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The screened polarons

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Abstract. We present a theory of polarons incorporating the screening of the Coulomb interaction, and we apply this theory to the case of anisotropic ionic crystals as the perovskites. We show that the "screened polarons" cannot be treated individually: all the polarons present in the material are coupled *via* the screening. We also show that, in the frame of this theory of large-scale polarons, the bipolarons are excluded and replaced by pairs of polarons; we propose to associate the pseudogap experimentally observed in perovskites with the binding energy of these pairs. Finally we suggest that the existence of the polarons pairs poses in new terms the problem of a polaronic theory of superconductivity.

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Introduction

Introducing polarons in the theory of superconductivity is *a priori* interesting because the interaction of two polarons, *via* their coupling with the lattice, may be much stronger than those of two dressed free electrons (interaction which produces the Cooper pairs in BCS theory). As a consequence a higher critical temperature may be expected in a polaronic theory of superconductivity.

Although the subject is a very old one (it traces back to the thirties with the pioneer work of Landau [1]), we think that some basic features of polaron theory still deserve to be clarified before embarking any theory of superconductivity.

The first point is: what are the conditions of existence of polarons? Curiously enough the existence problem was not posed to the inventors of polarons (Landau, Pekar, Fröhlich [1–3]). The reason is that they considered an electron-lattice interaction with infinite range, in which case polarons can be shown to always exist. But this situation is not generic, and also unphysical. An existence condition appears as soon as the interaction range is finite. Actually the condition is that the norm of $V(r)$, the electron-lattice interaction, is large enough, and it appears that this condition is satisfied when the range of $V(r)$ is infinite. In the general case a polaron results from the coupling of an electron with both optical and acoustical phonons (remember that the Landau or Fröhlich polaron is purely optical). This last coupling is responsible for the mutual attraction of polarons at large distance, – a property of obvious importance in a theory of superconductivity. But it can be shown (see for instance Haken [4]) that the interaction energy of an electron with the acoustic field diverges when the range λ of the acoustical part $V_{\rm ac}$ of $V(r)$ is infinite. Therefore λ must be finite. In the previous literature the acoustical coupling has been treated phenomenologically [5–10] by assuming a δ like form of $V_{\rm ac}$ (that is $\lambda \approx 0$). Then Emin *et al.* [5–7] indeed obtained an existence criterium for the polarons.

We propose, in this paper, to go beyond the phenomenological description of the acoustical coupling by taking account, in an ionic crystal, of the screening of the Coulomb interaction. Then λ is nothing else but the range of the screened Coulomb potential. Let us mention that the importance of the screening was foreseen long ago by Brazovskii [11], but not further investigated.

In the course of our work we have discovered that the screening phenomenon has much more implications than quantitatively improving the description of polarons. The major point is that one cannot treat the dynamics of one polaron independently from those of all the other polarons present in the material. Even if one ignores the polaron-polaron interaction, the polaron dynamics is a collective process. The reason is the following:
In a material where polarons do exist the charge carriers (density $n_{\rm cc}$) are distributed over the free electronic states (density $n_{\rm e}$) and the polaronic states (density $n_{\rm p}$), and we have $n_{\rm cc} = n_{\rm e} + n_{\rm p}$. The electronic states form two bands respectively associated with the free electrons and polaronic states. Now the screened potential $V(r)$ depends on

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n_e, that is on $n_p = n_{cc} - n_e$. But the width of the polaronic band, which is related to n_p, is a functional of $V(r)$. Therefore n_p, n_e and the various characteristics of the polarons are obtained through a self-consistent calculation in which all the polarons play a role.

The self-consistent aspect of the polaron dynamics has a decisive impact on the existence criterium. Indeed the formation of a set of polarons, which is energetically favorable, produces a diminution of n_e. As a consequence the effective range of $V(r)$ is increased, which makes easier the formation of polarons (this argument holds when the screening by the polarons may be neglected: a situation which is realized at low enough temperature). We find that this effect is responsible for the very existence of the polarons.

The choice of the screening model proves also to be of great importance. We had to decide between the Thomas-Fermi and the Lindhard model (see Ref. [12]). We know that the Lindhard correction to the Thomas-Fermi response function is appreciable for wave numbers k larger than $2k_F$ (Fermi wave number), and the efficiency of the screening is considerably decreased for $k > 2k_F$. Therefore the Lindhard correction may favor the formation of polarons if their width δ is of the order or smaller than $(2k_F)^{-1}$. Actually we show the existence of two classes of polarons:

1) the "weak polarons" which are large-scale and relatively small amplitude objects. They satisfy condition: $\delta > (2k_F)^{-1}$. Moreover their interaction with the lattice is characterized by a potential $\varphi(r)$, which decreases monotonically from the polaron center. The weak polarons are reminiscent of those of the standard theory.
2) The "strong polarons" whose width is much smaller and the amplitude larger. Their width is such that $\delta < (2k_F)^{-1}$, and, therefore they must be described using the Lindhard response function. Their potential φ has an oscillating behavior, which is associated with the Friedel oscillations of the screened potential.

The oscillating character of the strong polarons has an important implication: it is responsible for the formation of pairs of polarons with an appreciable binding energy. We propose to associate the binding energy of the polarons pairs with the pseudogap experimentally observed in perovskites. On the other hand we do not find bipolarons as solutions of the model equations (including the direct Coulomb repulsion between the two electrons).

We also find that the solution of the self-consistent problem is always a strong polaron. However the weak polarons play a role in the nucleation of the first polarons (non self- consistent problem) in a medium where the only charge carriers present at initial time are free electrons.

Our model deals with large-scale polarons: it is a continuous model in which the discreteness of the crystal is ignored. Remember that bipolaronic theories which usually deal with small polarons (according to Hölstein classification [13]) encounter serious difficulties due to the very large effective mass and poor mobility of the bipolarons. This led Emin [5–7] to look for large polarons (or bipolarons), and we adopt this point of view in this paper. Let us precise that the strong polarons we are considering here do not belong to the class of small polarons.

Our model can be *a priori* applied to two types of materials:

i) The metals, which can be conveniently described by a 3D isotropic model, the only relevant coupling being those with the acoustical phonons. Let us also mention that metals have a large density of charge carriers and therefore large values of k_F (of the order of the inverse lattice period).
ii) The strongly anisotropic materials such as the perovskites. Then we assume that the charge carriers are constrained to move in parallel planes (the CuO_2 planes), and the polarons would be flat disks in these planes. Here we have ions with charges of opposite sign and therefore we get a coupling with the optical phonons. On the other hand the excitation of acoustical phonons results from the coupling of the electrons with the uncompensated ionic charges. These charges are only a fraction ν of the total number of ions (ν is of the order of 10^{-2} in a cuprate: see Ref. [14]). Therefore k_F is expected to be much smaller than in metals.

We call this model the 2D model, although this terminology is somewhat misleading since the Coulomb field is actually 3D.

The polaron equations will be given for the two models, but they will be solved only in the case of the 2D model. Of course this last model is *a priori* more appealing since it refers to materials where polarons are known experimentally to exist. However one may wonder whether polarons are allowed in metals, and if they are not, it would be satisfactory to understand why. With the aim of shortening an already long paper we postpone the study of the metallic case to a further publication.

1 The model equations

As was said in the introduction, we are interested, in the case of the 2D model in a crystal made of ions with opposite charges and exhibiting a global charge defect ν. In the limit of a continuous description of this material, it can be shown that such a system is conveniently modelized by a density of dipoles (each cell of the periodic lattice containing one effective dipole made of opposite charges) and by a density ($\nu\rho$) of uncompensated electric charges. The uncompensated charges are responsible for the local deformation of the continuous medium under the field of the polaron charge and for the coupling of an electron with acoustical phonons.

The Hamiltonian describing the dynamics of one electron interacting with the continuous polarizable and elastic medium can be written as

$$H = H_0 + H_{\text{int}}, \tag{1}$$

H_0 is the Hamiltonian of the electron, the acoustic field and the optical field in the absence of interaction, and it reads:

$$H_0 = \int \Psi^+ \left(-\frac{\hbar^2}{2m^*} \Delta \right) \Psi \mathrm{d}\mathbf{x} + \int \left\{ \frac{\mathbf{P}^2}{2\nu\rho_\mathrm{m}} + \frac{\nu\chi}{2} (\mathrm{div}\, \mathbf{u})^2 \right\} \mathrm{d}\mathbf{x} + \int \left\{ \frac{\varepsilon_0}{2\gamma} \boldsymbol{\Pi}^2 + \frac{\varepsilon^\mathrm{f}}{2\varepsilon_0} \mathbf{Q}^2 \right\} \mathrm{d}\mathbf{x}. \quad (2)$$

In this expression the first integral is the free electron part, m^* being the effective mass of free electrons. The second integral represents the energy of elastic deformation, or the energy of acoustical phonons in the quantum description, the phonon dispersion being neglected. $\mathbf{P}$ is the momentum density, ρ_m is the mass density: $\rho_\mathrm{m} = M\rho$, ρ being the ion concentration and M an effective atomic ion mass. χ is related to sound velocity c by: $\chi = \rho_\mathrm{m} c^2$.

The third integral represents the polarization energy, or the energy of the optical phonons.

$\mathbf{Q}$ is the dipole density and $\boldsymbol{\Pi}$ is the canonically conjugated variable. ε_0 is the vacuum dielectric constant (MKS units), ω_0 is the frequency of optical phonons in the absence of dispersion; γ is related to Fröhlich dielectric constant ε^f by: $\gamma\omega_0^2 = \varepsilon^\mathrm{f}$, ε^f being defined as: $\frac{1}{\varepsilon^\mathrm{f}} = \frac{1}{\varepsilon_\mathrm{r}^0} - \frac{1}{\varepsilon_\mathrm{r}^\infty}$, ε_r^0 and $\varepsilon_\mathrm{r}^\infty$ being respectively the static and high frequency relative dielectric constants of the material.

The polarization part of H_0 has the same form as in the Fröhlich Hamiltonian [3]. In the sake of simplicity we have neglected the dispersion of the optical phonons. This can indeed be done (*cf.* Davydov [15]); however we do not think that it introduces new important qualitative features in the polarons properties. The form of the acoustical part is self-explanatory and does not deserve more comment. H_int reads:

$$H_\mathrm{int} = -\int \Psi^+(\mathbf{x})\Psi(\mathbf{x}) V(\mathbf{x}|\mathbf{x}') [\nu Z e \rho\, \mathrm{div}\, \mathbf{u}(\mathbf{x}') + \mathrm{div}\, \mathbf{Q}(\mathbf{x}')] \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}' \quad (3)$$

where Z represents an average ionization number per ion. $V(\mathbf{x}|\mathbf{x}')$ is the Green function of the screened Coulomb potential.

In the 3D model, V is actually a function of $\mathbf{x} - \mathbf{x}'$ in the homogeneous medium, and H_int may be rewritten as:

$$H_\mathrm{int} = \int \Psi^+(\mathbf{x})\Psi(\mathbf{x}) \{ V \otimes [\nu Z e \rho\, \mathrm{div}\, \mathbf{u} + \mathrm{div}\, \mathbf{Q}] \} \mathrm{d}\mathbf{x}, \quad (4)$$

where:

$$V \otimes A(\mathbf{x}) = \int V(\mathbf{x}|\mathbf{x}') A(\mathbf{x}') \mathrm{d}\mathbf{x}',$$

operator $\otimes$ being the 3D convolution product.

It is important to note that the screening of the Coulomb potential, although being a part of the linear response of the material to the field of the test charge, is not taken into account in the dielectric constants (ε^f and ε_r^0). Indeed it associated with a displacement of the electric charges, while the usual dielectric effect is due to the creation of electric dipoles on site. In general $V(\mathbf{x}|\mathbf{x}')$, the Green function of the screened potential which has the meaning of the potential created in $\mathbf{x}$ by a point charge located in $\mathbf{x}'$, obeys the Poisson equation:

$$-\varepsilon_0 \varepsilon_\mathrm{r}^0 \Delta V(\mathbf{x}|\mathbf{x}') = e\delta(\mathbf{x} - \mathbf{x}') + \rho^\mathrm{ind}(\mathbf{x}|\mathbf{x}') \quad (5)$$

where $\rho^\mathrm{ind}(\mathbf{x}|\mathbf{x}')$ is the charge density induced in $\mathbf{x}$ by the point charge at $\mathbf{x}'$. In the 3D model $\rho^\mathrm{ind}(\mathbf{x}|\mathbf{x}')$ has the form:

$$\frac{1}{\varepsilon_0} \rho^\mathrm{ind}(\mathbf{x}|\mathbf{x}') = -\int \chi(\mathbf{x} - \mathbf{x}'') V(\mathbf{x}''|\mathbf{x}') = -\chi \otimes V \quad (6)$$

where $\chi(\mathbf{x})$ is the response function of the material.

In the 2D model we assume that a confining vertical force constrains the electrons to move in the horizontal CuO_2 planes (the polaron we are considering lying in plane $z = 0$). For the same reason we make the simplifying assumption that $|\Psi|^2$ has the form:

$$|\Psi(\mathbf{x}, z)|^2 = |\Psi(\mathbf{x})|^2 \delta(z) \quad (7)$$

where $\mathbf{x}$ stands now for the horizontal coordinates.

The translational invariance with respect to variable z is broken but it can be shown that we still have the symmetry property:

$$V(\mathbf{x}, z|\mathbf{x}', z') = V(\mathbf{x}', z'|\mathbf{x}, z) = V(\mathbf{x} - \mathbf{x}'; z, z'). \quad (8)$$

Due to assumption (7), we need in expression (4) the value of potential V in the $z = 0$ plane. Therefore expression (4) for H_int is still valid provided the action of operator $V\otimes$ on any function $A(\mathbf{x}, z)$ is the following:

$$V \otimes A(\mathbf{x}, z) = \int V(\mathbf{x} - \mathbf{x}'; 0, z') A(\mathbf{x}', z') \mathrm{d}\mathbf{x}' \mathrm{d}z' \quad (9)$$

ρ^ind in equation (5) takes now the form:

$$\rho^\mathrm{ind}(\mathbf{x} - \mathbf{x}'; 0, z') = \sum_n \delta(z' - nl) \rho_n(\mathbf{x} - \mathbf{x}') \quad (10)$$

where l has the meaning of the average distance between the CuO_2 planes, and $\rho_n(\mathbf{x} - \mathbf{x}')$ is the 2D induced charge density in the nth plane. It is given by:

$$\frac{1}{\varepsilon_0} \rho_n(\mathbf{x} - \mathbf{x}') = -\chi \otimes V_n$$

where $V_n(\mathbf{x} - \mathbf{x}') = V(\mathbf{x} - \mathbf{x}'; 0, z' = nl)$. χ is here the 2D response function and $\otimes$ represents the 2D convolution product in the (x, y) plane. Summing up this results, the Poisson equation reads in the 2D model:

$$-\varepsilon_\mathrm{r}^0 \Delta V(\mathbf{x} - \mathbf{x}'; 0, z') = \frac{e}{\varepsilon_0} \delta(\mathbf{x} - \mathbf{x}') \delta(z') - \sum_n \delta(z' - nl) \chi \otimes V_n. \quad (11)$$

For simplicity $V(\mathbf{x};0,z)$ will be noted in the following $V(\mathbf{x},z)$.

The precise form of χ, the response function, will be analyzed in a next section.

The semi classical approximation amounts to consider the various operators Ψ, Ψ^+,$\mathbf{u}$, $\mathbf{P}$, $\mathbf{Q}$, $\boldsymbol{\Pi}$ as scalar or vector variables (see for instance Ref. [15]). The dynamical equations generated by Hamiltonian H are the following: Ψ obeys the Schrödinger equation:

$$(\mathrm{i}\hbar\partial_t + \frac{\hbar^2}{2m^*}\Delta + \varphi)\Psi = 0, \tag{12}$$

in which the potential φ has the form:

$$\varphi = \varphi_{\mathrm{ac}} + \varphi_{\mathrm{opt}}, \tag{13}$$

$$\varphi_{\mathrm{opt}} = V \otimes \mathrm{div}\,\mathbf{Q} \tag{14a}$$

$$\varphi_{\mathrm{ac}} = \nu Ze\rho V \otimes \mathrm{div}\,\mathbf{u} \tag{14b}$$

$$\partial_t \mathbf{Q} = \frac{\varepsilon_0}{\gamma}\boldsymbol{\Pi} \tag{15}$$

$$\partial_t \boldsymbol{\Pi} = \frac{\gamma}{\varepsilon_0}[\omega_0^2\mathbf{Q}] - \boldsymbol{\nabla}(V \otimes |\Psi(\mathbf{x})|^2) \tag{16}$$

$$\partial_t \mathbf{u} = \frac{1}{\nu\rho_{\mathrm{m}}}\mathbf{P} \tag{17}$$

$$\partial_t \mathbf{P} = \nu\chi\boldsymbol{\nabla}(\mathrm{div}\,\mathbf{u}) - \nu Ze\rho\boldsymbol{\nabla}[V \otimes |\Psi(\mathbf{x})|^2]. \tag{18}$$

Eliminating variables $\mathbf{P}$ and $\boldsymbol{\Pi}$, we obtain that $\mathbf{u}$ and $\mathbf{Q}$ obey the following equations:

$$(\partial_t^2 - c^2\Delta)\mathbf{u} = -\frac{Ze}{M}\boldsymbol{\nabla}(V \otimes |\Psi|^2) \tag{19a}$$

$$(\partial_t^2 + \omega_0^2)\mathbf{Q} = -\frac{\varepsilon_0}{\gamma}\boldsymbol{\nabla}(V \otimes |\Psi|^2). \tag{19b}$$

Equations (12-19) are the dynamical equations of our model.

We consider polaronic states whose electronic wave function is of the form:

$$\Psi = \exp\left(\mathrm{i}\frac{\mathbf{p}\cdot\xi}{\hbar}\right)\exp\left[\mathrm{i}\left(\frac{p^2}{2m^*} + E\right)\frac{t}{\hbar}\right]F(\xi) \tag{20}$$

where $\mathbf{p} = m^*\mathbf{v}$ and $\xi = \mathbf{x} - \mathbf{v}t$, $\mathbf{v}$ being the polaron velocity. Momentum p will be assumed to be quantized as those of a free electronic state.

The polaron equations read in terms of F:

$$\left(\frac{\hbar^2}{2m^*}\Delta + \varphi\right)F = E_{\mathrm{q}}F \tag{21}$$

$$\left[\Delta - \frac{(\mathbf{v}\cdot\boldsymbol{\nabla})^2}{c^2}\right]\mathrm{div}\,\mathbf{u} = \frac{Ze}{Mc^2}\Delta V \otimes |F|^2 \tag{22}$$

$$\left[1 + \frac{(\mathbf{v}\cdot\boldsymbol{\nabla})^2}{\omega_0^2}\right]\mathbf{Q} = -\frac{\varepsilon_0}{\varepsilon^{\mathrm{f}}}\boldsymbol{\nabla}V \otimes |F|^2 \tag{23}$$

φ_{ac} and φ_{opt} being obtained from $\mathrm{div}\,\mathbf{u}$ and $\mathbf{Q}$ through expressions (14). E_{q} has the meaning of the electronic part of the polaron energy.

Solving equations (22, 23) for $\mathrm{div}\,\mathbf{u}$ and $\mathbf{Q}$ is possible in the limit of small v. Indeed the kernel of the operator acting on $\mathrm{div}\,\mathbf{u}$ is void for $v < c$, and the existence of a regular solution of equation (23) for small v is shown in Appendix A, even though the kernel of the operator acting on $\mathbf{Q}$ is not void.

We shall restrict ourselves in this paper to study slow velocity polarons ($v \ll c$). Indeed one encounters mathematical difficulties when v is of the order of c, the polarons becoming strongly anisotropic. Besides a localized solution of the above equations is likely to disappear when v exceeds some critical velocity c_{m} of the order of c. This is easily seen in the case of the one-dimensional acoustical polaron. Then one gets from equation (14):

$$\varphi_{\mathrm{ac}} = \frac{(Ze)^2}{M(c^2 - v^2)}\nu\rho V \otimes V \otimes |F|^2.$$

One observes that φ_{ac} changes its sign when v becomes larger than c, and, as a consequence, there no longer exists any localized solution of the Schrödinger equation. This result has been already obtained by Wilson [16], and Arikabe *et al.* [17].

1.1 The ground polaronic state

The ground polaronic state proves to be the lowest energy state of the immobile polaron ($v = 0$). This ground state will be studied in some details in the following, the shape of slow polarons being close to those of the ground state.

For $v = 0$ we get from equations (22, 23):

$$\mathrm{div}\,\mathbf{u} = \frac{Z}{Mc^2}eV \otimes |\Psi|^2 \tag{24}$$

$$\mathrm{div}\,\mathbf{Q} = \frac{\varepsilon_0}{\varepsilon^{\mathrm{f}}}\Delta V \otimes |\Psi|^2. \tag{25}$$

It is now convenient to introduce an arbitrary length unit d, which will be conveniently chosen below in order to minimize the number of parameters entering the polarons equations. Then we put:

$$eV = WG, \tag{26}$$

where:

$$W = \frac{e^2}{\varepsilon_0\varepsilon_{\mathrm{r}}^0 d}\cdot \tag{27}$$

Then we obtain from expressions (24, 25), and using unit length d:

$$\varphi_{\mathrm{opt}} = -\frac{W}{\varepsilon^{\mathrm{f}}\varepsilon_{\mathrm{r}}^0}\Delta G \otimes G \otimes |\Psi|^2 \tag{28}$$

$$\varphi_{\mathrm{ac}} = \nu(\rho d^3)\frac{(ZW)^2}{Mc^2}G \otimes G \otimes |\Psi|^2, \tag{29}$$

and the total potential energy φ can be written, using $\bar{E} = \dfrac{\hbar^2}{2m^*d^2}$ as energy unit, in the form:

$$\varphi = (\mu - \mathcal{S}\Delta)G \otimes G \otimes |\Psi|^2 \tag{30}$$

where:

$$\mu = \frac{8\pi}{(\varepsilon_{\rm r}^0)^2}\frac{m^*}{m}\frac{\frac{e^2}{\varepsilon_0 a_0}}{Mc^2}(\nu\rho d^3) = \frac{8\pi}{\varepsilon_{\rm r}^0}W\frac{m^*}{m}\frac{d}{a_0}(\nu\rho d^3) \quad (31)$$

and:

$$\mathcal{S} = \frac{W}{\varepsilon^{\rm f}\varepsilon_{\rm r}^0\bar{E}} = \frac{8\pi}{(\varepsilon_{\rm r}^0)^2\varepsilon^{\rm f}}\frac{m^*}{m}\frac{d}{a_0} \quad (32)$$

a_0 being the Bohr radius:

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2}\cdot$$

Let us note that, in the above expressions, Ψ has been renormalized in order to preserve the original normalization ($\langle|\Psi|^2\rangle = 1$).

The value of μ measures the relative importance of the acoustical coupling, $\mu = 0$ corresponding to the case of a pure optical polaron.

In the 3D model φ may be rewritten, thanks to equation (5):

$$\varphi = \{\mu G\otimes G + \mathcal{S}(G - \chi\otimes G\otimes G)\}\otimes|\Psi|^2, \quad (33a)$$

while in the 2D model, we get through expression (11):

$$\varphi(\mathbf{x}) = \left\{\mu\int \mathrm{d}z\, G(\mathbf{x},z)\otimes G(\mathbf{x},z) + \mathcal{S}[G(\mathbf{x},0) - \chi\otimes\sum_n G(\mathbf{x},nl)\otimes G(\mathbf{x},nl)]\}\otimes|\Psi|^2\right\}. \quad (33b)$$

In this last expression of φ, the action of the convolution operator in $\{\mathbf{x},z\}$ space has been detailed, and $\otimes$ represents the 2D convolution product. Moreover we choose $d = l$, and put:

$$\nu\rho = \frac{n_{\rm cc}}{l},$$

where $n_{\rm cc}$ represents the effective 2D density of charge carriers in the CuO planes; moreover $\nu\rho$ has the meaning of the number of charge carriers in the cube of size l.

Our choice of d makes the numerical calculations easier. It may seem cumbersome and even unphysical that $\varphi(\mathbf{x})$ depends explicitly on the arbitrary length d through the expressions for μ and $\mathcal{S}$, making the solution of the Schrödinger equation itself depending on d. But one must remember that the Poisson equation obeyed by G (written in d length unit), and therefore G itself, also depends on d. As a result the polaron characteristics, such as their binding energy, are independent of d, as they must be.

In terms of d and $\bar{E}$ units, Schrödinger equation (21) reads:

$$(\Delta + \varphi)\Psi = k^2\Psi, \quad (34)$$

with:

$$k^2 = E_{\rm q}/\bar{E}.$$

In any case we shall write:

$$\varphi = \mathcal{A}|\Psi|^2 \quad (35)$$

where operator $\mathcal{A}$ is defined by expression (33a) or (33b), according to the model dimension.

2 Energy, stability, effective mass

2.1 Energy and effective mass of slow polarons

Parameter $E_{\rm q}$ entering Schrödinger equation (34) has the meaning of the electronic part of the ground-state polaron energy.

Let $E_{\rm p}$ be the total energy of the polaron, which includes the deformation of the crystal. Let us first evaluate the total energy E_0 of the immobile polaron. E_0 is the expectation value of H (given by Eq. (2)). It can be written as:

$$E_0 = E_{\rm q}\langle\Psi^2\rangle - (E_{\rm ac} + E_{\rm opt}), \quad (36)$$

where we leave the norm of Ψ unspecified; $E_{\rm ac} = \int\frac{\nu\chi}{2}(\mathrm{div}\,\mathbf{u})^2\mathrm{d}\mathbf{x}$; $E_{\rm opt} = \int\frac{\varepsilon^{\rm r}}{2\varepsilon_0}\mathbf{Q}^2\mathrm{d}\mathbf{x}$.

Using the above expressions for $\mathbf{Q}$ and $\mathrm{div}\,\mathbf{u}$, $E_{\rm ac}$ and $E_{\rm opt}$ can be written in the form:

$$E_{\rm ac} = \frac{\nu\rho}{2}\frac{(Ze)^2}{Mc^2}\langle[V\otimes\Psi^2]^2\rangle \quad (37a)$$

$$E_{\rm opt} = \frac{\varepsilon_0}{2\varepsilon^{\rm f}}\langle[\boldsymbol{\nabla}(V\otimes\Psi^2)]^2\rangle\cdot \quad (37b)$$

Then it is easily shown that $E_{\rm opt} + E_{\rm ac} = \frac{1}{2}\langle\varphi\Psi^2\rangle$. On the other hand we get from the Schrödinger equation $E_{\rm q}\langle\Psi^2\rangle = -\langle(\boldsymbol{\nabla}\Psi)^2\rangle + \langle\varphi\Psi^2\rangle$. Therefore we obtain:

$$E_0 = \frac{1}{2}[E_{\rm q}\langle\Psi^2\rangle - \langle(\boldsymbol{\nabla}\Psi)^2\rangle]\cdot \quad (38)$$

Let us now consider a moving polaron. For a given velocity v, the polaron energy will be obtained by minimizing $\langle H(E_{\rm q})\rangle$ with respect to $E_{\rm q}$. Now H can be written in the form:

$$H = -\int\Psi^+(\frac{\hbar^2}{2m^*}\Delta + \varphi_{\rm ac} + \varphi_{\rm opt})\Psi\mathrm{d}\mathbf{x} + \int\left\{\frac{\mathbf{P}^2}{2\nu\rho_{\rm m}} + \frac{\nu\chi}{2}(\mathrm{div}\,\mathbf{u})^2\right\}\mathrm{d}\mathbf{x} + \int\left\{\varepsilon_0\frac{\boldsymbol{\Pi}^2}{2\gamma} + \frac{\varepsilon^{\rm f}}{2\varepsilon_0}\mathbf{Q}^2\right\}\mathrm{d}\mathbf{x}.$$

Replacing Ψ by its expression (20) in $\langle H\rangle$, one obtains:

$$E_{\rm p} = -E_{\rm q} + \frac{m^*v^2}{2} - \mathrm{i}\hbar\int(\mathbf{v}\cdot\boldsymbol{\nabla})F\mathrm{d}\mathbf{x} + \int\left\{\frac{P^2}{2\nu\rho_{\rm m}} + \frac{\nu\chi}{2}(\mathrm{div}\,\mathbf{u})^2\right\}\mathrm{d}\mathbf{x} + \int\left\{\varepsilon_0\frac{\boldsymbol{\Pi}^2}{2\gamma} + \frac{\varepsilon^{\rm f}}{2\varepsilon_0}\mathbf{Q}^2\right\}\mathrm{d}\mathbf{x} \quad (39)$$

where:

$$\mathbf{P} = -\nu\rho_{\rm m}(\mathbf{v}\cdot\boldsymbol{\nabla})\mathbf{u}$$
$$\boldsymbol{\Pi} = -\frac{\varepsilon_0}{\gamma}(\mathbf{v}\cdot\boldsymbol{\nabla})\mathbf{Q},$$

and $E_{\rm q}$ is the eigenvalue of the Schrödinger equation (21).

$E_{\rm p}$ is evaluated in Appendix (B) in the limit $v \ll c$. One obtains that it can be written in the form:

$$E_{\rm p} = -E_0 + \frac{1}{2}M_{\rm p}v^2,$$

where:

$$M_{\rm p} = m^* + \frac{1}{D}\left\{\frac{1}{c^2}\langle F_0^2\varphi_{\rm ac}^0\rangle - \frac{1}{\omega_0^2}\langle F_0^2\Delta\varphi_{\rm opt}^0\rangle\right\}. \quad (40)$$

Assigning quantized values to the polaron momentum: $\mathbf{p} = M_{\rm p}\mathbf{v} = \hbar\mathbf{k}$, the slow polarons energy spectrum reads:

$$E_{\rm p} = -E_0 + \frac{\hbar^2}{2M_{\rm p}}k^2. \quad (41)$$

2.2 Energy and stability of the polaronic states

If $E_{\rm p}$, the total polaron energy, is positive, then the polaronic state is energetically favorable (compared with the unbounded states) and therefore it can be a ground state of the electron-lattice system. On the contrary a solution with negative energy cannot be a ground state. Such a solution is likely to be dynamically unstable.

Now the stability problem is posed here in rather peculiar terms. We first observe that the wave function of the actual physical system (electron + ionic sites) obeys a linear (multi-variables) Schrödinger equation, and stability considerations about this system are irrelevant. But the primitive dynamical system has been made non linear through the use of the semi-classical approximation, and the stability problem deserves now to be considered. And it may be asked whether there is a relation between the stability and the positiveness of the total energy.

The stability problem has been solved in the case of the NLS equation thanks to the Vakhitov-Kolokolov (V-K) criterium [18]: the stability of a localized solution (or soliton) is determined by the sign of $\frac{{\rm d}N}{{\rm d}E_{\rm q}}$. Since we have in this case $N \sim E_{\rm q}^{1-D/2}$ (D being the space dimension), only the 1D solitons are stable. It is remarkable (see Appendix C) that the sign of $E_{\rm p}$ behaves exactly as those of $\frac{{\rm d}N}{{\rm d}E_{\rm q}}$ as a function of $E_{\rm q}$. Therefore satisfying the V-K criterium or ensuring the positiveness of $E_{\rm p}$ are equivalent statements.

Clearly the conditions of validity of the V-K criterium are not fulfilled in the case of the complicated dynamical system defined by above equations (33, 34). An inviting conjecture is that the sign of the total energy still permits one to decide on the stability of a stationary solution, even in the case where the V-K criterium is not available: then only the polarons with positive total energy would be stable. We shall assume this conjecture to be true in the following.

It could happen that the energy domain of polarons be further limited by $c_{\rm m}$, the maximum allowed polaron velocity. This would happen if $E_0 > \frac{1}{2}M_{\rm p}c_{\rm m}^2$. We shall not consider here this possibility because, in the interesting physical situations, the polaron velocities are found much smaller than c. Then we shall assume that $E_{\rm pmax} = 0$ and expression (41) for the polaron energy spectrum to be valid all along the polaron energy spectrum and the maximum allowed wave number in expression (41) is $k_{\rm p}$ given by:

$$\frac{\hbar^2}{2M_{\rm p}}k_{\rm p}^2 = E_0. \quad (42)$$

2.3 Energy of the bipolaron and of a pair of polarons

We want to derive in this section expressions for the energy of the ground state of the bipolaron and of a pair of polarons.

The modifications which must be introduced in order to pass from the polaron Hamiltonian (expression (2)) to the bipolaron Hamiltonian are the following:
i) The polaron wave function will be noted $\Psi(\mathbf{x}_1, \mathbf{x}_2)$.
ii) In H_0 the kinetic energy reads: $\langle(\nabla_1\Psi(1,2))^2 + \nabla_2\Psi(1,2))^2\rangle$, with obvious notations

$$H_{\rm int} = H_{\rm el} + H_{\rm c}, \quad (43a)$$

where:

$$H_{\rm el} = \int \Psi^+(\mathbf{x}_1,\mathbf{x}_2)\Psi(\mathbf{x}_1,\mathbf{x}_2)\{V(\mathbf{x}|\mathbf{x}_1) + V(\mathbf{x}|\mathbf{x}_2)\}[\nu Ze\rho\,{\rm div}\,\mathbf{u}(\mathbf{x}) + {\rm div}\,\mathbf{Q}(\mathbf{x})]{\rm d}\mathbf{x}{\rm d}\mathbf{x}_1{\rm d}\mathbf{x}_2 \quad (43b)$$

$$H_{\rm c} = \int eV(\mathbf{x}_1,\mathbf{x}_2)\Psi^+(\mathbf{x}_1,\mathbf{x}_2)\Psi(\mathbf{x}_1,\mathbf{x}_2){\rm d}\mathbf{x}_1{\rm d}\mathbf{x}_2, \quad (43c)$$

$H_{\rm c}$ standing for the direct Coulomb interaction between the two electrons.

Then $E_{\rm bp}$, the bipolaron total energy reads:

$$E_{\rm bp} = 2\langle\Phi\varphi\rangle - \langle|\nabla_1\Psi(1,2)|^2 + |\nabla_2\Psi(1,2)|^2\rangle - \varepsilon^{\rm f}\varepsilon_{\rm r}^0\mathcal{S}\int G(1,2)|\Psi(1,2)|^2{\rm d}1{\rm d}2 \quad (44)$$

where:

$$\varphi = \mathcal{A}|\Psi|^2 \text{ and } \Phi(\mathbf{x}) = \int|\Psi(\mathbf{x},\mathbf{x}')|^2{\rm d}\mathbf{x}.$$

The bipolaron energy has been calculated by minimizing $E_{\rm bp}$ with respect to the parameters entering the expression for the chosen trial function $\Psi(\mathbf{x}_1, \mathbf{x}_2)$ (see below Sect. 6).

Let us now consider the problem of two well-separated (weakly interacting) polarons with antiparallel spins.

In the weak coupling approximation (WCA), the orbital part of the pair wave function $\Psi(\mathbf{x}_1, \mathbf{x}_2)$ is assumed factorized:

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = a\{\Psi_1(\mathbf{x}_1)\Psi_2(\mathbf{x}_2) + \Psi_1(\mathbf{x}_2)\Psi_2(\mathbf{x}_1)\}$$

where wave functions Ψ_1 and Ψ_2 are respectively centered at $\boldsymbol{\rho}_1$ and $\boldsymbol{\rho}_2$ ($\rho = |\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2| > l_\mathrm{w}$). At zero order $\Psi_i(\mathbf{x})$ reduces to $\Psi(\mathbf{x} - \boldsymbol{\rho}_i)$, which is the wave function of the unperturbed polaron centered at $\boldsymbol{\rho}_i$. and the normalization factor is $a \approx \frac{1}{\sqrt{2}}$.

At first order the energy of the pair of polarons is found to be:

$$E_\mathrm{pair} = 2E_\mathrm{q} + \Delta E, \text{ where } \Delta E = \delta E - \langle eV_\mathrm{c}\rangle$$

E_q has the same meaning as above: it is the electronic part of the unperturbed polaron energy. δE represents the specific polaron-polaron interaction; $-\langle eV_\mathrm{c}\rangle$ is the contribution of the direct Coulomb interaction. The contribution of the exchange terms are neglected for well-separated polarons $\langle eV_\mathrm{c}\rangle$ reads:

$$\begin{aligned}\langle eV_\mathrm{c}\rangle &= e\int V(\mathbf{x}-\mathbf{x}')|\Psi(\mathbf{x},\mathbf{x}')|^2 \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}' \\ &\approx e\int V(\mathbf{x}-\mathbf{x}')\Psi_1^2(\mathbf{x})\Psi_2^2(\mathbf{x}')\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}' \\ &\approx e\int V(\mathbf{x}-\mathbf{x}')\Psi^2(\mathbf{x}-\boldsymbol{\rho}_1)\Psi^2(\mathbf{x}-\boldsymbol{\rho}^2)\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{x}' \quad (45)\end{aligned}$$

δE is the sum of the energy variation of each polaron due to the field of the other one. Calling $\varphi(\mathbf{x} - \boldsymbol{\rho}_i)$ the field due to polaron i, we get (at lowest order):

$$\delta E = \int \Psi^2(\mathbf{x} - \boldsymbol{\rho}_1)\varphi(\mathbf{x} - \boldsymbol{\rho}_2)\mathrm{d}\mathbf{x}.$$

Summing the contributions of δE and $\langle eV_\mathrm{c}\rangle$ we obtain:

$$\Delta E(\rho) = \langle\tilde{\varphi}(\Psi_2), \Psi_1^2\rangle \quad (46)$$

with:

$$\tilde{\varphi}(\Psi^2) = \mathcal{S}\mathcal{A}|\Psi_2|^2 - \mathcal{S}\varepsilon^\mathrm{f}\varepsilon_\mathrm{r}^0 G \otimes |\Psi_2|^2 \quad (47)$$

where the last term is the contribution of the direct Coulomb interaction.

In the 2D model, we obtain:

$$\begin{aligned}\tilde{\varphi} = \Big\{\mu\int \mathrm{d}z\, G(\mathbf{x},z)\otimes G(\mathbf{x},z) + \mathcal{S}[(1-\varepsilon^\mathrm{f}\varepsilon_\mathrm{r}^0)G(\mathbf{x},0) \\ - \sum_n \chi\otimes G(\mathbf{x},nl)\otimes G(\mathbf{x},nl)]\Big\}\otimes|\Psi_2(\mathbf{x})|^2. \quad (48)\end{aligned}$$

3 The screened potential

Up to now the form of response function $\chi(\mathbf{x})$, which determines the screened Coulomb potential, has been left unspecified. This response function is at the very heart of the polaron physics because the existence and the dynamics of the polarons are determined by the screening. We shall only give here the expression for χ in the 2D model.

In the general case the charge carriers (density n_cc) are distributed over free electrons (density n_e) and polarons (density n_p), provided the polaronic states do exist. n_cc as well as χ, are the sum of two terms:

$$n_\mathrm{cc} = n_\mathrm{e} + n_\mathrm{p}, \quad (49)$$

$$\chi = \chi_\mathrm{e} + \chi_\mathrm{p}, \quad (50)$$

χ_e and χ_p being respectively the contributions of the free electrons and polarons.

The electronic states form two bands: the polaronic band ("P-band"), and the free states band ("FS-band"). If free electrons are present, the Fermi level is associated with a free state; the FS-band is defined in $[0, E_\mathrm{F}]$, while the P-band is defined in $[-E_0, 0]$. Moreover we have at $T = 0$:

$$2\pi n_\mathrm{e} = k_\mathrm{F}^2. \quad (51a)$$

Similarly the P-band is occupied up to k_p, and we have:

$$2\pi n_\mathrm{p} = k_\mathrm{p}^2. \quad (51b)$$

Finally we define k_cc by:

$$2\pi n_\mathrm{cc} = k_\mathrm{cc}^2. \quad (51c)$$

Then we have:

$$k_\mathrm{cc}^2 = k_\mathrm{F}^2 + k_\mathrm{p}^2. \quad (52)$$

Now it appears that, due to the finite energy domain of the polaronic states, the calculation of $\chi_\mathrm{p}(r)$ is different from those of $\chi_\mathrm{e}(r)$. We shall therefore study separately the characteristics of the electronic and the polaronic screening.

3.1 The electronic screening

The Lindhard calculation applies without any modification. It is detailed in Appendix D in the case of the isotropic 2D model. The assumption of anisotropy has been made for the sake of simplicity, and it is of course rather rough. We obtain at $T = 0$:

$$\begin{aligned}\chi(k) &= k_\mathrm{s} \qquad\qquad\qquad \text{for} \quad k \lesssim 2k_\mathrm{F} \\ &= k_\mathrm{s}\left\{1 - \sqrt{1 - \frac{4k_\mathrm{F}^2}{k^2}}\right\} \quad \text{for} \quad k \gtrsim 2k_\mathrm{F}, \quad (53)\end{aligned}$$

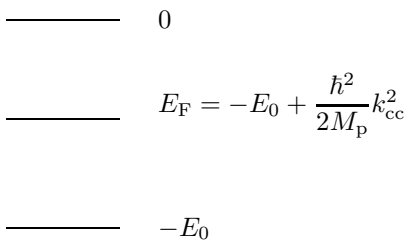
where:

$$k_\mathrm{s} = \frac{4}{\varepsilon_\mathrm{r}^0}\frac{m^*}{m}\frac{1}{a_0}\,. \quad (54)$$

The Thomas-Fermi model is defined by: $\chi(k) = k_\mathrm{s}\ \forall k$. (Using l as the unit length, k_s has the meaning of $k_\mathrm{s}l$).

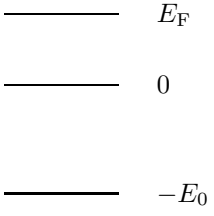
3.2 The polaronic screening

As was said above the finiteness of the polarons energy domain introduces a modification in the calculation of $\chi_{\rm p}$. Let us first consider the case of a pure polaronic screening. This implies that no free electrons would be present in the material, and the electric field of a given polaron would be screened by the surrounding polarons. Such a situation cannot be *a priori* ruled out since the polaron formation is energetically favorable. It would correspond to the following energy diagram:



In this case the Fermi level would be those of a polaronic state, and $E_{\rm F}$ would be negative. In other words the P-band would be incomplete and the standard Lindhard calculation holds, yielding the same expression for $\chi_{\rm p}$ as for $\chi_{\rm e}$, except for the replacement of m^* by $M_{\rm p}$. But $M_{\rm p}$ is much larger than m^*, which makes $\chi_{\rm p}(r)$ to take large values, and such a large screening kills the polaron. In other words no polaronic solution is expected in the case of the pure polaronic screening.

Let us therefore consider the case where free electrons are present. We have then the following diagram:



This situation corresponds to a filled P-band. Now it is shown in Appendix D that such a band yields a vanishingly small contribution in the limit $T \to 0$.

The calculation of $\chi_{\rm p}$ at finite T is given in Appendix D. In the limit $T \to 0$, $\chi_{\rm p}(k)$ vanishes except in a small interval around $k = 0$ where it takes a finite value. We have studied the polaronic solutions at finite T and found that they differ only moderately from those obtained at $T = 0$, as far as the polaron properties considered in this paper are concerned. For the sake of simplicity we shall present only the case $T = 0$ in the following, and therefore consider a pure free electrons screening.

4 Integrating the polaron equations. The existence criterium

Let us first briefly comment the method of integration of the polarons equations.

We look for the ground state of the system of equations (33, 34). Such a ground state is a bounded solution of Schrödinger equation (34), which keeps the same sign in all space: it looks like a ground state of an ordinary (linear) Schrödinger equation.

It is important to remark that Schrödinger equation (34) is actually non linear, through the dependence of potential φ on $|\Psi|^2$. As a result the norm condition:

$$N = \langle |\Psi|^2 \rangle = 1 \tag{55}$$

is not trivial, and it determines, together with the boundary conditions, eigenvalue $E_{\rm q}$ of this equation.

Equations (33, 34) has been solved numerically by iteration:
a) We start giving ourselves a trial function Ψ_0. For a given $E_{\rm q} = k^2$, Ψ_0 has a definite value at the origin: $C = \Psi_0(0)$.
b) φ is evaluated, according to equation (33a) or (33b), in terms of Ψ_0, giving $\varphi = \varphi_0$.
c) We look for the ground state (or eventually for one of the other bound states) of the Schrödinger equation in which φ is replaced by φ_0. We obtain $\Psi = \Psi_1$, and the new eigenvalue $E_1 = k_1^2$. Moreover Ψ_1 is given the same initial value C as Ψ_0.
d) φ is recalculated in terms of Ψ_1, etc.
This procedure converges fairly well, the norm of the solution being a definite function of C.

We want to show how satisfying the norm condition imposes a constraint on the model parameters. Let us first relax the norm condition. Then solving the Schrödinger equation yields the value of N for a given $E_{\rm q}$. If the function $N(E_{\rm q})$ has some lower bound $N_{\rm m}$, satisfying the norm condition gives an existence criterium, namely:

$$N_{\rm m} < 1. \tag{56}$$

Usually $N_{\rm m} > 0$ for $D > 1$ (see for instance Ref. [19]), an exception is the case of the standard 3D optical polaron in the absence of screening. In this case, indeed, we have $\varphi \sim \frac{1}{r} \otimes |\Psi|^2$. Then a simple scaling argument on the Schrödinger equation shows that the norm N is proportional to $\sqrt{E}$. Therefore $N_{\rm m} = 0$ and there is no lower bound for N and the norm condition can always be satisfied. We shall now see that, as soon as $k_{\rm s} \neq 0$, we get $N_{\rm m} \neq 0$ (for $D > 1$) and therefore an existence criterium has to be fulfilled. As a consequence the unscreened situation is pathological.

Let us now consider, in the 2D model, the variation of N with $E_{\rm q}$. Fixing the value of $k_{\rm cc}$ and $k_{\rm F}$, we find a unique solution of equation (34) corresponding to a given initial value $C = \Psi(0)$ of the wave function. Varying C we may study the variation of N with $E_{\rm q}$, without imposing the norm condition.

We observe that N is a monotonically growing function of $E_{\rm q}$. Therefore we get:

$$N_{\rm m} = N(E_{\rm q} = 0).$$

Let us mention that, in the 3D model, $N(E_{\rm q})$ exhibits a minimum $N_{\rm m}$ for a non-zero value of $E_{\rm q}$. Coming back to the 2D model, it is interesting to observe that, in the limit

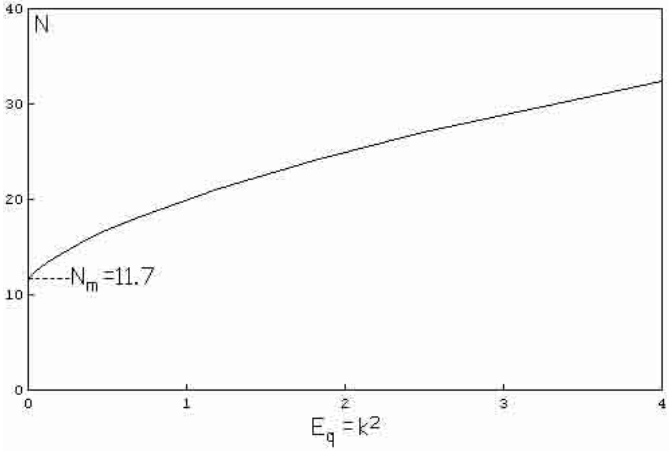


Fig. 1. Variation of $N = \langle \Psi^2 \rangle$ with E_q.

$E_q \to 0$, l_w, the width of the wave function, becomes very large and, as a result, potential φ takes the limiting form (see expression (35)):

$$\varphi = \langle \mathcal{A} \rangle |\Psi|^2. \tag{57}$$

With this form of φ, equation (34) reduces to the stationary non-linear Schrödinger equation (NLS equation) used in optics (see for instance Ref. [20]). Therefore the polarons obtained in the limit $k \to 0$ are nothing else but NLS solitons. Making the further change of variables $\sqrt{\langle \mathcal{A} \rangle}\Psi = kf$, and $\mathbf{x} \to k\mathbf{x}$, $(k = \sqrt{Eq})$ we obtain that f obeys the universal NLS equation:

$$(\Delta + f^2)f = f. \tag{58}$$

The norm Ω of the unique localized solution of this equation is found to be:

$$\Omega \approx 11.7,$$

a result already obtained in a previous publication [19].

Therefore N_m must be identified with Ω, and we can write:

$$\langle f^2 \rangle = \langle \mathcal{A} \rangle \langle |\Psi|^2 \rangle = \langle \mathcal{A} \rangle.$$

Then the existence criterium reads:

$$\langle \mathcal{A} \rangle > 11.7. \tag{59}$$

In the limit of small k, that is of very large polaron width, the use of the Thomas Fermi screened potential is certainly justified.

$\langle \mathcal{A} \rangle$ has been evaluated in Appendix E. In the limit of large k_s and μ, it takes the form:

$$\langle \mathcal{A} \rangle \approx \frac{2}{3}\frac{\mu}{k_s^2}, \tag{60}$$

where k_s is evaluated in $1/l$ unit.

Condition (59) then reads:

$$k_s < k_{smax}, \tag{61}$$

with:

$$k_{smax}^2 = \frac{2}{3}\frac{\mu}{11.7}\,. \tag{62}$$

Since k_s is known for a given material, condition (59) can be expressed as a condition to be satisfied by μ:

$$\mu > \mu_{crit},$$

where, from equation (60),

$$\mu_{crit} = 17.55 k_s^2. \tag{63}$$

Choosing the following values of the model parameters, adapted to a typical cuprate case (see for instance Ref. [14] pp. 14, 15): $m^* = 2m$; $\varepsilon_r^0 = 2$; $\nu = 3 \times 10^{-2}$; $l = 5$ Å; $\nu\rho l^3 \approx 0.64$; $Mc^2 = 7.5$ eV; $Z = 2.1$, one gets $\mu \approx 1600$, while $k_s \approx 37.7$ (in $1/l$ unit).

Then one finds, using expression (63), $\mu_{crit} \approx 2.5 \times 10^4$. Therefore μ_{crit} would be about 15 times the experimental μ. Therefore the existence criterium is not satisfied.

However it must be observed that a rather large uncertainty exists about the numerical values to be attributed to parameters μ and $\mathcal{S}$ of the model. Mc^2 is quite roughly estimated and we have used the Lindhard expression of the response function, expression that was derived for an isotropic system. Therefore we cannot draw a certain conclusion concerning the existence of weak polarons in a material of the perovskite type. We only suggest that the existence criterium is probably not satisfied in the bulk material, and that the nucleation of the first polarons can be realized only in particular regions of the crystal (for instance near a boundary or a defect).

5 The self-consistent problem. Weak and strong polarons

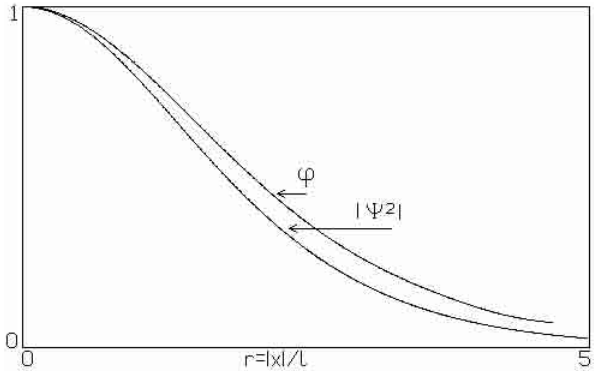
Considering the limit of zero temperature, we have seen that the screening is due to the only free electrons. Then $\chi(r)$ is a function of n_e, that is a functional of n_p, thanks to relation (49). On the other hand k_p^2 (or n_p) is proportional to $(M_p \cdot E_p)$ by relation (42). This relation can be rewritten, in $\bar{E}$ unit, as:

$$\left(\frac{M_p}{m^*}\right) E_0 = k_{cc}^2 - k_F^2, \tag{64}$$

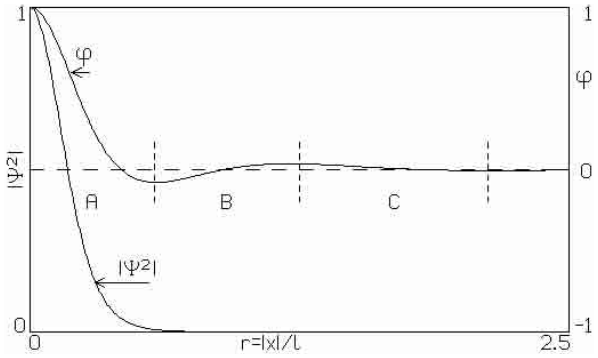
where $\frac{M_p}{m^*}$ is given by expression (40). $\frac{M_p}{m^*}$ and E_0 are known functionals of $\chi(r)$, that is known functions of k_{cc} and k_F. Therefore solving the polarons equations yields the value of k_F for a given k_{cc}, and also the P-band width k_p together with all the polarons characteristics (effective mass and binding energy).

In other words n_p and M_p are obtained through a self-consistent calculation, which means that χ cannot be *a priori* given.

It is worth observing that the polaron problem is no longer self-consistent in the 2D Thomas-Fermi model since χ_e is then independent of n_e or M_p.



(a)



(b)

Fig. 2. (a) $\mu = \mu_1$, (b) $\mu = \mu_2$.

Giving ourselves $\chi = \chi_e(r)$ independently of the polaron dynamics refers to two possible situations:

i) We are treating the one-polaron problem that is we study the formation of a first polaron in a system where only free electrons are present at initial time.
ii) We study the 2D Thomas-Fermi model where $\chi_e(r)$ does not depend on n_e.

Now we want to show that two types of polarons are obtained according as the Linhard correction is or is not relevant in the dynamics.

For that purpose let us fix k_F (which is actually done in the non self-consistent model: NSC model), and consider two particular values μ_1, μ_2 ($\mu_1 < \mu_2$) of the coupling parameter (which can be done by increasing n_{cc}). Solving the stationary polaron equations we find:
For $\mu = \mu_1 = 2500$, l_w, the polaron width, is relatively large ($l_w \approx 2.4$), and its total energy $E_q = 0.17$.

For $\mu = \mu_2 = 2800$, l_w is much smaller ($l_w \approx 0.25$), and its total energy $E_q = 17$. φ is now oscillating from the origin. In any case $|\Psi|^2$ is a monotonic decreasing function of r (see Figs. 2, 3).

These results are easily interpreted by inspecting the form of Lindhard potential $V_e(r)$. Indeed Lindhard response function $\chi_e(r)$ induces a potential $V_e(r)$ which exhibits the well-known Friedel oscillations where the abscissa of the first extremum is of the order of $(2k_F)^{-1}$.

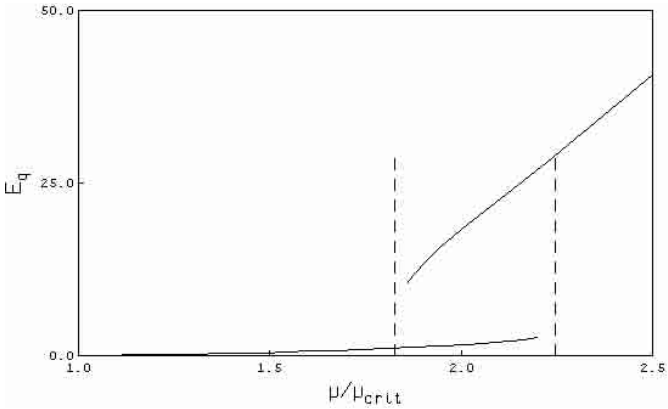


Fig. 3. Hysteresis cycle.

For small μ ($\mu = \mu_1$) l_w is larger than $(2k_F)^{-1}$, the relevant values of k in $\chi(k)$ are such as $k < 2k_F$ and the Lindhard correction to the screening can be ignored. Then the polaron sees a non-oscillating attractive field with small amplitude. For $\mu = \mu_2$ l_w is close to $(2k_F)^{-1}$. Then the maximum of the polaron amplitude and of $V_e(r)$ are close to each other, which makes the coupling with the lattice the most efficient. And the change of sign of $V_e(r)$ induces the oscillatory behavior of φ. $\varphi(r)$ is attractive near the origin (region A) then repulsive in region B, then attractive again in a rather large region C.

We call respectively "weak" and "strong" the polarons obtained for $\mu = \mu_1$ and $\mu = \mu_2$. A weak polaron is generated by a screened field of the Thomas-Fermi type, while a strong polaron is associated with the Lindhard oscillating field. One observes in Figures 2a, b that, in a weak polaron, φ and $|\Psi|^2$ are quite similar functions of r, which makes equation (34) close to the NLS equation. The weak polarons are reminiscent of the polarons of the standard theory.

On the contrary strong polarons look like different physical objects. Actually one observes a very sharp transition from weak to strong polarons when μ is increased. Therefore one can guess that the two types of polarons are to be found simultaneously in some range of μ, and that an hysteresis cycle can be observed when μ is first increased, then decreased. This is indeed the case (see Fig. 3).

Figure 3 represents, for a given value of k_F, the variation of E_q in terms of μ/μ_{crit}. The strong polarons must be studied in the frame of the self-consistent model, and it will be shown that the solutions of the SC model are always strong polarons.

However the nucleation of the first polarons from the free electrons initially present in the material calls for the NSC problem. We have shown before that the polarons for which the existence criterium is most easily satisfied are large scale ($E_q \to 0$). Therefore they are weak polarons, and this means that weak polarons are not only of academic interest.

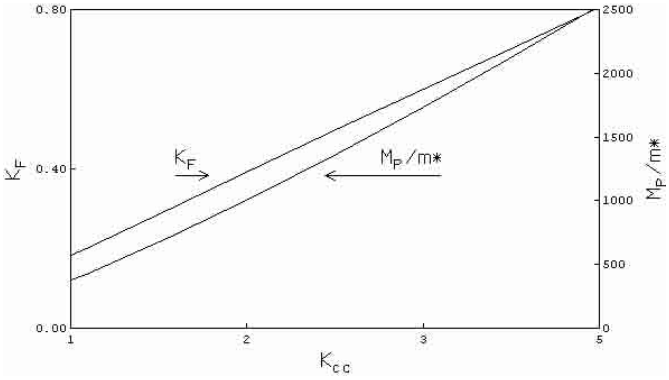


Fig. 4. Polaronic mass and Fermi level in function of k_{cc}.

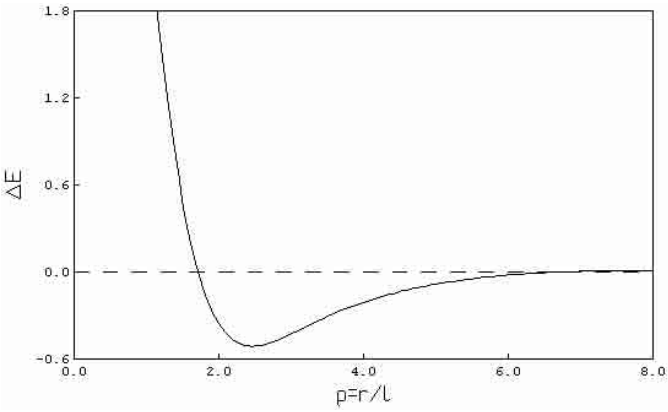


Fig. 5. Binding energy in function of ρ.

6 The strong polarons

The condition of existence of polarons drastically changes in the self-consistent model. Indeed the formation of polarons is accompanied by the diminution of the number of the free electrons which are responsible of the screening: the solution of the SC problem gives a much lower value of k_F ($k_F \sim 0.4$) that is a value of n_e which about 25 times smaller than n_{cc}. The closure of the SC problem is nothing but equation (64).

We have found solutions of equation (64) in a large range of k_{cc} values ($0.5 < k_{cc} < 5$ in 1/l unit). These solutions are always of the strong polaron type and they are characterized by a very small value of E_0 ($E_0 \sim 10^{-3}$), while electronic energy E_q remains finite. This means that, in a strong polaron, the gain of energy due to the electron field is almost compensated by the energy decrease due to the lattice deformation. And the total binding energy is quite small. On the contrary the amplitude of φ, the oscillating polaron field, remains finite. An important consequence is that the energy of the polaron pair is also finite (see below Sect. 6).

We also find that k_F is quite small (compared to its value in a crystal with electron density n_{cc}) and is a growing function of k_{cc} (see Fig. 4). The width of the FS band is quite small while that of the P-band is given by $k_p \approx k_{cc}$. The polaron effective mass is also a growing function of n_{cc}, and we find $M_p/m^* \approx 700$ for a typical perovskite ($k_{cc} \approx 1.7$).

The size of the polaron pair is found much larger than those of the individual polarons, which justifies the perturbative calculation of the pair energy given above. This also explains the existence of the pair, even when the direct repulsive Coulomb interaction is taken into account.

Let us consider a pair of polarons, whose inter distance is $\rho = r/l$. At large ρ, the dominant term in expression (48) for the interaction potential is due to acoustical term φ_{ac}. The force associated to φ_{ac} is attractive (while those associated to φ_{opt} is repulsive) and it can be shown that it dominates, at large distance, the contribution of the direct repulsive Coulomb interaction. As a consequence distant polarons always attract each other. We have represented in Figure 5 the variation of ΔE, the pair binding energy, as a function of ρ.

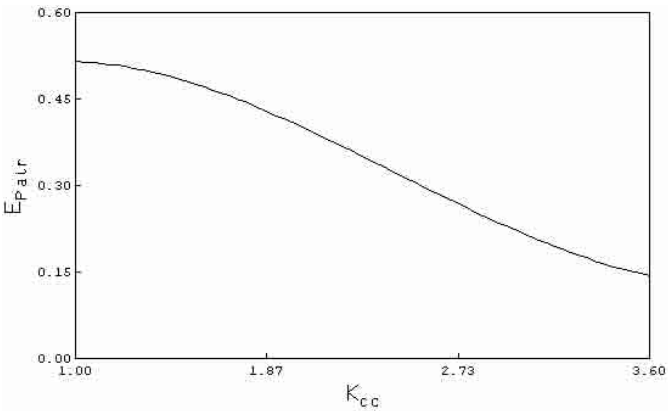


Fig. 6. E_{pair} as a function of k_{cc}.

The minimum E_{pair} of this function is the binding energy of the pair, and we verify that the weak coupling condition (namely: the size of the polaron pair is much larger than those of the individual polarons) is actually verified at the minimum of ΔE. (Remember that this condition is required in order that our above calculation of the pair energy holds.) One also finds that E_{pair} is much larger than E_0, the binding energy of the individual polarons. This fact is clearly connected with the oscillating character of $\varphi(r)$. Figure 6 is the graph of E_{pair} as a function of k_{cc}.

We have obtained that polarons are correlated in the CuO_2 horizontal planes, the correlation length being of the order of l, the average interdistance of these planes. Since the interaction potential between polarons is actually 3D, it may be guessed (and will be soon verified) that polarons are also vertically correlated (correlation between polarons located in adjacent planes). And this correlation could play a role in the c-axis conductivity. We are thus led to propose to associate E_{pair} and the perovskites pseudogap. Such a link between the horizontal and vertical dynamics of the charge carriers is considered by Basov *et al.* [21] in connection with the pseudogap problem. On the other hand we find that E_{pair} is of the order of 200 K, and falls down for large n_{cc}: properties which are in accordance with experimental observations [22].

We conclude from the above results that the direct repulsive Coulomb interaction is not able to oppose

the existence of pairs of polarons. This is explained by the relatively large size of these pairs. On the contrary bipolarons are expected to be more compact structures and the contribution of the direct Coulomb interaction is expected to be much larger. We have minimized expression (44) for the bipolaron energy, using a trial function of the form:

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = \alpha[1 + \frac{\lambda}{2}(|\mathbf{x}_1| + |\mathbf{x}_2|)]\exp\left\{-\frac{\lambda}{2}(|\mathbf{x}_1| + |\mathbf{x}_2|)\right\} \tag{65}$$

where α is related to λ in order to ensure the normalization of Ψ. This form of Ψ ensures the vanishing of the partial derivatives of Ψ at the origin, a property that generalizes those found to hold in the polaron case. We have also used a two parameters trial function (with a quadratic polynomial form multiplying the exponential) and the minimization of $E_{\rm bp}$ with this trial function yields comparable values of the bipolaron energy. More precisely we have solved the variational problem for a bipolaron Hamiltonian in which the prefactor $\varepsilon^{\rm f}\varepsilon_{\rm r}^0$ in the direct Coulomb term was replaced by some arbitrary ε. We then find a positive value of $E_{\rm bp}$ (that is a negative bipolaron energy) as long as ε is smaller than some $\varepsilon_{\max}$. But, for any value of $k_{\rm cc}$, in the large domain investigated, we have found $\varepsilon_{\max} < \varepsilon^{\rm f}\varepsilon_{\rm r}^0$. Therefore the action of the direct Coulomb term is too large to permit the existence of a bipolaron with negative energy. In other words stable bipolarons are not allowed in the frame of the present theory, and as far as our variational method works.

7 Conclusion

Screened polarons appear to be possible solutions of the equations of the electron- lattice interaction for materials of the perovskite type, even though the initial nucleation of these polarons deserves further studies. An important feature is the oscillating structure of the polaron field, related itself to the Friedel oscillations of the screened Coulomb potential.

The bipolarons seem to be excluded in the frame of our continuous theory. On the other hand the polarons are able to form pairs with a finite binding energy (of the order of 200 K). We propose to associate this energy with the pseudogap experimentally observed in perovskites.

It is worth remarking that our results have been obtained in the limit of zero temperature, the polarons properties being moderately sensitive to T. Actually we find that the pairing phenomenon exists up to $k_{\rm B}T \sim E_{\rm pair}(T = 0)$, that is for temperatures significantly higher than $T_{\rm c}$. Of course our results are expected to be considerably modified, at $T < T_{\rm c}$, when superconductivity occurs, that is when a collective interaction between polarons (or pairs of polarons) must be taken into account. The idea that a change in the pairing mechanism takes place at $T = T_{\rm c}$ in high $T_{\rm c}$ materials has been already given in the literature (see for instance Deutscher [23]).

We are not able, at present time, to foresee the structure of the super conducting state in a medium where most of the charge carriers are polarons. We may remark that we get here a basic difference with the situation described in BCS theory, the correlation between the charge carriers (giving the Cooper pairs) being the result of a collective interaction. The BCS point of view could eventually be generalized to a system where polarons are already associated in pairs (at $T > T_{\rm c}$). This generalization will be presented in a next publication.

The second point of view is those of the "molecular conductivity" initiated by Schaffroth *et al.* [24], and extensively developed, mainly by Alexandrov, in the eighties and the nineties (we only give the early references [25,26] in the Bibliography), under the generic name of bipolaronic theories. Since "screened bipolarons" are excluded in our theory, they ought to be replaced by the polarons pairs.

It must be clear that we are not opposing here the conventional bipolaronic theories which are based on small bipolarons. Indeed bipolarons cannot be described in the frame of our continuous theory. We only propose an alternative in polaron theory which has been suggested by some unexpected effects of the screening of the Coulomb interaction. By the way it may be remarked that our "strong polarons" are in an intermediate size domain between the conventional large polarons and the Hölstein small polarons.

Appendix A

We propose to solve equation (23) of the main text in the limit of small values of $\mathbf{v}$. Assuming $\mathbf{v}$ parallel to the coordinate this equation yields to ($\varphi = \boldsymbol{\nabla} \cdot \mathbf{Q}$):

$$\left[1 + \frac{v^2}{\omega_0^2}\partial_x^2\right]\varphi = -\frac{\varepsilon_0}{\varepsilon^{\rm f}}\Delta V \otimes |F|^2$$

or

$$\left[1 + \varepsilon\partial_x^2\right]\varphi = S \tag{A.1}$$

where: $S = -\frac{\varepsilon_0}{\varepsilon^{\rm f}}\Delta V \otimes |F|^2$ and $\varepsilon = v^2/\omega_0^2$. In these equations we shall use the unit of length d of the main text therefore ε is a dimensionnless quantity which we assume to be small.

Let $\mathcal{L}$ be the operator $1+\varepsilon\partial_x^2$. $\mathcal{L}$ depends only on x and (A.1) is a one dimensional equation invariant under space reflexion ($x \to -x$), therefore φ and also Ψ are functions of $|x|$. It is easily shown that the kernel $\mathcal{N}$ and the Green function $\mathcal{G}$ of operator $\mathcal{L}$ are given by:

$$\mathcal{G} = \frac{\varepsilon}{2}\sin\left(\frac{|x|}{\varepsilon}\right) \tag{A.2}$$

$$\mathcal{N} = \cos\left(\frac{x}{e}\right). \tag{A.3}$$

Since S, as φ and Ψ, is invariant under space reflection, the solvability condition of equation (A.1) is that S must be orthogonal to the unique function $\mathcal{N}$.

Finally the general solution of equation (A.1) reads:

$$\varphi = \mathcal{G} \otimes S + \lambda \mathcal{N} \tag{A.4}$$

where λ is an arbitrary parameter. In addition $S(|\Psi|^2)$ must satisfy orthogonality condition:

$$\langle \mathcal{N} | S(|\Psi|^2) \rangle = 0 \tag{A.5}$$

Ψ satisfies a Schrödinger equation in which φ depends on λ according to equation (A.4), which makes Ψ to be a function of λ. Equation (A.5) determines λ.

Now it can be verified that, for small ε (that is in the limit of small v), Green function $\mathcal{G}$ admits a regular expansion in terms of ε, which reads:

$$\mathcal{G} = [1 + \varepsilon \partial_x^2]^{-1} = \delta(x)\{1 - \varepsilon \partial_x^2 + ...\} \tag{A.6}$$

the first (not obvious) step is to show that we have $\mathcal{G} \to \delta(x)$ when $\varepsilon \to 0$. This is equivalent to show that $\langle \mathcal{G}, S \rangle = 0$, and this relation proves to hold provided orthogonality condition (A.5) is satisfied.

We shall now proceed to evaluate the parameter λ. Disregarding for simplicity the acoustic part of the potential, Ψ obeys the Schrödinger equation in which the potential is given by expression (A.4):

$$[\Delta + \mathcal{G} \otimes S + \lambda \mathcal{N}]\Psi = E\Psi. \tag{A.7}$$

If λ is small (an assumption which will be *a posteriori* verified) the λ term in equation (A.7) will be considered as a perturbation.

Let Ψ_0 and E_0 be the eigenfunction and eigenvalue of equation (A.7) for $\lambda = 0$. This equation reads:

$$[\Delta + \mathcal{G} \otimes S(\Psi_0^2)]\Psi_0 = E_0 \Psi_0. \tag{A.8}$$

Differentiating equation (A.8) with respect to E_0, we obtain:

$$H_1 = \frac{\partial \Psi_0}{\partial E_0} = \Psi_0 \tag{A.9}$$

where:

$$H_1 = \Delta + \mathcal{G} \otimes S(\Psi_0^2) + \frac{\delta\{\Psi_0 G \otimes S(\Psi_0^2)\}}{\delta \Psi_0} - E_0. \tag{A.10}$$

We now put:

$$\Psi = \Psi_0 + \Psi', E = E_0 + E'.$$

Linearizing equation (A.7) with respect to Ψ', we obtain:

$$H_1 \Psi' = (E' - \lambda \mathcal{N})\Psi_0. \tag{A.11}$$

Now differentiating equation (A.8) with respect to x it is easily seen that:

$$H_1(\frac{\mathrm{d}}{\mathrm{d}x}\Psi_0) = 0. \tag{A.12}$$

Therefore $\frac{\mathrm{d}}{\mathrm{d}x}\Psi_0$ belongs to the kernel of H_1. Moreover it can be shown that $\frac{\mathrm{d}}{\mathrm{d}x}\Psi_0$ is the only function of $\mathrm{Ker}(H_1)$.

Now we have: $\langle \frac{\partial \Psi_0}{\partial E_0}, H_1 \Psi' \rangle = \langle \Psi_0, \Psi' \rangle$, on account of the hermiticity of H_1. But, working at constant norm, the linear deviation $\langle \Psi_0, \Psi' \rangle$ of the norm must vanish. From equation (A.11) we obtain:

$$\begin{aligned} \langle \frac{\partial \Psi_0}{\partial E_0} H_1 \Psi' \rangle &= \langle \frac{\partial \Psi_0}{\partial E_0}(E' - \lambda \mathcal{N})\Psi' \rangle \\ &= \frac{1}{2}\left\{ E' \langle \frac{\partial \Psi_0^2}{\partial E_0} \rangle - \lambda \langle \mathcal{N}, \frac{\partial \Psi_0^2}{\partial E_0} \rangle \right\} \\ &= 0. \end{aligned} \tag{A.13}$$

Therefore we get:

$$E' = \lambda \frac{\langle \mathcal{N}, \partial \Psi_0^2 / \partial E_0 \rangle}{\langle \partial \Psi_0^2 / \partial E_0 \rangle} \tag{A.14}$$

λ will be determined thanks to orthogonality relation (A.5), which reads at first order in Ψ':

$$\langle \mathcal{N} | \Psi_0^2 \rangle + 2 \langle \mathcal{N} | \Psi_0 \Psi' \rangle = 0. \tag{A.15}$$

Equation (A.11) may be formally solved as:

$$\Psi' = H_1^{-1}(E' - \lambda \mathcal{N})\Psi_0. \tag{A.16}$$

The use of inverse operator H_1^{-1} in (B.15) is justified. Indeed the kernel of this operator is the odd function $\frac{\mathrm{d}}{\mathrm{d}x}\Psi_0$. But $(E' - \lambda \mathcal{N})\ \Psi_0$, which is a function of $|x|$, is an even function and therefore orthogonal to $\mathrm{Ker}(H_1)$. Replacing Ψ' by expression (A.15) in equation (A.13), we obtain:

$$0 = \langle \mathcal{N} | \Psi_0^2 \rangle + E' \langle \mathcal{N} | \frac{\partial \Psi_0^2}{\partial E_0} \rangle - 2\lambda \langle \mathcal{N} \Psi_0 H_1^{-1} \mathcal{N} \Psi_0 \rangle \tag{A.17}$$

Ψ_0^2 and $\partial \Psi_0^2 / \partial E_0$ are regular, non oscillating functions of $|x|$, while $\mathcal{N}$ is rapidly oscillating in the limit $\varepsilon \to 0$. Therefore the two first terms in equation (A.17) are extremely small: they are actually of the order of $\exp(-\sqrt{\frac{E_0}{\varepsilon}})$. On the other hand the third expectation value is not small (or, at least much larger than the first ones). This is due to the fact that H_1^{-1} is a regular operator depending only on $|x|$. As a result $H_1^{-1}\mathcal{N}\Psi_0$ oscillates at the same frequency than $\mathcal{N}$, and, generically it has a finite component on $\mathcal{N}$. This gives a finite value to $\langle \mathcal{N}\Psi_0 H_1^{-1} \mathcal{N}\Psi_0 \rangle$. Finally E' is proportional to λ according to (A.14), and the second term may be neglected in equation (A.17), compared to the third one. This leads to the following expression of λ:

$$2\lambda = \frac{\langle \mathcal{N}, \Psi_0^2 \rangle}{\langle \mathcal{N}\Psi_0, H_1^{-1}\mathcal{N}\Psi_0 \rangle}, \tag{A.18}$$

and, according to the above argument, the value of λ is of the same order as those of the numerator, that is $\lambda \sim \exp(-\sqrt{\frac{E_0}{\varepsilon}})$. λ is therefore vanishingly small in the cases of physical interest where E_0 is finite and ε is small. This result also shows that the solution of equation (A.7) has a non analytical dependence in λ. But λ is so small that

the λ extra term in the Schrödinger equation can be safely neglected. Then we are left with equation (A.8), in which the potential can be expanded thanks to expansion (A.6) of the Green function. At the end we obtain, in the limit of small v, a well-defined solution which can be expanded in terms of v^2/ω_0^2.

Appendix B

We propose to derive the expression of $E_{\rm p}$, the total energy of the moving polaron in the limit of small polaron velocity ($v \ll c$). $E_{\rm p}$ is defined by equation (38) of the main text.

Using equations (22, 23), one obtains that div $\mathbf{u}$ and $\mathbf{Q}$ obey the following equations

$$[\Delta - \frac{(\mathbf{v}\cdot\boldsymbol{\nabla})^2}{c^2}]\mathrm{div}\,\mathbf{u} = \frac{Ze}{Mc^2}\Delta B \tag{B.1}$$

$$[1 + \frac{(\mathbf{v}\cdot\boldsymbol{\nabla})^2}{\omega_0^2}]\mathbf{Q} = -\frac{\varepsilon_0}{\varepsilon^{\rm f}}\boldsymbol{\nabla}B \tag{B.2}$$

$$B = V \otimes |F|^2. \tag{B.3}$$

Solving equations (B.1, B.2) for div $\mathbf{u}$ and $\mathbf{Q}$ is possible in the limit of small v.

We shall write the formal solutions of equations (B1, B2) in the form:

$$\mathrm{div}\,\mathbf{u} = \frac{Ze}{Mc^2}L_{\rm ac}(v)B \tag{B.4}$$

$$\mathbf{Q} = -\frac{\varepsilon_0}{\varepsilon^{\rm f}}L_{\rm opt}(v)\boldsymbol{\nabla}B, \tag{B.5}$$

with

$$L_{\rm ac} = [1 - \frac{(\mathbf{v}\cdot\boldsymbol{\nabla})^2}{c^2}\Delta^{-1}]^{-1},$$

$$L_{\rm opt} = [1 + \frac{(\mathbf{v}\cdot\boldsymbol{\nabla})^2}{\omega_0^2}]^{-1},$$

$L_{\rm ac}$ and $L_{\rm opt}$ reducing to identity for $v = 0$.

Then $\varphi_{\rm ac}$ and $\varphi_{\rm opt}$ given by expressions (14) of the main text can be written as:

$$\varphi_{\rm ac} = \nu\rho\frac{(Ze)^2}{Mc^2}L_{\rm ac}V \otimes B \tag{B.6}$$

$$\varphi_{\rm opt} = -\frac{\varepsilon_0}{\varepsilon^{\rm f}}L_{\rm opt}V\Delta B. \tag{B.7}$$

It is easily shown that $E_{\rm q}$, the eigenvalue of Schrödinger equation (21) for a given v, actually minimizes $\langle H\rangle$.

Let us write $E_{\rm p}$ as:

$$E_{\rm p} = E_0 + \delta E_{\rm p}(v) \tag{B.8}$$

$\delta E(v)$ will be calculated perturbatively ($\delta E \ll \bar{E}$).

We first observe that we have for small v: $F = F_0(|\mathbf{x}|) + O(v^2)$, where F_0 is the wave function of the immobile polaron. Therefore the contribution of the second term in equation (2) is higher order than v^2. It will be neglected.

Let us now consider the momentum terms in equation (2) of the main text. They give, at first order in v^2:

$$\frac{\nu\rho_{\rm m}}{2}\int[\mathbf{v}\cdot\boldsymbol{\nabla}(\mathbf{u}_0)]^2\mathrm{d}\mathbf{x} + \frac{\varepsilon_0}{2\varepsilon^{\rm f}}\int[\mathbf{v}\cdot\boldsymbol{\nabla}(\mathbf{Q}_0)]^2\mathrm{d}\mathbf{x}$$
$$= \left(\frac{\omega^2}{2c^2}\right)\nu\rho\frac{(Ze)^2}{Mc^2}\langle B_0^2\rangle + \left(\frac{\omega^2}{2\omega_0^2}\right)\frac{\varepsilon_0}{\varepsilon^{\rm f}}\langle(\Delta B_0)^2\rangle, \tag{B.9}$$

where:

$$w^2 = \frac{v^2}{D},$$

and $\mathbf{u}_0$, $\mathbf{Q}_0$ and B_0 are the values of $\mathbf{u}$, $\mathbf{Q}$, B for $v = 0$. In particular $B_0 = V \otimes |F_0|^2$. Similarly we define $\varphi_{\rm ac}^0$ and $\varphi_{\rm opt}^{\rm o}$.

The last expression has been obtained by using expressions (B.4, B.5) (written at $v = 0$), and taking account of $\mathbf{u}_0$ and $\mathbf{Q}_0$ being isotropic and irrotational field vectors. Expression (B.9) reads in terms of $\varphi_{\rm ac}^0$ and $\varphi_{\rm opt}^0$ (*cf.* expressions (B.6, B.7)):

$$\frac{w^2}{2c^2}\langle F_0^2\varphi_{\rm ac}^0\rangle - \frac{w^2}{2w_0^2}\langle F_0^2\Delta\varphi_{\rm opt}^0\rangle.$$

Therefore we are left with the following expression for $\delta E_{\rm pol}$:

$$\delta E_{\rm p} = \frac{m^*v^2}{2} + \frac{w^2}{2c^2}\langle F_0^2\varphi_{\rm ac}^0\rangle - \frac{w^2}{2\omega_0^2}\langle F_0^2\Delta\varphi_{\rm opt}^0\rangle + \mathcal{A}, \tag{B.10}$$

with:

$$\mathcal{A} = \frac{\nu\chi}{2}\delta\langle(\mathrm{div}\,\mathbf{u})^2\rangle + \frac{\varepsilon^{\rm f}}{2\varepsilon_0}\delta\langle\mathbf{Q}^2\rangle - \delta E. \tag{B.11}$$

We shall now show that $\mathcal{A} = 0$.

First $\mathcal{A}$ can be rewritten, using expressions (B.4, B.5) as:

$$\mathcal{A} = \nu\rho\frac{(Ze)^2}{Mc^2}\langle B_0\delta(L_{\rm ac}B)\rangle - \frac{\varepsilon_0}{\varepsilon^{\rm f}}\langle B_0\delta(L_{\rm opt}\Delta B)\rangle - \delta E.$$

Now the variation (with respect to v) of Shrödinger equation (21) yields:

$$H_0\delta F + [\delta(\varphi_{\rm ac}) + \delta(\varphi_{\rm opt})]F_0 = F_0\delta E, \tag{B.12}$$

where

$$H_0 = \Delta + \varphi_{\rm ac}^0 + \varphi_{\rm opt}^0 - E_0.$$

Multiplying equation (B.12) by F_0 and space averaging, we get:

$$\delta E = \langle F_0^2[\delta(\varphi_{\rm ac}) + \delta(\varphi_{\rm opt})]\rangle$$
$$= \nu\rho\frac{(Ze)^2}{Mc^2}\langle F_0^2\delta(L_{\rm ac}V \otimes B)\rangle$$
$$- \frac{\varepsilon_0}{\varepsilon^{\rm f}}\langle F_0^2\delta(L_{\rm opt}V \otimes \Delta B)\rangle.$$

Finally it is easily verified that $\langle B_0\delta(L_{\rm ac}B)\rangle = \langle F_0^2\delta(L_{\rm ac}V\otimes B)\rangle$, and

$$\langle B_0\delta(L_{\rm opt}\Delta B)\rangle = \langle F_0^2\delta(L_{\rm opt}V\otimes\Delta B)\rangle.$$

Finally $\delta E_{\rm p}(v)$ is of the form $M_{\rm p}v^2$, that is the low energy spectrum of polaronic states coincides with the spectrum of a free particle with effective mass $M_{\rm p}$ given by:

$$M_{\rm p} = m^* + \frac{1}{D}\left\{\frac{1}{c^2}\langle F_0^2\varphi^0_{\rm ac}\rangle - \frac{1}{\omega_0^2}\langle F_0^2\Delta\varphi^0_{\rm opt}\rangle\right\}. \quad \text{(B.13)}$$

Appendix C

NLS equation in dimension D, which we shall write as $[{\rm i}\partial t + \Delta + \phi^2]\phi = 0$, has the following stationary form (obtained when ϕ has the time dependence $\exp(-{\rm i}Et)$)

$$[\Delta+\phi^2]\phi = E\phi, \quad \text{where} \quad \Delta = \frac{{\rm d}^2}{{\rm d}r^2} + \frac{D-1}{r}\frac{\rm d}{{\rm d}r}\cdot \quad \text{(C.1)}$$

Multiplying equation (C.1) successively by ϕ and $r^D\frac{{\rm d}\phi}{{\rm d}r}$, then integrating over r, we obtain the two relations:

$$\langle(\frac{{\rm d}\phi}{{\rm d}r})^2\rangle = \langle\phi^4\rangle - E\langle\phi^2\rangle \quad \text{(C.2)}$$

$$\langle(\frac{{\rm d}\phi}{{\rm d}r})^2\rangle = \frac{D}{2-D}[E\langle\phi^2\rangle - \frac{1}{2}\langle\phi^4\rangle]. \quad \text{(C.3)}$$

From these relations we get:

$$\langle\phi^4\rangle = \frac{4}{4-D}E\langle\phi^2\rangle \quad \text{(C.4)}$$

$$\langle(\frac{{\rm d}\phi}{{\rm d}r})^2\rangle = \frac{D}{4-D}E\langle\phi^2\rangle. \quad \text{(C.5)}$$

Thanks to expression (C.5) expression (38) of the main text for the total polaron energy can be written as:

$$E_{\rm pol} = \frac{2-D}{4-D}E\langle\phi^2\rangle. \quad \text{(C.6)}$$

We see that $E_{\rm pol}$ is positive for $D=1$ and negative for $D=3$, while it vanishes for $D=2$. Let us remark that the case $D>4$, where $E_{\rm pol}$ would be positive, must be disregarded. Indeed relation (C.4) would assign a negative value to $\langle\phi^4\rangle$, which is impossible: there does not exist any stationary solution of the NLS equation for $D>4$.

We conclude that relating the stability of the stationary solution and the positivity of the total polaron energy is quite justified: one obtains exactly the same result as by using the Vakhitov-Kolokolov criterium. (Note that for $D=2$ the two criteriums fail to decide. It is known that, a more refined argument is needed to conclude to the unstability of the solution.)

Appendix D

As was said in the main text, the k-domain of polaronic states is finite: $\mathcal{D}=[0,k_{\rm p}]$, and it appears that the calculation of Lindhard corrections (see Ref. [12]) is modified when $\mathcal{D}$ is finite. We shall therefore briefly recall the Lindhard derivation in this case.

In the presence of an external weak perturbative potential φ the wave function $|\Psi_{\mathbf{k}}\rangle$ of a charge carrier is modified as follows:

$$|\Psi_{\mathbf{k}}\rangle \to |\Psi_{\mathbf{k}} + \delta|\Psi_{\mathbf{k}}\rangle$$

with

$$\delta|\Psi_{\mathbf{k}}\rangle = \sum_{\mathbf{k}\neq\mathbf{k}',\mathbf{k}'\subset\mathcal{D}} \frac{1}{E_{\rm p}(\mathbf{k}) - E_{\rm p}(\mathbf{k}')}\langle\Psi_{\mathbf{k}'}\varphi\Psi_{\mathbf{k}}\rangle|\Psi_{\mathbf{k}'}\rangle \quad \text{(D.1)}$$

the induced space density fluctuation $\delta\rho(\mathbf{r})$ is given by:

$$\delta\rho(\mathbf{r}) = \sum_{\mathbf{k}\subset\mathcal{D}} \delta|\Psi_{\mathbf{k}}(r)|^2 f_{\mathbf{k}} \quad \text{(D.2)}$$

where $f_{\mathbf{k}}$ is the polaronic Fermi distribution. Inserting (D.1) in (D.2) and taking into account of the restrictions $\mathbf{k},\mathbf{k}'\subset\mathcal{D}$ we obtain finally for the linear response function $\chi(\mathbf{q})$:

$$\chi_{\rm j}(\mathbf{q}) = \frac{4}{a_0}\frac{1}{\varepsilon_{\rm r}^0}\frac{1}{2\pi}\frac{m_{\rm j}}{m}\int_{|\mathbf{k}\pm\frac{\mathbf{q}}{2}|<k_{\rm p}} {\rm d}\mathbf{k}\frac{f(\mathbf{k}-\frac{\mathbf{q}}{2}) - f(\mathbf{k}+\frac{\mathbf{q}}{2})}{\mathbf{k}\cdot\mathbf{q}} \quad \text{(D.3)}$$

where index j refers to the class of charge carriers (free electrons or polarons). We take as $f(\mathbf{k})$ the isotropic Fermi function:

$$f(\mathbf{k}) = \frac{1}{\exp[\beta(E_{\rm p}-E_{\rm F})]+1}$$

($E_{\rm F}$: chemical potential of the electrons).

Calculating $\chi_{\rm e}$ (the contribution of the free electronic states) k_m is infinite; the evaluation of the above unbounded integral is easy, and equation (D.3) gives (with $m_{\rm j}=m^*$) gives:

$$\chi_{\rm e}(q) = \tilde{k}_{\rm s} \quad \text{for } k\le 2k_{\rm F}$$
$$= \tilde{k}_{\rm s}\left\{1-\sqrt{1-\frac{4k_{\rm F}^2}{k^2}}\right\} \quad \text{for } k\ge 2k_{\rm F},$$

where $\tilde{k}_{\rm s} = \frac{4}{a_0}\frac{1}{\varepsilon_{\rm r}^0}\frac{m^*}{m}$. This is the 2D version of the 3D Lindhard formula.

Let us now consider the polaronic contribution. We first obtain from expression (D.3) for $\chi_{\rm p}(\mathbf{q})$ that:

$$\chi_{\rm p}(0) = -\frac{4}{a_0}\frac{M_{\rm p}}{m_{\rm e}}[f(0)-f(k_{\rm p})] \quad \text{(D.4)}$$

$$\chi_{\rm p}(q) = 0 \quad \text{for } |q|\ge 2k_{\rm p}. \quad \text{(D.5)}$$

An important remark is that χ vanishes in the case when the polaronic band is fully occupied. We have indeed in this case: $\chi_{\rm p}(0)=0$ since $f(0)=f(k_{\rm p})=1$.

In terms of energy unit $\bar{E} = \frac{\hbar^2}{2m^* d^2}$ of the main text, E_p reads:

$$E_\mathrm{p} = -E_0 + \frac{m^*}{M_\mathrm{p}} k^2 = \frac{m^*}{M_\mathrm{p}} k_\mathrm{m}^2 (x^2 - 1) \tag{D.6}$$

where $\mathbf{x} = \mathbf{k}/k_\mathrm{m}$. With these notations we get:

$$\begin{aligned} \beta(E_\mathrm{p} - E_\mathrm{F}) &= \beta[\frac{m^*}{M_\mathrm{p}} k_\mathrm{m}^2 (x^2 - 1) - E_\mathrm{F}] \\ &= B(x^2 - 1) - A \end{aligned} \tag{D.7}$$

with

$$B = \beta \frac{m^*}{M_\mathrm{p}} k_\mathrm{m}^2; \quad A = \beta(E_\mathrm{F} + E_\mathrm{max}).$$

It is worth noting the limit $\beta \to \infty$ does not imply $B \to \infty$.

Putting $\mathbf{z} = \mathbf{q}/k_\mathrm{m}$, expression (A.5) is rewritten as:

$$\begin{aligned} \chi_\mathrm{p}(\mathbf{z}) &= \frac{4}{a_0} \frac{1}{\varepsilon_\mathrm{r}^0} \frac{1}{2\pi} \frac{M_\mathrm{p}}{m_\mathrm{e}} I \\ I(\mathbf{z}) &= \int_{|\mathbf{x} \pm \frac{\mathbf{z}}{2}| \langle 1} \mathrm{d}\mathbf{x} \frac{f(\mathbf{x} - \frac{\mathbf{z}}{2}) - f(\mathbf{x} + \frac{\mathbf{z}}{2})}{\mathbf{x} \cdot \mathbf{z}} \end{aligned} \tag{D.8}$$

with:

$$f(\mathbf{x}) = \frac{1}{\exp[B(x^2 - 1) - A] + 1} \cdot \tag{D.9}$$

Evaluating quantity I for reasonable values of parameters A and B can only be done numerically, except in the limit $B \to \infty$. Let us write in this case:

$$B(x^2 - 1) - A = B(x^2 - x_\mathrm{f}^2) \text{ with } x_\mathrm{f}^2 = 1 + A/B.$$

Two cases are to be considered:
a) $x_\mathrm{f} \ll 1$ (then A is negative).
the limitation $|\mathbf{x} \pm \frac{\mathbf{z}}{2}| < 1$ can be disregarded and we obtain:

$$\begin{aligned} I(\mathbf{z}) &= 1 && \text{for } |\mathbf{z}| \leq 2x_\mathrm{f} \\ I(\mathbf{z}) &= 1 - \sqrt{1 - \frac{4x_\mathrm{f}^2}{z^2}} && \text{for } |\mathbf{z}| \geq 2x_\mathrm{f}. \end{aligned}$$

In other words $I(x)$ has the same form as for the free electronic states.
b) $x_\mathrm{f} \gtrsim 1$
In this case the limitation $|\mathbf{x} \pm \frac{\mathbf{z}}{2}| < 1$ plays a central role and we find after some geometry:

$$\begin{aligned} I(\mathbf{z}) &= 1 - \frac{1}{\exp(-A) + 1} = \frac{\exp(-A)}{\exp(-A) + 1} \quad \text{for } |\mathbf{z}| = 0 \\ I(\mathbf{z}) &= 0 \quad \text{for } |\mathbf{z}| \neq 0. \end{aligned}$$

A quite non-analytical result! If the order of the limits was reversed: making first $B \to \infty$, then $|\mathbf{z}| \to 0$, then we should get $I = 0$ every where. It is clear that this last procedure is unphysical. In the following we shall always assume that $A > 0$, therefore the limitation $|\mathbf{x} \pm \frac{\mathbf{z}}{2}| < 1$ plays an important role. From equation (D.4) we obtain immediately:

$$I(0) = \frac{1}{\exp(-B - A) + 1} - \frac{1}{\exp(-A) + 1} \cdot \tag{D.10}$$

Although not very large even for $\beta \to \infty$ quantity B is noticeably larger than one therefore

$$I(0) \approx \frac{\exp(-A)}{\exp(-A) + 1} \cdot \tag{D.11}$$

Let us remember that $I(\mathbf{z}) = 0$ for $|\mathbf{z}| \geq 2$. Numerical calculations show that $I(\mathbf{z}) < I(0)$ for $|\mathbf{z}| \neq 0$. In the domain $0 < |\mathbf{z}| < 2$, $I(\mathbf{z})$ is generally a gentle decreasing function except, for large values of B, near $|\mathbf{z}| = 2$ where I is non analytical, and $I(0)$ vanishes for $B \to \infty$. The following are asymptotic expansions of $I(z)$:

$$\begin{aligned} I(z) &\approx I(0) G(B, z). \quad (I(0) \approx \exp(-A)) \\ &\text{for } \exp(-A) \ll 1 \end{aligned} \tag{D.12}$$

$$\begin{aligned} I(z) &\approx I(0) \frac{2}{\pi} \left[\arccos(\frac{z}{2}) - \frac{z}{2} \sqrt{1 - \frac{z^2}{4}} \right] \\ &\text{for } B \ll 1. \end{aligned} \tag{D.13}$$

We have $\exp(-A) \ll 1$ and $I(\mathbf{z})/I(0) \approx G(B, z)$.

In Figure 7 we have represented $G(z)$ for $B = 0$ and $B = 20$.

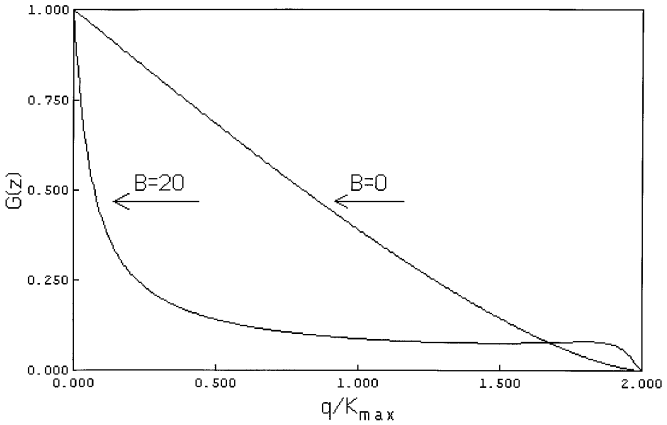


Fig. 7. Function $G(z)$ for $B = 0$ and $B = 20$.

Appendix E

We want to solve the equation obeyed by Green function $G(\mathbf{x}, z)$ of the main text when the response function is those of the Thomas Fermi model, that is $\chi = k_\mathrm{s}$ in Fourier space:

$$-\Delta G(\mathbf{x}, z) = \delta(\mathbf{x})\delta(z) - k_\mathrm{s}\delta(\mathbf{x}) G(\mathbf{x}, z) \sum_n (z - n) \tag{E.1}$$

where the adopted unit length is $d = l$.

We shall proceed in Fourier space with respect to variable **x**. Equation (E.1) becomes:

$$(-\sigma^2+\partial_z^2)G(\boldsymbol{\sigma},z)=-\delta(z)+k_{\mathrm{s}}G(\boldsymbol{\sigma},z)\sum_n(z-n) \tag{E.2}$$

where $\boldsymbol{\sigma}$ is the Fourier variable associated with **x**.

Let now $G_n(\sigma)$ be the solution of equation (E.2) in interval $[n<z<n+1]$. $G_n(\boldsymbol{\sigma})$ and its derivative with respect to z have the form:

$$G_n=A_n\mathrm{e}^{-\sigma z}+B_n\mathrm{e}^{\sigma z} \tag{E.3a}$$

$$\partial_z G_n=\sigma(-A_n\mathrm{e}^{-\sigma z}+B_n\mathrm{e}^{\sigma z}). \tag{E.3b}$$

Now $\partial_z G_n$ exhibits a finite jump at $z=ln$, due to the presence of the δ function in equation (E.2).

This jump is defined by:

$$\partial_z G_n(z+\varepsilon)-\partial_z G_n(z-\varepsilon)=k_{\mathrm{s}}G_n(\varepsilon\ll 1). \tag{E.4}$$

If $\{A_n,B_n\}$ are defined as the amplitudes just above $z=n(z-n=\varepsilon)$, we have the following relations between $\{A_{n+1},B_{n+1}\}$ and $\{A_n,B_n\}$:

$$A_{n+1}+B_{n+1}=A_n\mathrm{e}^{-\sigma}+B_n\mathrm{e}^{\sigma} \tag{E.5a}$$

$$\sigma(-A_{n+1}+B_{n+1})=\sigma(-A_n\mathrm{e}^{-\sigma}+B_n\mathrm{e}^{\sigma})+k_{\mathrm{s}}(A_{n+1}+B_{n+1}). \tag{E.5b}$$

The first relation expresses the continuity of G on $z=(l+1)n$, the second one expresses relation (B.4) on the same frontier.

Putting $X_n=\begin{pmatrix}A_n\\B_n\end{pmatrix}$ these two relations can be put in the following matricial form:

$$X_{n+1}=QX_n \tag{E.6}$$

Q being the matrix:

$$Q=\begin{pmatrix}(1-a)\mathrm{e}^{-\varphi} & -a\mathrm{e}^{\varphi}\\ a\mathrm{e}^{-\varphi} & (1+a)\mathrm{e}^{\varphi}\end{pmatrix}$$

where $\varphi=\sigma$, $a=\frac{k_{\mathrm{s}}}{2\sigma}$.

Eigenvalues of matrix Q are: $\xi\pm=\mathrm{e}^{\pm\theta}$, where θ is given by:

$$\cosh\theta=\cosh\varphi+a\sinh\varphi. \tag{E.7}$$

We look for a solution of equation (C.6) which does not diverge when $n\to\infty$. This is obtained by choosing initial vector X_0 parallel to ξ_-, the eigenvector associated with ζ_-. This implies that we have:

$$\frac{B_0}{A_0}=\left(\frac{1}{a}\right)[(1-a)\mathrm{e}^{-2\varphi}-\mathrm{e}^{-(\theta+\varphi)}]. \tag{E.8}$$

On the other hand, the continuity relations written on $z=0$, with the additional statement that $\partial_z G$ is antisymmetric ($\partial_z G(z)=-\partial_z G(-z)$), permit one to express A_0 and B_0 in terms of initial value $G_0=G(\boldsymbol{\sigma},0)$. We get:

$$2A_0=(1-a)G_0+\frac{1}{2\sigma}$$

$$2B_0=(1+a)G_0-\frac{1}{2\sigma} \tag{E.9}$$

G_0 can be obtained from equations (E.8) and (E.9).

Then the solution of equations (E.6) reads:

$$X_n=\mathrm{e}^{-n\theta}X_0,$$

from which we get:

$$G(\mathbf{k},z)=\sum_n Y(z-n)Y[(n+1)-z]\mathrm{e}^{-n\theta}\times\left\{\mathrm{e}^{-\sigma(z-n)}A_0+\mathrm{e}^{\sigma(z-n)}B_0\right\} \tag{E.10}$$

where Y is the Heaviside step function.

$$\int G(\boldsymbol{\sigma},z)^2\mathrm{d}z.$$

Let us now evaluate the average value of operator $\mathcal{A}$ of the main text. It is given by:

$$\langle\mathcal{A}\rangle=\left\{\mu\int G(\boldsymbol{\sigma},z)^2\mathrm{d}z+\mathcal{S}[G(\boldsymbol{\sigma},0)-k_{\mathrm{s}}\sum_n G(\boldsymbol{\sigma},n)\otimes G(\boldsymbol{\sigma},n)]\right\}_{\sigma=0}.$$

In the limit $\sigma\to 0$, we find:

$$G(\boldsymbol{\sigma},0)=G_0=\frac{1}{k_{\mathrm{s}}}\frac{1+k_{\mathrm{s}}-\mathrm{e}^{-\theta}}{3+k_{\mathrm{s}}-\mathrm{e}^{-\theta}}$$

$$\sum_n G(\boldsymbol{\sigma},n)\otimes G(\boldsymbol{\sigma},n)=\frac{1+\mathrm{e}^{-2\theta}}{1-\mathrm{e}^{-2\theta}}G_0^2$$

$$\int G(\boldsymbol{\sigma},z)^2\mathrm{d}z=\frac{2}{k_{\mathrm{s}}^2}\frac{1+\mathrm{e}^{-2\theta}}{1-\mathrm{e}^{-2\theta}}\times\frac{(1-\mathrm{e}^{-\theta})(1+k_{\mathrm{s}}-\mathrm{e}^{-\theta})+\frac{(ks)^2}{3}}{(3+k_{\mathrm{s}}-\mathrm{e}^{-\theta})^2},$$

where:

$$\mathrm{e}^{-\theta}=1+\frac{k_{\mathrm{s}}}{2}-\sqrt{(1+\frac{k_{\mathrm{s}}}{2})^2-1}\,.$$

In the limit of large k_{s}, $\mathrm{e}^{-\theta}$ is negligible and we get: $G_0\approx\frac{1}{k_{\mathrm{s}}}(1-\frac{2}{k_{\mathrm{s}}})$. Then $\langle\mathcal{A}\rangle$ reduces to:

$$\langle\mathcal{A}\rangle\approx\frac{2}{k_{\mathrm{s}}^2}\left\{\mathcal{S}+\frac{\mu}{3}\right\}\ \text{(in l unit)}.$$

In the limit of large μ we are left with:

$$\langle\mathcal{A}\rangle\approx\frac{2}{3}\frac{\mu}{k_{\mathrm{s}}^2}\,.$$

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