.t. to translations in the phonon coordinate (i.e. (3.17)) forces, at low energies, also the centering w.r.t. translations in the electron coordinate, at least approximately. At this point, it is also easy to verify that $\theta = O(v)$ (and, as an aside, that $|y'| = O(v)$), since, by the upper bound derived in the first step and the coercivity of $\mathcal{E}$, we have

$$\|\psi_{\mathrm{P}}^{y'} - \mathrm{e}^{\mathrm{i}\theta}\,\psi_{\mathrm{P}}^{y}\|_2 \leqslant \|\psi_{\mathrm{P}}^{y'} - \psi_0\|_2 + \|\mathrm{e}^{\mathrm{i}\theta}\,\psi_{\mathrm{P}}^{y} - \psi_0\|_2 = O(v). \tag{3.21}$$

In particular, we conclude that

$$\|\delta_1\|_{H^1} \leqslant \|\mathrm{e}^{\mathrm{i}\theta}\,\psi_{\mathrm{P}}^{y} - \psi_0\|_{H^1} + \|\psi_{\mathrm{P}} - \mathrm{e}^{\mathrm{i}\theta}\,\psi_{\mathrm{P}}^{y}\|_{H^1} = O(v). \tag{3.22}$$

Using again (3.7) and that $Q(H_{\mathrm{P}} - 4X_{\mathrm{P}})Q \geqslant 0$, we conclude that for any $(\psi_0, \varphi_0) \in I_v$ satisfying (3.16) and (3.17), as well as $\mathcal{G}(\psi_0, \varphi_0) \leqslant e_{\mathrm{P}} + O(v^2)$, we have

$$\mathcal{G}(\psi_0, \varphi_0) \geqslant e_{\mathrm{P}} + \langle \mathrm{Im}\,\psi_0 | H_{\mathrm{P}} | \mathrm{Im}\,\psi_0 \rangle + \|\mathrm{Im}\,\varphi_0\|_2^2 + O(v^3). \tag{3.23}$$

By arguing as in (3.14), we see that the conditions $\mathrm{X}_{\mathrm{ph}}(0) = 0$ and $\mathrm{V}_{\mathrm{ph}}(0) = v$ imply that

$$P_{\nabla\varphi_{\mathrm{P}}}(\mathrm{Im}\,\varphi_0 + v\alpha^2\partial_1\mathrm{Re}\,\varphi_0) = 0, \tag{3.24}$$

where $P_{\nabla\varphi_{\mathrm{P}}}$ denotes the projection onto the span of $\partial_j\varphi_{\mathrm{P}}$, $1 \leqslant j \leqslant 3$. Since $P_{\nabla\varphi_{\mathrm{P}}}\partial_1$ is a bounded operator, and $\|\delta_2\|_2 = O(v)$, we find

$$\|\mathrm{Im}\,\varphi_0\|_2^2 \geqslant \|P_{\nabla\varphi_{\mathrm{P}}}\mathrm{Im}\,\varphi_0\|_2^2 = v^2\alpha^4\|\partial_1\varphi_{\mathrm{P}} + P_{\nabla\varphi_{\mathrm{P}}}\partial_1\mathrm{Re}\,\delta_2\|_2^2 \geqslant v^2\alpha^4\|\partial_1\varphi_{\mathrm{P}}\|_2^2 - O(v^3). \tag{3.25}$$

We are left with giving a lower bound on $\langle \mathrm{Im}\,\psi_0 | H_{\mathrm{P}} | \mathrm{Im}\,\psi_0 \rangle$, under the condition that

$$2\langle \psi_0 | -i\nabla | \psi_0 \rangle = 4\langle \mathrm{Im}\,\psi_0 | \nabla\,\mathrm{Re}\,\psi_0 \rangle = v(1, 0, 0). \tag{3.26}$$

We already argued in (3.22) that $\|\psi_0 - \psi_{\mathrm{P}}\|_{H^1} = O(v)$, and therefore

$$4\langle \mathrm{Im}\,\psi_0 | \nabla\psi_{\mathrm{P}} \rangle = v(1, 0, 0) + O(v^2). \tag{3.27}$$

Completing the square, we find

$$\begin{aligned}\langle \mathrm{Im}\,\psi_0|H_\mathrm{P}|\mathrm{Im}\,\psi_0\rangle &= \langle H_\mathrm{P}\,\mathrm{Im}\,\psi_0 - v\partial_1\psi_\mathrm{P}|H_\mathrm{P}^{-1}|H_\mathrm{P}\,\mathrm{Im}\,\psi_0 - v\partial_1\psi_\mathrm{P}\rangle \\ &\quad + 2v\langle \mathrm{Im}\,\psi_0|\partial_1\psi_\mathrm{P}\rangle - v^2\langle\partial_1\psi_\mathrm{P}|H_\mathrm{P}^{-1}|\partial_1\psi_\mathrm{P}\rangle \\ &\geqslant 2v\langle \mathrm{Im}\,\psi_0|\partial_1\psi_\mathrm{P}\rangle - v^2\langle\partial_1\psi_\mathrm{P}|H_\mathrm{P}^{-1}|\partial_1\psi_\mathrm{P}\rangle. \end{aligned} \tag{3.28}$$

From the constraint (3.27) and (3.10), it thus follows that

$$\langle \mathrm{Im}\,\psi_0|H_\mathrm{P}|\mathrm{Im}\,\psi_0\rangle \geqslant \frac{v^2}{4} + O(v^3). \tag{3.29}$$

By combining (3.23), (3.25) and (3.29), we arrive at the final lower bound

$$E(v) \geqslant e_\mathrm{P} + v^2\left(\frac{1}{4} + \alpha^4\|\partial_1\varphi_\mathrm{P}\|_2^2\right) + O(v^3). \tag{3.30}$$

Again, since φ_P is radial, this is of the desired form, and hence the proof is complete. □

4. Further considerations

In this section, we carry out the details related to remarks 2.2 and 2.3.

4.1. Effective mass through traveling wave solutions

A possible way of formalizing the derivation of the effective mass in [1, 15] relies on traveling wave solutions of the LP equations. A traveling wave of velocity $v \in \mathbb{R}^3$ is a solution (ψ_t, φ_t) of (1.1) of the form

$$(\psi_t, \varphi_t) = (\mathrm{e}^{-\mathrm{i}e_v t}\,\psi_v^\mathrm{TW}(\cdot - vt), \varphi_v^\mathrm{TW}(\cdot - vt)), \tag{4.1}$$

for all $t \in \mathbb{R}$, with $e_v \in \mathbb{R}$ defining a suitable phase factor. As before, by rotation invariance we can restrict our attention to velocities of the form $v(1, 0, 0)$ with $v \in \mathbb{R}$ in the following.

Note that in the case $\alpha = 0$, where $\varphi_t = -\sigma_{\psi_t}$ for all $t \in \mathbb{R}$, the LP equations simplify to a non-linear Schrödinger equation (also known as Choquard equation). In this case, a traveling wave is given by $\psi_v^\mathrm{TW}(x) = \mathrm{e}^{\mathrm{i}x_1 v/2}\,\psi_\mathrm{P}(x)$ with $e_v = \mu_\mathrm{P} + \frac{v^2}{4}$, and its energy can be computed to be

$$\mathcal{G}\left(\psi_v^\mathrm{TW}, -\sigma_{\psi_v^\mathrm{TW}}\right) = e_\mathrm{P} + \frac{v^2}{4}, \tag{4.2}$$

yielding an effective mass $m = 1/2$ at $\alpha = 0$. For the case $\alpha > 0$, on the other hand, we conjecture that there are no traveling wave solutions of the form (4.1).

Conjecture 4.1. For $\alpha > 0$, there are no solutions to the LP equation (1.1) of the form (4.1) with $v \neq 0$.

The motivation for this conjecture comes from the vanishing of the sound velocity in the medium. An initially moving electron can be expected to be slowed down to zero speed by emitting radiation. Establishing this effect rigorously for the LP equations remains an open problem, however.

If one *assumes* the existence of traveling wave solutions, at least for small v, one can predict an effective mass that agrees with our formula (2.20), as we shall now demonstrate.

From the LP equation (1.1) one easily sees that a traveling wave solution needs to satisfy

$$\begin{aligned} -iv\partial_1\psi_v^{\mathrm{TW}} &= \left(h_{\varphi_v^{\mathrm{TW}}} + e_v\right)\psi_v^{\mathrm{TW}} \\ -i\alpha^2 v\partial_1\varphi_v^{\mathrm{TW}} &= \varphi_v^{\mathrm{TW}} + \sigma_{\psi_v^{\mathrm{TW}}}. \end{aligned} \tag{4.3}$$

We shall denote by $E^{\mathrm{TW}}(v)$ the energy of the traveling wave as a function of the velocity $v \in \mathbb{R}$, i.e.

$$E^{\mathrm{TW}}(v) := \mathcal{G}(\psi_v^{\mathrm{TW}}, \varphi_v^{\mathrm{TW}}). \tag{4.4}$$

In the following, we assume that $e_v = \mu_{\mathrm{P}} + O(v^2)$ and that the traveling wave is of the form

$$(\psi_v^{\mathrm{TW}}, \varphi_v^{\mathrm{TW}}) = \left(\frac{\psi_{\mathrm{P}} + v\xi_v}{\|\psi_{\mathrm{P}} + v\xi_v\|_2}, \varphi_{\mathrm{P}} + v\eta_v\right), \tag{4.5}$$

with both ξ_v and η_v bounded in v and converging to some (ξ, η) as $v \to 0$. In other words, we assume that the traveling waves have a suitable differentiability in v, at least for small v, and converge to the standing wave solution $(\mathrm{e}^{-\mathrm{i}\mu_{\mathrm{P}}t}\psi_{\mathrm{P}}, \varphi_{\mathrm{P}})$ for $v = 0$. W.l.o.g. we may also assume that ξ_v is orthogonal to ψ_P.

We can then use that

$$\frac{1}{\|\psi_{\mathrm{P}} + v\xi_v\|_2^2} = 1 - v^2\frac{\|\xi_v\|_2^2}{\|\psi_{\mathrm{P}} + v\xi_v\|_2^2} = 1 - v^2\|\xi\|_2^2 + o(v^2), \tag{4.6}$$

in order to linearize the traveling wave equation (4.1), obtaining that (ξ, η) solves

$$\begin{pmatrix} i\partial_1\psi_{\mathrm{P}} \\ i\alpha^2\partial_1\varphi_{\mathrm{P}} \end{pmatrix} = \begin{pmatrix} H_{\mathrm{P}} & 2\psi_{\mathrm{P}}(-\Delta)^{-1/2}\,\mathrm{Re} \\ 2(-\Delta)^{-1/2}\psi_{\mathrm{P}}\,\mathrm{Re} & 1 \end{pmatrix}\begin{pmatrix} \xi \\ \eta \end{pmatrix}, \tag{4.7}$$

where $H_{\mathrm{P}} = h_{\varphi_{\mathrm{P}}} - \mu_{\mathrm{P}}$, as defined in (2.3). Splitting into real and imaginary parts, we equivalently find

$$H_{\mathrm{P}}\,\mathrm{Im}\,\xi = \partial_1\psi_{\mathrm{P}} \tag{4.8}$$

$$\mathrm{Im}\,\eta = \alpha^2\partial_1\varphi_{\mathrm{P}} \tag{4.9}$$

$$H_{\mathrm{P}}\mathrm{Re}\xi + 2\psi_{\mathrm{P}}(-\Delta)^{-1/2}\mathrm{Re}\,\eta = 0 \tag{4.10}$$

$$2(-\Delta)^{-1/2}\psi_{\mathrm{P}}\,\mathrm{Re}\,\xi + \mathrm{Re}\,\eta = 0. \tag{4.11}$$

Combining (4.10) and (4.11) gives $(H_{\mathrm{P}} - 4X_{\mathrm{P}})\mathrm{Re}\,\xi = 0$, with X_{P} defined after (3.6). It was shown in [16] that the kernel of $H_{\mathrm{P}} - 4X_{\mathrm{P}}$ is spanned by $\nabla\psi_{\mathrm{P}}$, hence $\mathrm{Re}\,\xi \in \mathrm{span}\{\nabla\psi_{\mathrm{P}}\}$. Equation (4.11) then implies that $\mathrm{Re}\,\eta \in \mathrm{span}\{\nabla\varphi_{\mathrm{P}}\}$.

Using these equations and (4.6) in the expansion (3.7), it is straightforward to obtain

$$E^{\mathrm{TW}}(v) = e_{\mathrm{P}} + v^2\left(\frac{1}{4} + \alpha^4\|\partial_1\varphi_{\mathrm{P}}\|_2^2\right) + o(v^2), \tag{4.12}$$

which agrees with (4.2) for the case $\alpha = 0$, and also with (2.19) to leading order in v. In particular, (2.22) holds.

4.2. Effective mass with alternative definition for the electron's velocity

In this section, we discuss a different approach to the definition of the effective mass. This approach is based on an alternative way of defining the electron's position and velocity. While in section 2.2 we use the standard definition from quantum mechanics, here we use a definition similar to the one of the phonons' position and velocity (2.16). For this purpose, we recall remark 2.1 and that δ^* has been chosen such that the condition $\mathcal{E}(\psi_0) \leqslant \mathcal{G}(\psi_0, \varphi_0) \leqslant e_{\mathrm{P}} + \delta^*$ ensures that for all times there exists a unique L^2-projection $\mathrm{e}^{\mathrm{i}\theta(t)}\,\psi_{\mathrm{P}}^{y(t)}$ of ψ_t onto the manifold $\mathcal{M}_{\mathcal{E}}$. Then, we define the electron's position and velocity by

$$\widetilde{\mathrm{X}}_{\mathrm{el}}(t) = y(t), \qquad \widetilde{\mathrm{V}}_{\mathrm{el}}(t) = \dot{y}(t). \tag{4.13}$$

Similarly to the conditions (a) and (b) in section 2.2, we define the set of admissible initial data as

$$\widetilde{I}_v = \{(\psi_0, \varphi_0)|(\mathrm{a}), (\mathrm{b}') \text{ are satisfied}\}, \tag{4.14}$$

where

(b′) $\widetilde{\mathrm{V}}_{\mathrm{el}}(t) = \mathrm{V}_{\mathrm{ph}}(0) = v(1, 0, 0)$.

Note that we are leaving the parameter $\dot{\theta}(0)$ free, which in this case is also relevant. In other words, we have

$$\widetilde{I}_v = \cup_{\kappa\in\mathbb{R}} \widetilde{I}_{v,\kappa}, \tag{4.15}$$

where

$$\widetilde{I}_{v,\kappa} = \{(\psi_0, \varphi_0)|(\mathrm{a}), (\mathrm{b}') \text{ are satisfied and } \dot{\theta}(0) = \kappa\}. \tag{4.16}$$

Minimizing now the energy over all states of the set $\widetilde{I}_v$

$$\widetilde{E}(v) := \inf_{(\psi_0,\varphi_0)\in\widetilde{I}_v} \mathcal{G}(\psi_0, \varphi_0), \tag{4.17}$$

leads to an energy expansion in v that differs from the one of theorem 2.1 in its second order.

Proposition 4.1. *As* $v \to 0$, *we have*

$$\widetilde{E}(v) = e_{\mathrm{P}} + v^2 \left(\frac{\|\nabla\psi_{\mathrm{P}}\|_2^4}{3\|\nabla\varphi_{\mathrm{P}}\|_2^2} + \frac{\alpha^4}{3}\|\nabla\varphi_{\mathrm{P}}\|_2^2 \right) + O(v^3). \tag{4.18}$$

The energy expansion in (4.18) leads to the effective mass

$$\widetilde{m}_{\mathrm{eff}} = \lim_{v\to 0} \frac{\widetilde{E}(v) - e_{\mathrm{P}}}{v^2/2} = \frac{2\|\nabla\psi_{\mathrm{P}}\|_2^4}{3\|\nabla\varphi_{\mathrm{P}}\|_2^2} + \frac{2\alpha^4}{3}\|\nabla\varphi_{\mathrm{P}}\|_2^2, \tag{4.19}$$

which agrees with (2.20) and (2.22) in leading order for large α only (and thus still confirms the LP prediction [15]), but differs in the $O(1)$ term. In fact, it turns out that $\widetilde{m}_{\mathrm{eff}} < m_{\mathrm{eff}}$ with m_{eff} defined in (2.22).

This follows from the observation that the trial state

$$(\widetilde{\psi}_0, \widetilde{\varphi}_0) = \left(\frac{f_v \psi_{\mathrm{P}} + ivH_{\mathrm{P}}^{-1}\partial_1\psi_{\mathrm{P}}}{\|f_v\psi_{\mathrm{P}} + ivH_{\mathrm{P}}^{-1}\partial_1\psi_{\mathrm{P}}\|}, \varphi_{\mathrm{P}} + iv\alpha^2\partial_1\varphi_{\mathrm{P}} \right), \tag{4.20}$$

with $f_v = \frac{1}{2}\left(1 + \sqrt{1 - v^2/(4\|\partial_1\psi_{\mathrm{P}}\|_2^2)}\right)$ (which coincides up to terms of order v^2 with the trial state (3.8)) is an element of $\widetilde{I}_{v,\bar{\kappa}}$ for $\bar{\kappa} = -\mu_{\mathrm{P}} + 4\|\partial_1\psi_{\mathrm{P}}\|_2^2(f_v - 1)$ and is such that $\mathcal{G}(\widetilde{\psi}_0, \widetilde{\varphi}_0) = e_{\mathrm{P}} + m_{\mathrm{eff}}\, v^2/2 + O(v^3)$. Thus, $\widetilde{m}_{\mathrm{eff}} \leqslant m_{\mathrm{eff}}$ and equality holds if and only if equality (up to terms $o(v^2)$) holds in (4.36). This is the case if and only if

$$Q_{\psi_{\mathrm{P}}}\left(\mathrm{Im}\,\widetilde{\psi}_0 - cv\partial_1\psi_{\mathrm{P}}\right) = o(v). \tag{4.21}$$

Using (4.20), equality holds if and only if

$$0 = H_{\mathrm{P}}^{-1}\partial_1\psi_{\mathrm{P}} - c\partial_1\psi_{\mathrm{P}} = -\left(x_1/2 + c\partial_1\right)\psi_{\mathrm{P}}, \tag{4.22}$$

i.e. recalling the radiality of ψ_{P}, if and only if ψ_{P} is a Gaussian with variance $\sigma^2 = 1/(2c)$. Since ψ_{P} satisfies the Euler–Lagrange equation

$$H_{\mathrm{P}}\psi_{\mathrm{P}} = 0 \iff V_{\varphi_{\mathrm{P}}}\psi_{\mathrm{P}} = (-\Delta + \mu_{\mathrm{P}})\psi_{\mathrm{P}}, \tag{4.23}$$

it cannot be a Gaussian and therefore $\tilde{m}_{\mathrm{eff}} < m_{\mathrm{eff}}$.

We present only a sketch of proof of proposition 4.1, since it uses very similar arguments as the proof of theorem 2.1.

Sketch of proof of proposition 4.1. **Upper bound**: we use the alternative trial state

$$(\widetilde{\psi}_0, \widetilde{\varphi}_0) = \left(\frac{f_v \psi_{\mathrm{P}} + ivc\partial_1\psi_{\mathrm{P}}}{\|f_v\psi_{\mathrm{P}} + ivc\partial_1\psi_{\mathrm{P}}\|}, \varphi_{\mathrm{P}} + iv\alpha^2\partial_1\varphi_{\mathrm{P}} \right), \tag{4.24}$$

with

$$f_v := \frac{1 + \sqrt{1 + 4c^2v^2\|\partial_1\psi_{\mathrm{P}}\|^2}}{2}, \quad c := \frac{\|\partial_1\psi_{\mathrm{P}}\|^2}{\|\partial_1\varphi_{\mathrm{P}}\|^2}. \tag{4.25}$$

With similar arguments as in the previous section, one can verify that $(\widetilde{\psi}_0, \widetilde{\varphi}_0) \in \widetilde{I}_v$, in particular $(\widetilde{\psi}_0, \widetilde{\varphi}_0) \in \widetilde{I}_{v,\kappa}$ with $\kappa = -\mu_{\mathrm{P}} + \frac{-1+\sqrt{1+4c^2v^2\|\partial_1\psi_{\mathrm{P}}\|^2}}{2c}$.

Note that, similarly to (3.14), one can derive necessary conditions for the velocities $\dot{y}(0), \dot{\theta}(0)$ (using $\widetilde{\mathrm{X}}_{\mathrm{el}}(0) = 0, \theta(0) = 0$), namely

$$\langle [h_{\mathrm{Re}\,\widetilde{\varphi}_0} + \dot{\theta}(0)]\mathrm{Im}\,\widetilde{\psi}_0 - \dot{y}(0)\cdot\nabla\,\mathrm{Re}\,\widetilde{\psi}_0 | (u\cdot\nabla)\psi_{\mathrm{P}}\rangle = 0 \quad \text{for all } u \in \mathbb{S}^2, \tag{4.26}$$

and

$$\langle \psi_{\mathrm{P}} | (h_{\mathrm{Re}\,\widetilde{\varphi}_0} + \dot{\theta}(0))\mathrm{Re}\,\widetilde{\psi}_0 + \dot{y}(0)\cdot\nabla\,\mathrm{Im}\,\widetilde{\psi}_0\rangle = 0. \tag{4.27}$$

Straightforward computations then show that

$$\widetilde{E}(v) \leqslant \mathcal{G}(\widetilde{\psi}_0, \widetilde{\varphi}_0) = e_{\mathrm{P}} + v^2 \left(\frac{\|\partial_1 \psi_{\mathrm{P}}\|_2^4}{\|\partial_1 \varphi_{\mathrm{P}}\|_2^2} + \alpha^4 \|\partial_1 \varphi_{\mathrm{P}}\|_2^2 \right) + O(v^3). \tag{4.28}$$

Lower bound: we proceed similarly to the lower bound in the previous section. First, we assume w.l.o.g. that

$$P_{L^2}^{\mathcal{M}_{\mathcal{E}}}(\psi_0) = \psi_{\mathrm{P}}^{y(0)}, \qquad P_{L^2}^{\mathcal{M}_{\mathcal{F}}}(\varphi_0) = \varphi_{\mathrm{P}}, \tag{4.29}$$

i.e. centering with respect to translations and changes of phase. We can then substitute the two conditions of (b′) and the conditions for $\psi_{\mathrm{P}}^{y(0)}$ (resp. φ_{P}) to be the L^2-projection of ψ_0 (resp. φ_0) onto $\mathcal{M}_{\mathcal{E}}$ (resp. $\mathcal{M}_{\mathcal{F}}$) with their analogue necessary conditions (whose computations proceed along the lines of (4.26) and (4.27)). With this discussion, we are left with the task of minimizing $\mathcal{G}$ over the set

$$\widetilde{I}'_v := \bigcup_{\kappa \in \mathbb{R}} \widetilde{I}'_{v,\kappa}, \tag{4.30}$$

with

$$\begin{aligned} \widetilde{I}'_{v,\kappa} := \Big\{ (\psi_0, \varphi_0) \in \widetilde{I}^* \,|\, & P_{\nabla \psi_{\mathrm{P}}^{y(0)}} \left[(h_{\mathrm{Re}\,\varphi_0} + \kappa) \mathrm{Im}\,\psi_0 - v\partial_1 \mathrm{Re}\,\psi_0 \right] = 0, \\ & P_{\psi_{\mathrm{P}}^{y(0)}} \left[(h_{\mathrm{Re}\,\varphi_0} + \kappa) \mathrm{Re}\,\psi_0 + v\partial_1 \mathrm{Im}\,\psi_0 \right] = 0, \\ & P_{\nabla \varphi_{\mathrm{P}}} (\mathrm{Im}\,\varphi_0 - v\alpha^2 \partial_1 \mathrm{Re}\,\varphi_0) = 0 \Big\}, \end{aligned} \tag{4.31}$$

and

$$\widetilde{I}^* := \left\{ (\psi_0, \varphi_0) | \mathcal{G}(\psi_0, \varphi_0) \leqslant e_{\mathrm{P}} + \delta^*, \|\psi_0\|_2^2 = 1, \mathrm{Re}\,\psi_0 \perp \nabla \psi_{\mathrm{P}}^{y(0)}, \mathrm{Re}\,\varphi_0 \perp \nabla \varphi_{\mathrm{P}} \right\}. \tag{4.32}$$

As in the previous section, one can argue by coercivity of $\mathcal{E}$ and $\mathcal{F}$ and the upper bound that it is possible to restrict to initial conditions such that $\|\delta_2\|_2, \|\delta_1\|_{H^1}, y(0)$ are all $O(v)$. Moreover, the second constraint of the rhs of (4.31) shows that $\kappa = -\mu_{\mathrm{P}} + O(v)$. Thus, we are left with minimizing $\mathcal{G}$ over the set

$$\widetilde{I}''_v := \widetilde{I}'_v \cap \{\kappa + \mu_{\mathrm{P}} = O(v), \|\delta_1\|_{H^1} = O(v), \|\delta_2\|_2 = O(v)\}. \tag{4.33}$$

The lower bound is proven in the same way as before. But instead of the constraint (3.27), this time we need to minimize w.r.t.

$$P_{\nabla \psi_{\mathrm{P}}^{y(0)}} \left[(h_{\mathrm{Re}\varphi_0} + \kappa) \mathrm{Im}\,\psi_0 - v\partial_1 \mathrm{Re}\,\psi_0 \right] = 0. \tag{4.34}$$

Since $\kappa + \mu_{\mathrm{P}}, y_0, \|\delta_1\|_{H^1}$ and $\|\delta_2\|_2$ are all order v and $\psi_{\mathrm{P}} \in C_0^\infty(\mathbb{R}^3)$ (and these facts also allow to infer that $\psi_{\mathrm{P}}^{y(0)} = \psi_{\mathrm{P}} + O(v)$), the constraint (4.34) can be written as

$$\langle \nabla \psi_{\mathrm{P}} | H_{\mathrm{P}} | \mathrm{Im}\,\psi_0 \rangle = v \|\partial_1 \psi_{\mathrm{P}}\|_2^2 (1, 0, 0) + O(v^2). \tag{4.35}$$

Denoting $c = \|\partial_1\psi_\mathrm{P}\|_2^2/\|\partial_1\varphi_\mathrm{P}\|_2^2$, we complete the square

$$\begin{aligned}\langle \mathrm{Im}\,\psi_0|H_\mathrm{P}|\mathrm{Im}\,\psi_0\rangle &= \langle \mathrm{Im}\,\psi_0 - vc\partial_1\psi_\mathrm{P}|H_\mathrm{P}|\mathrm{Im}\,\psi_0 - vc\partial_1\psi_\mathrm{P}\rangle \\ &\quad + 2vc\langle \mathrm{Im}\,\psi_0|H_\mathrm{P}|\partial_1\psi_\mathrm{P}\rangle - c^2v^2\langle\partial_1\psi_\mathrm{P}|H_\mathrm{P}|\partial_1\psi_\mathrm{P}\rangle \\ &\geqslant 2cv\langle \mathrm{Im}\,\psi_0|H_\mathrm{P}\partial_1\psi_\mathrm{P}\rangle - c^2v^2\langle\partial_1\psi_\mathrm{P}|H_\mathrm{P}|\partial_1\psi_\mathrm{P}\rangle. \end{aligned} \tag{4.36}$$

With the constraint (4.34) and $\langle\partial_i\psi_\mathrm{P}|H_\mathrm{P}|\partial_j\psi_\mathrm{P}\rangle = \delta_{i,j}\|\partial_j\varphi_\mathrm{P}\|_2^2$, we arrive at (4.18). □

5. Conclusions

While a rigorous determination of the effective mass of a polaron described by the Fröhlich model remains an outstanding open problem, we solve here the classical analog of this problem, where the polaron is described by the LP equations. Even though these equations are often invoked in heuristic derivations of the effective polaron mass, it is not at all obvious how to make such derivations rigorous since they rely, in one form or another, on the assumption of the existence of traveling waves. As argued above, the latter can not be expected to exist, however. We overcome this problem by introducing a novel variational principle, minimizing the Pekar energy functional over states of given initial velocity v, which can be defined in a natural way for all low-energy states. We hope that this novel point of view may in the future also shed some light on the corresponding problem for the Fröhlich polaron, in particular in view of the recent derivation [17] of the LP equations from the Fröhlich model in the strong coupling limit.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Appendix A. Well-posedness and regularity of the projections onto $\mathcal{M}_\mathcal{F}$

Similar arguments to the ones used in the following proof are contained in [4], where the functional $\mathcal{F}$ is investigated in the case of a torus in place of $\mathbb{R}^3$. Remark 2.1 on the properties $\mathcal{M}_\mathcal{E}$ can be shown with a similar approach, but we omit its proof.

Proof of lemma 2.1. We need to prove that there exists $\delta > 0$ such that for any $\varphi \in (\mathcal{M}_\mathcal{F})_\delta$ there exists a unique z_φ identifying the projection of φ onto $\mathcal{M}_\mathcal{F}$, and such that z_φ is differentiable at any $\varphi \in (\mathcal{M}_\mathcal{F})_\delta$. As the problem is invariant w.r.t. translations, we can w.l.o.g. restrict to show differentiability at $\varphi_0 \in (\mathcal{M}_\mathcal{F})_\delta$ such that $z_{\varphi_0} = 0$.

We define the function $F : L^2(\mathbb{R}^3) \times \mathbb{R}^3 \to \mathbb{R}^3$ given, component-wise, by

$$F_i(\varphi, z) = \mathrm{Re}\langle\varphi|\partial_i\varphi_{\mathrm{P}}^z\rangle \quad \text{for } i = 1, 2, 3. \tag{A.1}$$

By definition of z_φ, we have $F(\varphi_0, 0) = 0$ and $F(\varphi, z_\varphi) = 0$, for any φ in a sufficiently small neighborhood of φ_0. Hence, we set out to use the implicit function theorem to determine properties of z_φ. Observe that, for any $\eta \in L^2(\mathbb{R}^3)$, $z \in \mathbb{R}^3$ and $i, j \in \{1, 2, 3\}$, we have

$$\partial_t F_i(\varphi + t\eta, z) = \mathrm{Re}\langle\eta|\partial_i\varphi_{\mathrm{P}}^z\rangle \quad \text{and} \quad \partial_{z_j} F_i(\varphi, z) = -\mathrm{Re}\langle\varphi|\partial_i\partial_j\varphi_{\mathrm{P}}^z\rangle. \tag{A.2}$$

Since $\varphi_{\mathrm{P}} \in C^\infty(\mathbb{R}^3)$, the map $(\mathcal{M}_{\mathcal{F}})_\delta \ni \varphi \mapsto \det\left(\frac{\partial F_i}{\partial z_j}(\varphi, z)\right)_{i,j=1,\dots,3}$ is continuous w.r.t the L^2-norm and, by radiality of φ_{P},

$$\det\left(\frac{\partial F_i}{\partial z_j}(\varphi_{\mathrm{P}}, 0)\right)_{i,j=1,\dots,3} = \frac{1}{9}\|\nabla\varphi_{\mathrm{P}}\|_2^2 > 0. \tag{A.3}$$

Thus, it follows that $\det\left(\frac{\partial F_i}{\partial z_j}(\varphi_0, 0)\right)_{i,j=1,\dots,3} > 0$, uniformly in φ_0 for sufficiently small $\delta > 0$. By the implicit function theorem, there exists a unique differentiable $z_\varphi : (\mathcal{M}_{\mathcal{F}})_\delta \to \mathbb{R}^3$ whose partial derivative in the direction $\eta \in L^2(\mathbb{R}^3)$ at φ_0 is given by

$$\partial_t z_{\varphi_0 + t\eta}\restriction_{t=0} = \left[\left(\frac{\partial F_i}{\partial z_j}(\varphi_0, z_{\varphi_0})\right)_{i,j=1,\dots,3}\right]^{-1} \mathrm{Re}\langle\eta|\partial_i\varphi_{\mathrm{P}}^{z_{\varphi_0}}\rangle. \tag{A.4}$$

□

ORCID iDs

Simone Rademacher https://orcid.org/0000-0001-5059-4466
Robert Seiringer https://orcid.org/0000-0002-6781-0521

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