Mathematical analysis of a nonparabolic two-band Schrödinger-Poisson problem.

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Abstract

A mathematical model for the quantum transport of a two-band semiconductors that includes the self-consistent electrostatic potential is analyzed. Corrections beyond the usual effective mass approximation are considered. Transparent boundary conditions are derived for the multi-band envelope Schrödinger model. The existence of solution of the nonlinear system is proved by using an asymptotic procedure. Some numerical examples are included. They illustrate the behavior of the scattering and the resonant states.

I. INTRODUCTION

In the modern semiconductor devices, the electrons are confined nanometric regions. In this context, the quantum mechanical behavior of the particles becomes important. Quantum devices like the resonant tunneling diodes are applied in the nowadays high-speed electronic systems [1]. Differing from the usual particle transport phenomena where the electronic current flows inside a single band, the remarkable feature of such devices is the presence of strong interband effects. Under certain regimes, an important contribution to the particle transport arises from the inter-band tunneling. A very popular approach for modeling the multi-band devices, is so called kp theory. It has been derived by Kane [2], Luttinger and Kohn [3] (see Ref. [4, 5] for an exhaustive review of the kp models including various applications). The kp approach provides an accurate description of the energy band structure of bulk semiconductors and heterostructures. This method is based on the decomposition of the particle wave function on a particular set of Bloch functions. The kp models have been theoretically investigated and their applications to the solid state physics have been explored. The description of the particle motion can be preformed at different levels. The more direct approach is to use of the original Schrödinger-like multiband picture. As an alternative, formulations based on the density matrix or on the Wigner function have been considered [6–9]. Moreover, hybrid models have been also developed. In these approaches, the quantum and classical transport equations are combined. Coherent and phase-breaking phenomena are included [10, 11].

The study of multiband models is a very active area of research [12–22]. A considerable effort has been made in order to develop mathematical models that reproduce the steady states and the out-of-equilibrium dynamics in heterostructure devices [23]. In order to model a quantum device, it is necessary to devise special boundary conditions that describe a net flux of current through the contacts of the device [24, 25]. In this way, it is possible to restrict the original physical model, that usually is derived for an unbounded domain, to a finite interval. Different methods are proposed in literature (see for example Ref. [26] for the boundary element methods or Ref. [27] for the infinite element methods). In this contribution, we adopt the so called transparent boundary conditions (TBC) [28, 29]. The derivation of the TBC is addressed in sec. II.

The paper is organized as follows. In sec. II we present the two-band quantum model for the charge carriers. In sec. III A we describe the nonlinear problem and we enunciate the existence of a solution for the two-band Schrödinger-Poisson system that is the main result of this contribution. In sec. III B we study the existence and uniqueness of solution for a non-hermitian two-band system. In secs. IV A-V we prove the existence of a solution of the non-linear asymptotic model. The proof is based on the Leray-Schauder fixed point theorem. The asymptotic limit is addressed in secs. IV-VI. Finally, in sec. VII some numerical tests are performed.

II. MEF SYSTEM WITH TBC

We describe a crystal with the multiband envelope function kp theory. In this context, the particle wave function is constituted by a sequence of smooth functions ψ_n. The quantity $|\psi_n|^2$ is proportional to the probability to find the electron in the $n-$th band (more details are given in Ref. [3, 30] and in Appendix A). The linear Schrödinger problem that describes a one-dimensional crystal where only the conduction and the valence bands are take into account, is given by [31]

$$-b_c \frac{\mathrm{d}^2 \psi_c}{\mathrm{d}x^2} + (E_c + V)\psi_c - \gamma \frac{\mathrm{d}V}{\mathrm{d}x}\psi_v = E\psi_c \tag{1}$$

$$a\frac{\mathrm{d}^4\,\psi_v}{\mathrm{d}x^4} + b_v \frac{\mathrm{d}^2 \psi_v}{\mathrm{d}x^2} + (E_v + V)\psi_v - \gamma \frac{\mathrm{d}V}{\mathrm{d}x}\psi_c = E\psi_v\ . \tag{2}$$

Here, $a > 0$ is a constant that describes the non parabolicity of the valence band, $b_c = \frac{\hbar}{2m_c}$, $b_v = \frac{\hbar}{2m_v}$ where $\hbar$ is the Planck constant and m_c, m_v are, respectively, the effective mass in conduction and in valence band. Moreover, $\gamma = \frac{P\hbar^2}{mE_g}$, where m is the bare electron mass and $E_g = E_c - E_v$ is the energy gap between the top of the valence band E_v and the bottom of the conduction band E_c. The symbol P is denoted as the Kane parameter and represents the matrix element in the Wigner-Sietz cell $\mathcal{C}$ of the gradient operator

$$P = \int_{\mathcal{C}} \overline{u_c}(\mathbf{r})\nabla_{\mathbf{r}}\, u_v\,(\mathbf{r})\ \mathrm{d}\mathbf{r}\ . \tag{3}$$

Here, the function u_c (u_v) denotes the Bloch wave function for the conduction (valence) band for $\mathbf{k} = 0$. Finally, V is the sum of the electrostatic and built-in potential.

We denote the system of Eqs. (1)-(2) by multi envelope function (MEF) model. For the sake of compactness, we rewrite the MEF model in the matrix form $\mathcal{H}\boldsymbol{\psi} = E\boldsymbol{\psi}$, where

$$\mathcal{H} := \begin{pmatrix} -b_c \dfrac{\mathrm{d}^2}{\mathrm{d}x^2} + E_c + V & -\gamma \dfrac{\mathrm{d}V}{\mathrm{d}x} \\ \\ -\gamma \dfrac{\mathrm{d}V}{\mathrm{d}x} & a\dfrac{\mathrm{d}^4}{\mathrm{d}x^4} + b_v \dfrac{\mathrm{d}^2}{\mathrm{d}x^2} + E_v + V \end{pmatrix}, \quad \boldsymbol{\psi} = \begin{pmatrix} \psi_c \\ \psi_v \end{pmatrix}. \tag{4}$$

Differing from the standard effective mass approach, where the kinetic energy is proportional to the second-order derivative of the wave function, in Eq. (2) a fourth order derivative of ψ_v is present (ψ_v represents the component of the wave function in the valence band). This term takes into account the non parabolicity effects and provides a lower bound in the spectrum of the Hamiltonian operator. This can be easily verified by writing formally $\mathcal{H}$ in the Fourier space (it is sufficient make the substitution $\frac{d}{dx} \to ik$). The eigenvalues of $\mathcal{H}$ are bounded from below. The existence of a minima in the spectrum, is crucial for the regularity of the system. From a mathematical point of view, the presence of the high order derivative provides a control of the norm of the particle density and prevents the blow up of the solution (see theorem 6 in the following).

We remark that in this formulation, the MEF problem is an eigenvalue problem and E is the eigenvalue. We study of the MEF problem in the bounded domain $\Omega = [x_l, x_r]$. At the boundary, we assume the so called "transparent boundary conditions" (TBC). The TBC are widely used for modeling open quantum systems. In particular, they describe the particles that enter and leave Ω without reflection. The eigenvalue problem is formulated as the restriction to the domain Ω of the unbounded problem defined on $\mathbb{R}$. More into details, we extend Eqs. (1)-(2) to $\mathbb{R}$ and we assume that the potential V is constant outside Ω ($V(x) = V(x_l)$ for $x < x_l$ and $V(x) = V(x_l)$ for $x > x_r$). The solution of Eqs. (1)-(2) outside Ω is easily found (the derivative of V vanishes and the two equations decouple). We obtain

$$\psi_j(x) = \sum_{r=1}^{n_j} A_r^j e^{ik_r^j(x-x_0)} \qquad j = c, v\ , \tag{5}$$

where A_k^j and x_0 are coefficients, $n_c = 2$ ($n_v = 4$) and k_r^j are the $n_c + n_v$ roots of the secular equation $E_{s,p}(k_r^j) = 0$ with

$$E_{s,p}(k) = \begin{cases} E_c + V(x_p) + b_c k^2 & \text{for} \quad s = c \\ E_v + V(x_p) - b_v k^2 + ak^4 & \text{for} \quad s = v\ , \end{cases} \tag{6}$$

where $p = l, r$. We require that the solution inside the domain Ω is compatible with Eq. (5). This is obtained by requiring that $\boldsymbol{\psi}$ has the same high-order derivatives of the plane wave expansion (6). In order to ensure that the MEF problem in Ω is well-defined, we should impose at the boundaries $n_c + n_v$ independent equations. By imposing symmetric conditions in $x = x_l$ and $x = x_r$, only $(n_c + n_v)/2$ constraints are necessary. Equation (5) contains $n_c + n_v$ free parameters A_r^j (for simplicity, in the following we assume $x_0 = 0$). By evaluating $n_c/2$ and $n_v/2$ derivatives, we can eliminate $(n_c + n_v)/2$ parameters by expressing the high-order derivative of ψ_j in terms of the lower order derivative. $\psi_j^{(m_j)} = \psi_j^{(m_j)}\left(\psi_j^{(1)}, \cdots, \psi_j^{(n_j/2)}\right)$ with $n_j/2 \leq m_j < n_j$.

In this procedure we are free to choose $n_j/2$ parameters A_k^j among the n_j. In the present case, the choice is driven by physical considerations. We impose the boundary conditions that describe plane waves entering and leaving Ω in $x = x_l$ and $x = x_r$. We classify each term of Eq. (5) as incoming, transmitted or reflected modes. The traveling modes incoming from the left (the right) have positive (negative) group velocity $v_g = \left.\frac{\mathrm{d}E_{s,p}}{\mathrm{d}k}\right|_{k_r^j}$. They represent the particles that enter in Ω. The reflected waves have velocity with opposite sign and the transmitted waves have velocity with the same sign of the incoming waves at the opposite boundary. The boundary conditions are obtained as follows. We define the parameter "injection energy" $\overline{E} \equiv E_{s_0,p_0}(q)$. We fix the value of the vector (s_0, p_0, q) in the range $[c, v] \times [l, r] \times [0, +\infty)$. The energy $E_{s_0,p_0}(q)$ is given by Eq. (6) and represents the energy of the incoming waves. More into details, they have momentum equal to q, enters in Ω from the left or the right side according to $p_0 = l, r$ and belongs to the conduction or the valence band according to $s_0 = c, v$. We choose $(s, p) \neq (s_0, p_0)$ and we solve the equation $E_{s,p}(k) = \overline{E}$ with respect to k. We obtain n_s solutions and, according to the expansion given in Eq. (5), we associate to each root k_r^j the corresponding plane wave $A_r^j\, e^{ik_r^j x}$. We assign $A_r^j \neq 0$ only for the outgoing waves. As explained before, for $p = r$ ($p = l$) they have positive (negative) group velocity v_g and $\Im\{k_r^j\} < 0$ ($\Im\{k_r^j\} > 0$), where $\Im$ denotes the imaginary part. It is easy to verify that there are at least $n_s/2$ of such solutions. As explained before, we derive Eq. (5) $n_s/2 - 1$ times and we express the parameters A_r^j in terms of the spatial derivative of $\psi_j(x)$. Concerning the case $(s, p) = (s_0, p_0)$ (that was excluded before), we proceed in the same way, with the only difference that we include also the solution $k_r^j = q$. This provides an additional parameter $\iota \equiv a_k^s$ for the wave $\iota e^{\pm iqx}$. Differing from the former cases, this term describes an incoming wave. The parameter ι (that can be chosen equal to one without loss of generality) leads to an homogenous term in the differential equation.

For sake of clearness, we describe the details of the calculations that leads to the TBC for the valence band ($s = v$) in $x = x_l$. These the boundary conditions describe the particles that enter in Ω through the valence band. The other cases $(s,p),(s_0,p_0) = \{(v,l);(v,r);(c,r);(c,l)\}$ are treated in the same way. We choose $q \in \mathbb{R}^+$ and we assume $(s_0,p_0) = (s,p) = (v,l)$. The choice $(s_0,p_0) \neq (s,p)$ can be treated as the particular case with $\iota = 0$. The MEF problem extended to $\mathbb{R}$ gives (without loss of generality we assume $V(x_l) = 0$):

$$a\frac{\mathrm{d}^4\,\psi_v}{\mathrm{d}x^4} + b_v\frac{\mathrm{d}^2\psi_v}{\mathrm{d}x^2} + E_v\psi_v = \overline{E}\psi_v \tag{7}$$

It is easy to verify that in addition to $k_r^v = q$, the equation $\overline{E} = E_v + V(x_p) - b_v k^2 + ak^4$ (see Eq. (6)) has two solutions such that $v_g(q_\pm) \leq 0$ and $\Im(q_\pm) \leq 0$. We denote these solutions by q_+ and q_- respectively. The solution of Eq. (7) becomes

$$\psi_v(x) = \iota e^{-iq_-x} + r_-e^{iq_-x} + r_+e^{iq_+x}\ . \tag{8}$$

We derive the previous expression three times and we eliminate the parameters $r_\pm$. After few calculations, we obtain

$$\begin{cases} \dfrac{\mathrm{d}^2\psi_v(x_l)}{\mathrm{d}x^2} &= -2q_-(q_+ + q_-)\iota + i\dfrac{\mathrm{d}\psi_v(x_l)}{\mathrm{d}x}(q_+ + q_-) + q_+q_-\psi_v(x_l) \\ \dfrac{\mathrm{d}^3\,\psi_v(x_l)}{\mathrm{d}x^3} &= -i2q_+q_-(q_+ + q_-)\iota + \dfrac{\mathrm{d}\psi_v(x_l)}{\mathrm{d}x}\left(-q_-q_+ - \dfrac{b_c}{a}\right) + iq_+q_-(q_+ + q_-)\psi_v(x_l)\ . \end{cases} \tag{9}$$

Proceeding in the same way for the other cases we obtain the MEF problem with TBC

$$\mathcal{S}_V(\boldsymbol{\psi}_\mathfrak{q}) = 0 \equiv \begin{cases} \mathcal{H}\boldsymbol{\psi}_\mathfrak{q} - \overline{E}(\mathfrak{q})\boldsymbol{\psi}_\mathfrak{q} &= 0 \\ \dfrac{\mathrm{d}\psi_c(x_s)}{\mathrm{d}x} &= iq_c^s[2\iota^s - \psi_c(x_s)] \\ \dfrac{\mathrm{d}^2}{\mathrm{d}x^2}\begin{pmatrix} \psi_v(x_s) \\ \frac{\mathrm{d}\psi_v(x_s)}{\mathrm{d}x} \end{pmatrix} &= \mathcal{A}^s\begin{pmatrix} \psi_v(x_s) \\ \frac{\mathrm{d}\psi_v(x_s)}{\mathrm{d}x} \end{pmatrix} + \mathbf{I}^s\ , \end{cases} \tag{10}$$

where $s = r, l$. For the sake of compactness, we defined $\mathfrak{q} = (s_0, p_0, q)$, $\iota^s = \delta_{s_0,s}\delta_{p_0,c}$ and

$$\mathbf{I}^s = \begin{pmatrix} 1 \\ -iq_+^s \end{pmatrix} 2\delta_{s_0,s}\delta_{p_0,v}(-q_+^s - q_-^s)q_-^s \tag{11}$$

$$\mathcal{A}^s = \begin{pmatrix} q_+^s q_-^s & i(q_+^s + q_-^s) \\ i(q_+^s + q_-^s)q_+^s q_-^s & -\frac{b}{a} - q_-^s q_+^s \end{pmatrix}\ , \tag{12}$$

with

$$q_c^s = -\sigma^s \chi_c^s \sqrt{\frac{1}{b_c} \left| V(x_s) + E_c - \overline{E} \right|} \; . \tag{13}$$

$$q_\pm^s = -\sigma^s \chi_\pm^s \sqrt{\frac{1}{2a} \left| b_v \pm \sqrt{b_v^2 - 4a \left(V(x_s) + E_v - \overline{E} \right)} \right|}. \tag{14}$$

We defined $\sigma^l = -1$, $\sigma^r = 1$. The parameters χ^s are given in table II of the Appendix.

In summary, we write system (10) as a class of Schrödinger problems. Every problem is characterized by a different $\mathfrak{q}$. In order to put evidence on this, we denote the solution of the MEF system by $\boldsymbol{\psi}_\mathfrak{q}$. We remark that, differing from the unbounded problem, the MEF system with TBC is no longer an eigenvalue problem. Here, $\overline{E}(\mathfrak{q})$, is an explicit function of $\mathfrak{q}$. We study the behavior of the solution $\boldsymbol{\psi}_\mathfrak{q}$ when $\mathfrak{q}$ spans the domain $\omega_\mathfrak{q} = [c, v] \times [l, r] \times [0, +\infty)$.

III. SCHRÖDINGER-POISSON PROBLEM: NON-LINEAR SYSTEM

A. Poisson equation

We consider a distribution of charged particles inside the domain Ω. We requires the compatibility between the charge and the electrostatic potential inside Ω. At the mean field level, this is obtained by calculating the electrostatic potential V with the Poisson equation

$$\mathcal{V}_n(V) = 0 \equiv \begin{cases} \dfrac{\mathrm{d}^2 V}{\mathrm{d}x^2} = \dfrac{n(x)}{\varepsilon_r} \\ V(x_l) = V_1 \\ V(x_r) = V_2 \end{cases} \tag{15}$$

Here, $n(x)$ is the charge density, ε_r is the dielectric constant and the boundary values V_1 and V_2 are given. According to Ref. [31], the charge density is given by

$$n(x) = \int_0^\infty \mathcal{M}\boldsymbol{\psi}_\mathfrak{q} \, G(q) \, \mathrm{d}q \; , \tag{16}$$

where

$$\mathcal{M}\boldsymbol{\psi}_\mathfrak{q} = |\psi_{\mathfrak{q},c}(x)|^2 + |\psi_{\mathfrak{q},v}(x)|^2 + 2\gamma \, \frac{\mathrm{d}\, \Re \left(\overline{\psi_{\mathfrak{q},c}} \, \psi_{\mathfrak{q},v} \right)}{\mathrm{d}x} \tag{17}$$

and $\Re$ denotes the real part. The function $G(q)$ is assigned. From a physical point of view, $G(q)$ is proportional to the number of particles with momentum q that enter into Ω. For technical reasons, we assume that G is a compactly supported in $\mathbb{R}^+$. The derivation of Eqs.

(16)-(17) is addressed in Appendix A. Thermodynamical considerations ensure that $G(q)$ vanishes exponentially when q goes to infinity. For this reason, we fix a cutoff for G. We assume that there exists q_0 such that $G(q) = 0$ for $q > q_0$. Our model deals with the envelope function representation of the particle motion. For this reason, the particle density is not equal to the sum of the squared modulus of the solution. In particular, the non-conventional form of the particle density of Eqs. (16)-(17), ensures that the particle density is bounded.

In the present contribution, we preform the mathematical analysis of the nonlinear Schröringer-Poisson problem (10) (MEF problem with TBC). The electrostatic potential V is obtained by the Poisson equation (16). One of the major difficulties encountered in the present study is that the linear Schrödinger problem is not well-posed. In particular, the analysis shows that the two-band Hamiltonian has a countable set of discrete eigenvalues embedded in the continuous spectrum. In the proximity of the discrete eigenvalues (resonant states), the norm of the solution diverges. The study of the linear Schrödinger problem and the behavior of the solution around the discrete eigenvalues in addressed in sec. IV and ends with the theorem 4. The absence of good estimates for the linear system prevents the direct application of a fixed point technique for the study of the nonlinear Schrödinger-Poisson problem. We proceed as follows. We modify the form of the linear MEF model, by adding to the Hamiltonian a non-Hermitian term proportional to a small parameter ε (hereafter we will denote the nonlinear Schödinger Poisson problem constituted by the Eqs. (10)-(15) by MEF-P problem). The correction is chosen in such a way that the modified MEF problem (that we will denote as MEF-ε problem) admits a unique solution (see theorem 3). By applying the Leray-Schauder fixed point theorem we prove the existence of the solution for the nonlinear problem. As a final step, we study of the limit $\varepsilon \to 0$. One of the major difficulties is to prove that the density of particles and the electrostatic potential are bounded. This is stated in lemma IV.1. The presence of resonant states embedded in the continuous spectrum leads to a non-trivial form of the limit density of particles (see theorem 8). We state here the major result of the present work. Existence of the solution for the MEF-P problem

Theorem 1 *For every positive function G compactly supported in $\mathbb{R}^+$, the MEF-P problem*

$$MEF - P \quad \begin{cases} \mathcal{S}_V(\boldsymbol{\psi}_{\mathrm{q}}) = 0 \ ; \ Eq. \ (10) \\ \mathcal{N}_{\boldsymbol{\psi}_{\mathrm{q}}}(n) = 0 \ ; \ Eq. \ (16) \\ \mathcal{V}_n(V) = 0 \ ; \ Eq. \ (15) \end{cases} \tag{18}$$

admits a solution $(\boldsymbol{\psi}_{\mathfrak{q}}, n, V)$ *such that* $\boldsymbol{\psi}_{\mathfrak{q}} \in \boldsymbol{H}^2(\Omega) \times \boldsymbol{H}^4(\Omega)$*,* $n \in \boldsymbol{L}^\infty$ *and* $V \in \boldsymbol{H}^2$*.*

As discussed before, we modify the MEF-P problem by adding a term proportional to a small quantity ϵ to the linear Schödinger equations $\mathcal{S}_V(\boldsymbol{\psi}_{\mathfrak{q}}) = 0$. We denote the modified problem by MEF-P-ϵ (and we make the substitution $\mathcal{S}_V(\boldsymbol{\psi}_{\mathfrak{q}}) = 0 \rightarrow \mathcal{S}_V^\varepsilon(\boldsymbol{\psi}_{\mathfrak{q}}) = 0$). In order to avoid confusion between the MEF-P and the MEF-P-ϵ problems, we denote the solution with the superscript ε when necessary.

B. The non-hermitian formulation

The MEF-ε problem ($\mathcal{S}_V^\varepsilon(\boldsymbol{\psi}_{\mathfrak{q}}) = 0$) is obtained by adding the term $i\boldsymbol{\psi}$ to the right side of Eq. (10). For the sake of clearness we report the explicit formulation of the problem

$$\mathcal{S}_V^\varepsilon(\boldsymbol{\psi}_{\mathfrak{q}}) = 0 \equiv \begin{cases} \mathcal{H}\boldsymbol{\psi}_{\mathfrak{q}} - (\overline{E}(\mathfrak{q}) + i\varepsilon)\boldsymbol{\psi}_{\mathfrak{q}} = 0 \\ \dfrac{\mathrm{d}\psi_c(x_s)}{\mathrm{d}x} = iq_c^s[2\iota^s - \psi_c(x_s)] \\ \dfrac{\mathrm{d}^2}{\mathrm{d}x^2}\begin{pmatrix} \psi_v(x_s) \\ \frac{\mathrm{d}\psi_v(x_s)}{\mathrm{d}x} \end{pmatrix} = \mathcal{A}^s \begin{pmatrix} \psi_v(x_s) \\ \frac{\mathrm{d}\psi_v(x_s)}{\mathrm{d}x} \end{pmatrix} + \mathbf{I}^s \end{cases} \tag{19}$$

where $s = r, l$. We have the following

Theorem 2 *For every positive function* G *compactly supported in* $\mathbb{R}^+$ *and every* $\varepsilon > 0$*, the MEF-P-*ε *problem*

$$MEF - P - \varepsilon \quad \begin{cases} \mathcal{S}_{V^\varepsilon}^\varepsilon(\boldsymbol{\psi}_{\mathfrak{q}}^\varepsilon) = 0 \;\; ; \;\; Eq.\ (19) \\ \mathcal{N}_{\boldsymbol{\psi}_{\mathfrak{q}}^\varepsilon}(n^\varepsilon) = 0 \;\; ; \;\; Eq.\ (16) \\ \mathcal{V}_{n^\varepsilon}(V^\varepsilon) = 0 \;\; ; \;\; Eq.\ (15) \end{cases} \tag{20}$$

admits a solution $(\boldsymbol{\psi}_{\mathfrak{q}}^\varepsilon, n^\varepsilon, V^\varepsilon)$ *such that* $\boldsymbol{\psi}_{\mathfrak{q}}^\varepsilon \in \boldsymbol{H}^2(\Omega) \times \boldsymbol{H}^4(\Omega)$*,* $n^\varepsilon \in \boldsymbol{L}^\infty$ *and* $V^\varepsilon \in \boldsymbol{H}^2$*.*

The theorem 2 is proved by a fix point technique. As a first step, we show that the linear Schrödinger problem $\mathcal{S}_V^\varepsilon(\boldsymbol{\psi}_{\mathfrak{q}}^\varepsilon) = 0$ admits a unique solution.

Theorem 3 *For every* $V \in \boldsymbol{L}^\infty$ *and* $\mathfrak{q} \in \omega_{\mathfrak{q}}$*, the MEF-*$\varepsilon$ *problem* $\mathcal{S}_V^\varepsilon(\boldsymbol{\psi}_{\mathfrak{q}}^\varepsilon) = 0$ *has a unique solution* $\boldsymbol{\psi}_{\mathfrak{q}}^\varepsilon \in \boldsymbol{H}^2 \times \boldsymbol{H}^4$*.*

Proof of the theorem 3

The MEF-ε has the following weak formulation. Find $\boldsymbol{\psi} \in \mathbf{H}^1(\Omega) \times \mathbf{H}^2(\Omega)$ such that

$$c(\boldsymbol{\psi}, \boldsymbol{\varphi}) + h(\boldsymbol{\psi}, \boldsymbol{\varphi}) - \left(\overline{E}(\mathfrak{q}) + i\varepsilon\right)(\boldsymbol{\psi}, \boldsymbol{\varphi}) = \mathcal{L}(\boldsymbol{\varphi}) \quad \forall \boldsymbol{\varphi} \in \mathbf{H}^1(\Omega) \times \mathbf{H}^2(\Omega) \quad . \tag{21}$$

Some details of the calculation are given in Appendix B. The sesquilinear form $h(\boldsymbol{\psi},\boldsymbol{\varphi})$, the anti-linear form $c(\boldsymbol{\psi},\boldsymbol{\varphi})$ and the linear operator $\mathcal{L}(\boldsymbol{\varphi})$ are defined as follow

$$h(\boldsymbol{\psi},\boldsymbol{\varphi}) = b_c\,(\psi_c,\varphi_c)_{\mathbf{H}^1} + E_c\,(\psi_c,\varphi_c)_{\mathbf{L}^2} + a\,(\psi_v,\varphi_v)_{\mathbf{H}^2} + E_v\,(\psi_v,\varphi_v)_{\mathbf{L}^2} \tag{22}$$

$$\mathcal{L}(\boldsymbol{\varphi}) = -\mathbf{I}^s\widetilde{\boldsymbol{\varphi}_v}^t + \sum_{s=l,r} 2i\sigma^s b_c \iota^s q^s \overline{\varphi_c}(x_s) \tag{23}$$

$$\begin{aligned} c(\boldsymbol{\psi},\boldsymbol{\varphi}) = &\int_{x_l}^{x_r}\left[(V-b_c)\psi_c\overline{\varphi}_c + (V-a)\psi_v\overline{\varphi}_v - \gamma\frac{\mathrm{d}V}{\mathrm{d}x}(\psi_c\overline{\varphi}_v + \psi_v\overline{\varphi}_c)\right]\,\mathrm{d}x \\ &+ \sum_{\substack{j\,=\,1,2;\\ k\,=\,l,r}} i\sigma^k\zeta_j^k\ \left[\overline{\Theta^i\widetilde{\boldsymbol{\varphi}_v}}\right]_j \left[\Theta^i\widetilde{\boldsymbol{\psi}_v}\right]_j + \sigma^k\lambda_j^k\ \left[\overline{\Theta^r\widetilde{\boldsymbol{\varphi}_v}}\right]_j \left[\Theta^r\widetilde{\boldsymbol{\psi}_v}\right]_j \\ &+ i\sigma^k b_c q_c^k \psi_c(x_k)\overline{\varphi_c}(x_k) - (b_v+a)\left(\frac{\mathrm{d}\psi_v}{\mathrm{d}x},\frac{\mathrm{d}\varphi_v}{\mathrm{d}x}\right)_{\mathbf{L}^2}. \end{aligned} \tag{24}$$

By using the Riesz representation it is easy to verify that there exists a unique

(i) - $\mathcal{A}_c \in \mathcal{C}(\mathbb{H})$, compact linear operator such that

$$(\mathcal{A}_c\boldsymbol{\psi},\boldsymbol{\varphi})_{\mathbb{H}} = c(\boldsymbol{\psi},\boldsymbol{\varphi}) - \left(\overline{E}(\mathfrak{q}) + i\varepsilon\right)(\boldsymbol{\psi},\boldsymbol{\varphi})_{\mathbf{L}^2\times\mathbf{L}^2} \quad \forall\,\boldsymbol{\varphi}\in\mathbb{H}\,.$$

(ii) - $\mathcal{A}_h \in \mathcal{B}(\mathbb{H})$, invertible bounded linear operator such that

$$(\mathcal{A}_h\boldsymbol{\psi},\boldsymbol{\varphi})_{\mathbb{H}} = h(\boldsymbol{\psi},\boldsymbol{\varphi}) \quad \forall\,\boldsymbol{\varphi}\in\mathbb{H}\,.$$

(iii) - $\mathbf{f}_{\mathcal{L}} \in \mathbb{H}$ such that

$$\mathcal{L}(\boldsymbol{\varphi}) = (\mathbf{f}_{\mathcal{L}},\boldsymbol{\varphi})_{\mathbb{H}} \quad \forall\,\boldsymbol{\varphi}\in\mathbb{H}\,.$$

Here, we denoted the Hilbert space $\mathbf{H}^1\times\mathbf{H}^2$ by $\mathbb{H}$. Concerning (i), we have

$$|c(\boldsymbol{\psi},\boldsymbol{\varphi})| \le C\|\boldsymbol{\psi}\|_{\mathcal{C}^0\times\mathcal{C}^1}\ \|\boldsymbol{\varphi}\|_{\mathbb{H}}$$

and $\|\mathcal{A}_c\boldsymbol{\psi}\|_{\mathbb{H}} \le C\|\boldsymbol{\psi}\|_{\mathcal{C}^0\times\mathcal{C}^1}$. The operator $\mathcal{A}_c$ is compact since $\mathbb{H}\hookrightarrow\mathcal{C}^0\times\mathcal{C}^1$ is a compact injection. The proposition (ii) follows from the inequality

$$\|\mathcal{A}_h\boldsymbol{\psi}\|_{\mathbb{H}}\ \|\boldsymbol{\psi}\|_{\mathbb{H}} \ge C\|\boldsymbol{\psi}\|_{\mathbb{H}}^2$$

and $\mathcal{A}_h$ is invertible. The problem (21) becomes

$$(\mathcal{I} + \mathcal{A}_h^{-1}\mathcal{A}_c)\boldsymbol{\psi} = \mathcal{A}_h^{-1}\mathbf{f}_{\mathcal{L}} \tag{25}$$

The product $\mathcal{A}_h^{-1}\mathcal{A}_c$ is compact. We apply the Fredholm alternative [32]. The existence of a solution of Eq. (25) can be proved by analyzing the dimension of the kernel of the operator $\mathcal{A}_h + \mathcal{A}_c$. The latter, is equivalent to the problem (21) with $\mathcal{L}(\boldsymbol{\varphi}) \equiv 0$ (homogeneous problem). We fix $\boldsymbol{\varphi} = \boldsymbol{\psi}$. The imaginary part of (21) gives

$$\sum_{j=1,2;k=l,r} \sigma^k \left(\zeta_j^k \left| \left[\Theta^i \widetilde{\boldsymbol{\psi}} \right]_j \right|^2 + b_c \Re \left(q_c^k \right) |\psi_c(x_k)|^2 \right) = \varepsilon \|\boldsymbol{\psi}\|^2_{\mathbf{L}^2 \times \mathbf{L}^2} \tag{26}$$

where we used Eq. (B9) in Appendix. Tables I, II and Eq. (13) ensure that all the terms in Eq. (26) are negative. Consequently, the kernel of the operator $\mathcal{A}_h + \mathcal{A}_c$ has dimension zero. This ends the proof of the theorem 3. ■

IV. LINEAR MEF PROBLEM: $\varepsilon = 0$

Before to take the limit $\varepsilon \to 0$ in Eq. (20), we focus on original problem MEF with $\varepsilon = 0$. We find that the MEF-ε problem converges to Eq. (10), only for nearly all the values of the parameter q in $\mathbb{R}^+$. More precisely, there is a countable set of values of q for which our procedure, based on the Fredholm alternative, does not apply. However, the almost everywhere convergence is sufficient to ensure the existence of the integral (16) that provides the particle density n. We have

Theorem 4 *For every $V \in \boldsymbol{L}^\infty$, there exists a positive sequence E_n with $n = 1, \ldots, \infty$, such that the linear MEF problem (Eq. (10)) admits a unique solution in $\boldsymbol{\psi}_{\mathfrak{q}} \in \boldsymbol{H}^2 \times \boldsymbol{H}^4$ for every $\overline{E}(\mathfrak{q}) \neq E_n$.*

We proceed similarly to proof of the theorem 3. The MEF problem is equivalent to the following weak formulation

$$h(\boldsymbol{\psi}, \boldsymbol{\varphi}) + c(\boldsymbol{\psi}, \boldsymbol{\varphi}) - \overline{E}(\mathfrak{q})(\boldsymbol{\psi}, \boldsymbol{\varphi})_{\mathbf{L}^2 \times \mathbf{L}^2} = \mathcal{L}(\boldsymbol{\varphi}) \quad \forall \boldsymbol{\varphi} \in \mathbf{H}^1(\Omega) \times \mathbf{H}^2(\Omega) \tag{27}$$

where the forms $h(\boldsymbol{\psi}, \boldsymbol{\varphi})$, $c(\boldsymbol{\psi}, \boldsymbol{\varphi})$ and $\mathcal{L}(\boldsymbol{\varphi})$ are defined by Eqs. (22)-(25). The application of the Fredholm alternative requires the study of the homogenous problem ($\mathcal{L} \equiv 0$), that we report here for future references

$$h(\boldsymbol{\psi}, \boldsymbol{\varphi}) + c(\boldsymbol{\psi}, \boldsymbol{\varphi}) - \overline{E}(\mathfrak{q})(\boldsymbol{\psi}, \boldsymbol{\varphi})_{\mathbf{L}^2 \times \mathbf{L}^2} = 0 \quad \forall \boldsymbol{\varphi} \in \mathbf{H}^1(\Omega) \times \mathbf{H}^2(\Omega) \quad . \tag{28}$$

A simple analysis of the sesquilinear form $c(\boldsymbol{\psi}, \boldsymbol{\varphi})$ in Eq. (24) reveals that c is the sum of two form, respectively Hermitian and anti-Hermitian, denoted by $c'(\boldsymbol{\psi}, \boldsymbol{\varphi})$ and $c_a(\boldsymbol{\psi}, \boldsymbol{\varphi})$,

$$c_a(\boldsymbol{\psi}, \boldsymbol{\varphi}) = i\zeta_j^k \left[\overline{\Theta^i\widetilde{\varphi_v}}\right]_j \left[\Theta^i\widetilde{\psi_v}\right]_j + i\sigma_k b_c q_c^k \psi_c(x_k)\overline{\varphi_c}(x_k) \tag{29}$$

$$c'(\boldsymbol{\psi}, \boldsymbol{\varphi}) = c(\boldsymbol{\psi}, \boldsymbol{\varphi}) - c_a(\boldsymbol{\psi}, \boldsymbol{\varphi}) \; . \tag{30}$$

It is useful to use the kernel of $c_a(\boldsymbol{\psi}, \boldsymbol{\varphi})$ as the set of the test functions that appear in the weak formulation of the problem. We denote this set by $\mathcal{D}$:

$$\mathcal{D} = \left\{\boldsymbol{\varphi} \in \mathbb{H} \equiv \mathbf{H}^1 \times \mathbf{H}^2 \text{ such that } c_a(\boldsymbol{\psi}, \boldsymbol{\varphi}) = 0 \; ; \forall \; \boldsymbol{\psi} \in \mathbb{H}\right\} . \tag{31}$$

We consider the homogeneous problem (28) restricted to $\mathcal{D}$

$$h(\boldsymbol{\psi}, \boldsymbol{\varphi}) + c'(\boldsymbol{\psi}, \boldsymbol{\varphi}) - \overline{E}(\mathfrak{q})(\boldsymbol{\psi}, \boldsymbol{\varphi})_{\mathbf{L}^2\times\mathbf{L}^2} = 0 \quad \forall \boldsymbol{\varphi} \in \mathcal{D} \quad . \tag{32}$$

Every time the only solution of Eq. (32) is $\boldsymbol{\psi} = 0$, the same is true for the original problem (where $c'(\boldsymbol{\psi}, \boldsymbol{\varphi}) \to c(\boldsymbol{\psi}, \boldsymbol{\varphi})$ and $\boldsymbol{\varphi} \in \mathbb{H}$). In such cases, we conclude that the MEF problem of Eq. (10) has a unique solution. At the contrary, when Eq. (32) admits a non-vanishing solution, the Fredholm method cannot be used to predict the behavior of Eq. (28). We address to following theorem (the proof can be found, i. e., in [34]).

Theorem 5 *Given a Hermitian continuous and coercive sesquilinear form $a(\boldsymbol{\psi}, \boldsymbol{\varphi})$ defined on a Hilbert space $\mathbb{H}' \subset \boldsymbol{L}^2 \times \boldsymbol{L}^2$, then there exists a constant $C > 0$, a sequence ξ_k such that*

$$0 < C \leq \xi_k \to +\infty \quad \text{when} \quad k \to +\infty \; ,$$

and $\boldsymbol{w}^k \in \mathbb{H}'$ for which

$$\begin{aligned} & a(\boldsymbol{w}^k, \boldsymbol{\varphi}) = \xi_k(\boldsymbol{w}^k, \boldsymbol{\varphi})_{\boldsymbol{L}^2\times\boldsymbol{L}^2} \quad \forall \; \boldsymbol{\varphi} \in \mathbb{H}' \\ & \|\boldsymbol{w}^k\|_{\boldsymbol{L}^2\times\boldsymbol{L}^2} = 1 \quad . \end{aligned} \tag{33}$$

Furthermore, the set $\boldsymbol{w}^k$ is an orthogonal basis of $\boldsymbol{L}^2 \times \boldsymbol{L}^2$.

It is easy to verify that the hypotheses of theorem 5 are satisfied by $h(\boldsymbol{\psi}, \boldsymbol{\varphi}) + c'(\boldsymbol{\psi}, \boldsymbol{\varphi})$ and for $\mathbb{H}' = \mathcal{D}$. The sequence ξ_k is given by the min-max formula

$$\xi_k = \max_{V_{n-1}\subset\mathbb{H}} \left\{ \min_{\boldsymbol{\psi}\in V_{n-1}^{\perp};\|\boldsymbol{\psi}\|_{\mathbf{L}^2}=1} h(\boldsymbol{\psi}, \boldsymbol{\psi}) + c'(\boldsymbol{\psi}, \boldsymbol{\psi}) \right\} \tag{34}$$

where V_n is a vectorial subspace of $\mathbb{H}$ with dimension n. By comparing Eq. (33) with Eq. (32), we see that the function $\boldsymbol{w}^k$ is a non-vanishing solution of the homogenoeous problem given in Eq. (32) if

$$\overline{E}(\mathfrak{q}) = \xi_k \ . \tag{35}$$

In our problem $\mathfrak{q} = (s_0, p_0, q)$. Here, s_0 and p_0 are discrete values and q belongs to $\mathbb{R}^+$. In order to establish for which values of k and $\mathfrak{q}$ the relationship $\overline{E}(\mathfrak{q}) = \xi_k$ is satisfied, we assign to the couple (s_0, p_0), one of the four possible values and we study the solution of Eq. (35) when q spans into the interval $\mathbb{R}^+$. The functions ξ_k are continuous with respect to q. We consider the derivative

$$\frac{\mathrm{d}\left[h(\boldsymbol{\psi},\boldsymbol{\psi}) + c(\boldsymbol{\psi},\boldsymbol{\psi}) - c_a(\boldsymbol{\psi},\boldsymbol{\psi})\right]}{\mathrm{d}q} = \sum_{j=1,2;k=l,r} \sigma^k \frac{\mathrm{d}\lambda_j^k}{\mathrm{d}q} \left| \left[\Theta^r \widetilde{\boldsymbol{\psi}_v}\right]_j \right|^2 .$$

We we have that the functions $\overline{E}$ and ξ_k have the opposite behavior. When $\overline{E}$ increases, ξ_k decreases and viceversa. This proves that there exists a sequence of points (k_j, q_j) with $j \in \mathbb{N}$ for which Eq. (35) holds true. Theorem 4 is thus proved.

A. Non linear MEF-P-ε problem: a priori estimates

We analyze the nonlinear MEF-P-ε problem.

Theorem 6 *Let $(V^\varepsilon$, $n^\varepsilon)$ be the solution of the MEF-P-ε problem (see Eq.* (20)*). Then V^ε and n^ε are bounded in $\boldsymbol{L}^\infty$ by a constant that is independent to ε.*

It is convenient to consider the following lemma

Lemma IV.1 *Let $\boldsymbol{\psi}$ be a solution of the MEF-P-ε problem* (20) *and ϵ_1, $\epsilon_2 > 0$, then there is a constant $C(\epsilon_1, \epsilon_2) \geq 0$ such that*

i)

$$\|\psi_c\|^2_{\boldsymbol{L}^2} + \|\psi_v\|^2_{\boldsymbol{L}^2} \leq 4 \int \mathcal{M}\boldsymbol{\psi} \ dx + \epsilon_1 \left\| \frac{d^2\,\psi_v}{dx^2} \right\|_{\boldsymbol{L}^2} + C \tag{36}$$

ii)

$$\epsilon_1 \left\|\psi_v\right\|^2_{\boldsymbol{H}^2} + \epsilon_2 \left\|\psi_c\right\|^2_{\boldsymbol{H}^1} \geq \|\mathcal{M}\boldsymbol{\psi}\|_{\boldsymbol{L}^2} - \frac{1}{C} \int \mathcal{M}\boldsymbol{\psi} \ dx - C \tag{37}$$

Proof: i) Hereafter, we denote the constants by C (sometime we insert a subscript that highlights the dependence of C by some parameters). We have

$$\int \mathcal{M}\boldsymbol{\psi}\,\mathrm{d}x = \int \left(|\psi_c|^2 + |\psi_v|^2\right)\,\mathrm{d}x + 2\gamma\,\Re(\psi_v\overline{\psi_c})\,\Big|_{x_l}^{x_r}. \tag{38}$$

The term $\Re(\psi_v\overline{\psi_c})$ can be estimated as

$$\Re(\psi_c\,\overline{\psi_v})\big|_{x_l}^{x_r} \leq \epsilon_1 \left\|\frac{\mathrm{d}^2\psi_v}{\mathrm{d}x^2}\right\|_{\mathbf{L}^2}^2 + C_{\epsilon_1}\|\psi_v\|_{\mathbf{L}^2}^2\,, \tag{39}$$

where we used Eq. (B12) and the Gagliardo-Niremberg inequality

$$|\psi_v(x_s)|^2 \leq \|\psi_v\|_{\mathbf{L}^\infty}^2 \leq \epsilon_1 \left\|\frac{\mathrm{d}^2\psi_v}{\mathrm{d}x^2}\right\|_{\mathbf{L}^2}^2 + C_{\epsilon_1}\,\|\psi_v\|_{\mathbf{L}^2}^2\,.$$

By using Eq. (39), Eq. (38) we have

$$\int \left(|\psi_c|^2 + |\psi_v|^2\right)\,\mathrm{d}x \leq \int \mathcal{M}\boldsymbol{\psi}\,\mathrm{d}x + \epsilon_1 \left\|\frac{\mathrm{d}^2\,\psi_v}{\mathrm{d}x^2}\right\|_{\mathbf{L}^2} + C_{\epsilon_1}\|\psi_v\|_{\mathbf{L}^2}$$

By using the well known inequality $(a+b)^2 \leq 2(a^2+b^2)$, we obtain

$$\|\psi_c\|_{\mathbf{L}^2} + \|\psi_v\|_{\mathbf{L}^2} \leq \frac{C_{\epsilon_1}}{2} + \sqrt{\frac{C_{\epsilon_1}^2}{4} + \left(2\int \mathcal{M}\boldsymbol{\psi}\,\mathrm{d}x + \epsilon_1\left\|\frac{\mathrm{d}^2\,\psi_v}{\mathrm{d}x^2}\right\|_{\mathbf{L}^2}\right)}$$

and we get Eq. (36).

ii) : We have

$$\|\mathcal{M}\boldsymbol{\psi}\|_{\mathbf{L}^2} = \left(\int \left[|\psi_c|^2 + |\psi_v|^2 + 2\gamma\,\frac{\mathrm{d}\,\Re(\psi_v\overline{\psi_c})}{\mathrm{d}x}\right]^2\,\mathrm{d}x\right)^{\frac{1}{2}} \leq C\left(\|\psi_c\|_{\mathbf{L}^2}^2 + \|\psi_v\|_{\mathbf{L}^2}^2\right)$$

$$+\epsilon_1\left\|\frac{\mathrm{d}\,\psi_c}{\mathrm{d}x}\right\|_{\mathbf{L}^2}^2 + \epsilon_2\left\|\frac{\mathrm{d}^2\,\psi_v}{\mathrm{d}x^2}\right\|_{\mathbf{L}^2}^2\,,$$

where we used (that follows from the Gagliardo-Niremberg inequality)

$$\left\|\frac{\mathrm{d}\,\xi}{\mathrm{d}x}\right\|_{\mathbf{L}^2}\|\chi\|_{\mathbf{L}^\infty} \leq C(\epsilon_1,\epsilon_2)\left(\|\chi\|_{\mathbf{L}^2}^2 + \|\xi\|_{\mathbf{L}^2}^2\right) + \epsilon_1\left\|\frac{\mathrm{d}\,\chi}{\mathrm{d}x}\right\|_{\mathbf{L}^2}^2 + \epsilon_2\left\|\frac{\mathrm{d}^2\,\xi}{\mathrm{d}x^2}\right\|_{\mathbf{L}^2}^2\,,$$

and the embedding $\mathbf{L}^4 \hookrightarrow \mathbf{L}^2$. In conclusion, by using Eq. (36) we have

$$\|\mathcal{M}\boldsymbol{\psi}\|_{\mathbf{L}^2} - \frac{1}{C}\int \mathcal{M}\boldsymbol{\psi}\,\mathrm{d}x - \epsilon_1\left\|\frac{\mathrm{d}^2\,\psi_v}{\mathrm{d}x^2}\right\|_{\mathbf{L}^2} - C \leq \|\mathcal{M}\boldsymbol{\psi}\|_{\mathbf{L}^2} - C\left(\|\psi_c\|_{\mathbf{L}^2}^2 + \|\psi_v\|_{\mathbf{L}^2}^2\right)$$

$$\leq \epsilon_1\left\|\frac{\mathrm{d}\,\psi_c}{\mathrm{d}x}\right\|_{\mathbf{L}^2}^2 + \epsilon_2\left\|\frac{\mathrm{d}^2\,\psi_v}{\mathrm{d}x^2}\right\|_{\mathbf{L}^2}^2\,,$$

and Eq. (37) follows. ■

Proof of the theorem 6: The real part of Eq. (21) with $\boldsymbol{\varphi} = \boldsymbol{\psi}$ gives

$$
\begin{aligned}
&\int_{x_l}^{x_r} \left(V - \overline{E}(\mathfrak{q})\right) \mathcal{M}\boldsymbol{\psi} \, \mathrm{d}x - (b_v + a) \left\| \frac{\mathrm{d}\,\psi_v}{\mathrm{d}x} \right\|_{\mathbf{L}^2}^2 \\
&+ a \left\|\psi_v\right\|_{\mathbf{H}^2}^2 + b_c \left\|\psi_c\right\|_{\mathbf{H}^1}^2 + (E_c - b_c) \left\|\psi_c\right\|_{\mathbf{L}^2}^2 + (E_v - a) \left\|\psi_v\right\|_{\mathbf{L}^2}^2 = \\
&- \sum_{j=1,2;k=l,r} \lambda_j^k \left| \left[\Theta^r \widetilde{\boldsymbol{\psi}_v}\right]_j \right|^2 - i\sigma_k b_c q_c^k \left|\psi_c(x_k)\right|^2 - \sum_{s=l,r} 2\sigma^s b_c \iota^s \Im\left(q^s \overline{\psi_c}(x_s)\right) \\
&+ 2\gamma \left(V - \overline{E}\right) \Re(\psi_c \overline{\psi_v})\Big|_{x_l}^{x_r} - \Re\left(\mathbf{I}^s \widetilde{\boldsymbol{\psi}_v}^t\right) .
\end{aligned}
\tag{40}
$$

The solution at the boundaries can be easily estimated by using Eq. (B12) and the Gagliardo-Niremberg inequality in same way as in Eq. (39). Proceeding as in Eqs. (39)-(40) we obtain

$$
\begin{aligned}
&\int_{x_l}^{x_r} \left(V - \overline{E}(\mathfrak{q})\right) \mathcal{M}\boldsymbol{\psi} \, \mathrm{d}x + (a - \epsilon_1) \left\|\psi_v\right\|_{\mathbf{H}^2}^2 + b_c \left\|\psi_c\right\|_{\mathbf{H}^1}^2 \\
&\leq C_{\epsilon_1} \left(\left\|\psi_v\right\|_{\mathbf{L}^2}^2 + \left\|\psi_c\right\|_{\mathbf{L}^2}^2\right) + C \leq C_1 \int_{x_l}^{x_r} \mathcal{M}\boldsymbol{\psi} \, \mathrm{d}x + \epsilon_1 \left\| \frac{\mathrm{d}^2\,\psi_v}{\mathrm{d}x^2} \right\|_{\mathbf{L}^2}^2 + C_2 ,
\end{aligned}
\tag{41}
$$

where in the second inequality we used Eq. (36). By using Eq. (37), Eq. (41) becomes

$$
\int_{x_l}^{x_r} V \, \mathcal{M}\boldsymbol{\psi} \, \mathrm{d}x + C_1 \|\mathcal{M}\boldsymbol{\psi}\|_{\mathbf{L}^2} \leq C_2 \int_{x_l}^{x_r} \mathcal{M}\boldsymbol{\psi} \, \mathrm{d}x + C_3 . \tag{42}
$$

We multiply Eq. (42) by G and we integrate over $\mathbb{R}^+$. We obtain

$$
\int_{x_l}^{x_r} V \, n \, \mathrm{d}x + C_1 \left\|n\right\|_{\mathbf{L}^2}^2 \leq C_2 \int_0^L n(x) \, \mathrm{d}x + C_3 , \tag{43}
$$

where we used the definition of n given in Eq. (16) and

$$
\int_{\mathbb{R}^+} \|\mathcal{M}\boldsymbol{\psi}\|_{\mathbf{L}^2}^2 \, G(q) \, \mathrm{d}q \geq \frac{1}{G_M} \int_{x_l}^{x_r} \int_{\mathbb{R}^+} \left|\mathcal{M}\boldsymbol{\psi}\right|^2 G^2(q) \, \mathrm{d}q \, \mathrm{d}x \geq \frac{1}{G_M} \left\|n\right\|_{\mathbf{L}^2}^2 .
$$

Here, G_M denotes the maximum of G. Since G has a compact support we can exchange the order of the integrals. From the Poisson equation (15), we have the following standard estimate

$$
\|n\|_{\mathbf{L}^2} \geq C \|V\|_{\mathbf{H}^2} \geq C \left\| \frac{\mathrm{d}\,V}{\mathrm{d}x} \right\|_{\mathbf{H}^1}
$$

and

$$
\begin{aligned}
&\int_{x_l}^{x_r} V \, n \, \mathrm{d}x = \varepsilon_r \int V \, \frac{\mathrm{d}^2\,V}{\mathrm{d}x^2} \, \mathrm{d}x = \left\| \frac{\mathrm{d}\,V}{\mathrm{d}x} \right\|_{\mathbf{L}^2}^2 - V \, \frac{\mathrm{d}\,V}{\mathrm{d}x}\Big|_{x_l}^{x_r} \\
&\int n \, \mathrm{d}x = \varepsilon_r \, \frac{\mathrm{d}\,V}{\mathrm{d}x}\Big|_{x_l}^{x_r} .
\end{aligned}
$$

Since the values of the potential V at the boundary are prescribed, Eq. (43) yields

$$\left\|\frac{\mathrm{d}V}{\mathrm{d}x}\right\|^2_{\mathbf{L}^2} + \left\|\frac{\mathrm{d}V}{\mathrm{d}x}\right\|_{\mathbf{H}^1} \le C\left\|\frac{\mathrm{d}V}{\mathrm{d}x}\right\|_{\mathbf{L}^\infty} .$$

In order to homogenize the two sides of the previous equation, we apply the interpolation inequality (see i.e. Ref. [32])

$$\left\|\frac{\mathrm{d}V}{\mathrm{d}x}\right\|_{\mathbf{L}^\infty} \le C\left\|\frac{\mathrm{d}V}{\mathrm{d}x}\right\|^{\frac{1}{2}}_{\mathbf{H}^1}\left\|\frac{\mathrm{d}V}{\mathrm{d}x}\right\|^{\frac{1}{2}}_{\mathbf{L}^2} \le \frac{C}{2-2\delta_1}\left\|\frac{\mathrm{d}V}{\mathrm{d}x}\right\|^{1-\delta_1}_{\mathbf{H}^1} + \frac{C}{2+2\delta_2}\left\|\frac{\mathrm{d}V}{\mathrm{d}x}\right\|^{1+\delta_2}_{\mathbf{L}^2} ,$$

that follows from the Young inequality. We have $\delta_1, \delta_2 < 1$ and

$$\begin{cases} 2-2\delta_1 < 2 \\ \dfrac{1-\delta_1}{1-2\delta_1} = 1+\delta_2 > 1 . \end{cases}$$

Finally, for $\delta_1 = 1/4$ $\delta_2 = 1/2$, we obtain

$$\left\|\frac{\mathrm{d}V}{\mathrm{d}x}\right\|_{\mathbf{H}^1} + \left\|\frac{\mathrm{d}V}{\mathrm{d}x}\right\|^2_{\mathbf{L}^2} \le C\left(\left\|\frac{\mathrm{d}V}{\mathrm{d}x}\right\|^{\frac{3}{4}}_{\mathbf{H}^1} + \left\|\frac{\mathrm{d}V}{\mathrm{d}x}\right\|^{\frac{3}{2}}_{\mathbf{L}^2}\right) .$$

This shows that V is $\mathbf{H}^2-$bounded. ■

V. NONLINEAR SCHRÖDINGER-POISSON PROBLEM: EXISTENCE OF A SOLUTION.

The theorem 2 ensures the existence of the solution of the nonlinear MEF-P-ε problem (20).

Proof of the theorem 2: We consider the Gummel map

$$V^\varepsilon_{j+1} = \mathcal{T}(V^\varepsilon_j) \quad \text{with} \quad V^\varepsilon_0 = V \in \mathbf{L}^\infty , \tag{44}$$

defined by

$$\mathcal{T}: \quad V^\varepsilon_j \stackrel{\mathcal{S}^\varepsilon_{V^\varepsilon}(\psi^\varepsilon_{\mathsf{q}})=0}{\longrightarrow} \quad \boldsymbol{\psi}^\varepsilon_{\mathsf{q}} \stackrel{\mathcal{N}_{\psi^\varepsilon_{\mathsf{q}}}(n^\varepsilon_j)=0}{\longrightarrow} \quad n^\varepsilon_j \stackrel{\mathcal{V}_{n^\varepsilon_j}(V^\varepsilon_{j+1})=0}{\longrightarrow} \quad V^\varepsilon_{j+1} . \tag{45}$$

Explicitly, the map $V^* = \mathcal{T}(V)$ is obtained by the following steps. For every V we solve the modified Schrödinger MEF-ε problem (19) and we obtain the family of wave functions $\boldsymbol{\psi}^\varepsilon_{\mathsf{q}}$ parameterized by q. By integrating the quantity $\mathcal{M}\boldsymbol{\psi}^\varepsilon_{\mathsf{q}}$ (see Eq. (17)),we obtain the density n^ε_j (see Eq. (16)). The Poisson equation (15) gives the potential V^*. The theorem 2 states that there exists a fixed point for the map $\mathcal{T}$. We verify that $\mathcal{T}$ is a continuous and compact map. The proof of the theorem follows from the Leray-Schauder theorem [33].

Theorem 7 *The map $\mathcal{T}$ defined by Eq. (44) is continuous and compact in $\boldsymbol{L}^\infty$.*

Compactness: We consider a bounded sequence U_j in $\mathbf{L}^\infty$, and we define $U_j^* = \mathcal{T}(U_j)$. The theorem 3 ensures the existence of a sequence $\boldsymbol{\psi}^\varepsilon_{\mathfrak{q},j}$. By equation (B11) we have that the $\boldsymbol{\psi}^\varepsilon_{\mathfrak{q},j}$ are bounded in $\mathbf{L}^2 \times \mathbf{L}^2$

$$\|\psi^\varepsilon_{c,j}\|_{\mathbf{L}^2} + \|\psi^\varepsilon_{v,j}\|_{\mathbf{L}^2} \leq C \ . \tag{46}$$

From Eq. (41) we obtain

$$\left\|\psi^\varepsilon_{v,j}\right\|^2_{\mathbf{H}^2} + \left\|\psi^\varepsilon_{c,j}\right\|^2_{\mathbf{H}^1} \leq C\|U_j\|_{\mathbf{W}^{1,\infty}} \left(\|\psi^\varepsilon_{c,j}\|_{\mathbf{L}^2} + \|\psi^\varepsilon_{v,j}\|_{\mathbf{L}^2}\right)$$

where we used Eq. (37),

$$\left|\int_{x_l}^{x_r} U_j\, \mathcal{M}\boldsymbol{\psi}\ \mathrm{d}x\right| \leq \|U_j\|_{\mathbf{W}^{1,\infty}} \|\mathcal{M}\boldsymbol{\psi}^\varepsilon_j\|_{\mathbf{L}^2} \tag{47}$$

and

$$\int \mathcal{M}\boldsymbol{\psi}^\varepsilon_j\ \mathrm{d}x \leq C\left(\|\psi^\varepsilon_{c,j}\|_{\mathbf{L}^2} + \|\psi^\varepsilon_{v,j}\|_{\mathbf{L}^2}\right) + \epsilon_1 \left\|\frac{\mathrm{d}^2\,\psi^\varepsilon_{v,j}}{\mathrm{d}x^2}\right\|_{\mathbf{L}^2} + \epsilon_2 \left\|\frac{\mathrm{d}\,\psi^\varepsilon_{c,j}}{\mathrm{d}x}\right\|_{\mathbf{L}^2} . \tag{48}$$

Equation (48) follows from Eq. (38) and Eq. (39). From Eq. (46) we have that the sequence $\boldsymbol{\psi}^\varepsilon_{\mathfrak{q},j}$ is bounded in $\mathbf{H}^1 \times \mathbf{H}^2$ and in $\mathbf{L}^\infty \times \mathbf{L}^\infty$. The equivalence of the strong (Eq. (19)) and the weak formulation (Eq. (21)) of the MEF-ε problem, guarantee that the solutions $\boldsymbol{\psi}^\varepsilon_{\mathfrak{q},j}$ belong to the space $\mathbf{H}^2 \times \mathbf{H}^4$. The boundness of the density n in $\mathbf{L}^\infty$ follows from Eq. (16). Since the sequence U_j^* is obtained by the solving the Poisson equation (15) is bounded in $\mathbf{W}^{2,\infty}$. By using the compactness of the injection $\mathbf{W}^{2,\infty} \hookrightarrow \mathbf{L}^\infty$, the compactness part of the theorem 7 follows.

Continuity: We consider a sequence V_j^ε that converges to V^ε in $\mathbf{L}^\infty$. Since $\mathcal{T}$ is compact, there exists a converging subsequence of $\overline{V_j^\varepsilon} = \mathcal{T}(V_j^\varepsilon)$ (still denoted by $\overline{V_j^\varepsilon}$) with limit $\overline{V^\varepsilon}$. It is sufficient to prove that $\overline{V^\varepsilon} = \mathcal{T}(V)$. We illustrate the proof with the help of the following scheme

$$\begin{array}{ccccccc} V_j^\varepsilon & \longrightarrow & \boldsymbol{\psi}^\varepsilon_j & \longrightarrow & n^\varepsilon_j & \longrightarrow & V^\varepsilon_{j+1} = \mathcal{T}\left(V_j^\varepsilon\right) \\ & & & & & & \Big\downarrow j \to \infty \\ V^\varepsilon & \longrightarrow & \boldsymbol{\psi}^\varepsilon & \longrightarrow & n^\varepsilon & \longrightarrow & \mathcal{T}(V^\varepsilon) \end{array} \tag{49}$$

We will prove the continuity of each step moving from the left to the right of the scheme. Proceedings as in the proof of the compactness, the bondness of V_j^ε implies that the sequence

$\boldsymbol{\psi}_j^\varepsilon$ (the sequence of the solutions of the MEF-ε problem with potential V_j^ε) is bounded in $\mathbf{H}^2 \times \mathbf{H}^4$. The compact injection of $\mathbf{H}^2 \times \mathbf{H}^4$ in $\mathcal{C}^1 \times \mathcal{C}^2$ ensures the existence of a subsequence of $\boldsymbol{\psi}_j^\varepsilon$ strongly convergent in $\mathcal{C}^1 \times \mathcal{C}^2$. It is easy to verify that the limit of this sequence, denoted by $\boldsymbol{\psi}^\varepsilon$, is the solution of $\mathcal{S}^\varepsilon_{V^\varepsilon}(\boldsymbol{\psi}^\varepsilon) = 0$. This proves that the first and the second column of the scheme (49) define a continuous map. The sequence n_j^ε is bounded in $\mathbf{L}^\infty$. This ensures the existence of a convergent subsequence in the weak$-*$ topology. We denote the limit by $\overline{n^\varepsilon}$. From Lemma V.1 (see below) we infer that $\overline{n^\varepsilon}$ coincides with n^ε (the density related to $\boldsymbol{\psi}^\varepsilon$). We have strong convergence in $\mathcal{C}^0$.

We denote by $\overline{V_j^\varepsilon}$ the potential obtained from n_j^ε by the Poisson equation. By using the following estimate

$$\|\overline{V_j^\varepsilon}\|_{\mathbf{W^{2,\infty}}} \leq C \|n_j^\varepsilon\|_{\mathbf{L}^\infty}$$

and the compact embedding $\mathbf{W}^{2,\infty} \hookrightarrow \mathbf{W}^{1,\infty}$, we have that $\overline{V_j^\varepsilon}$ converges to V^ε (it is sufficient to take the limit in the Poisson equation and to use the uniqueness of the solution). This prove that $\mathcal{T}(V_j^\varepsilon) \xrightarrow{\mathbf{W}^{1,\infty}} \mathcal{T}(V^\varepsilon)$ and, consequently, the continuity statement of theorem 7. ∎

In order to complete the proof of the theorem 2 we prove the following lemma

Lemma V.1 *We have*

$$n_j^\varepsilon \xrightarrow{\mathcal{C}^0} n^\varepsilon$$

Proof: From the definition of n given in Eq. (16) we have

$$|n_j^\varepsilon(x) - n^\varepsilon(x)| \leq \int \left(\left\|\psi_{j,c}^\varepsilon\right\|_{\mathbf{L}^\infty} + \|\psi_c^\varepsilon\|_{\mathbf{L}^\infty} \right) \left\|\psi_{j,c}^\varepsilon - \psi_c^\varepsilon\right\|_{\mathbf{L}^\infty} G(q)\,\mathrm{d}q \tag{50}$$
$$+ \int \left(\left\|\psi_{j,v}^\varepsilon\right\|_{\mathbf{L}^\infty} + \|\psi_v^{\varepsilon,q}\|_{\mathbf{L}^\infty} \right) \left\|\psi_{j,v}^\varepsilon - \psi_v^\varepsilon\right\|_{\mathbf{L}^\infty} G(q)\,\mathrm{d}q$$
$$+ 2\gamma \int \left\|\psi_{j,c}^\varepsilon \psi_{j,v}^\varepsilon - \psi_c^\varepsilon \psi_v^\varepsilon\right\|_{\mathbf{W}^{1,\infty}} G(q)\,\mathrm{d}q$$

From the proof of theorem 7 we have that $\left(\psi_{c,j}^\varepsilon, \psi_{v,j}^\varepsilon\right) \xrightarrow{\mathcal{C}^1} (\psi_c^\varepsilon, \psi_v^\varepsilon)$, completing the proof of the lemma. ∎

We proved the existence of the solution for the linear and the nonlinear case. Few remarks are necessary. In the nonlinear problem the existence of the limit is ensured by the estimates of the lemma IV.1. They are based on the Poisson equation and thus are valid only for the nonlinear problem. Although the nonlinear problem MEF-P-ε is regular in $\varepsilon = 0$ (see theorem 8), this is no longer true for the linear problem.

VI. MEF-P-ε PROBLEM: LIMIT $\varepsilon \to 0$.

We focus on the derivation of the limit ε going to zero for the nonlinear problem. The result is given by the following theorem.

Theorem 8 *There exists a positive sequence Δ_j such that*

$$\lim_{\varepsilon\to 0} n^\varepsilon(x) = n^0(x) + \sum_j \Delta_j \left(\left|\boldsymbol{w}^j\right|^2_{\ell^2} + 2\gamma \frac{d\Re\left(\overline{\boldsymbol{w}_c^j}\boldsymbol{w}_v^j\right)}{dx} \right) \tag{51}$$

where we defined $|\psi|_{\ell^2} = |\psi_c| + |\psi_v|$.

Remark VI.1 *In order to ease the subsequent analysis, we will assume that the spectrum of the form a in Eq.* (33) *consists only of non-degenerate eigenvectors, i. e., the eigenspace related to each ξ_k is of dimension one. All the following results, with straightforward extensions, are also valid without this assumption.*

Proof: We define the set $\Omega_\delta = \bigcup_{j=1}^\infty \varpi_j$ where $\varpi_j = [E_j - \delta, E_j + \delta]$ and we denote the complementary of Ω_δ by $\mho_\delta = \complement\Omega_\delta$. We use the notation

$$n^\varepsilon_\Sigma = \int_\Sigma G(q)\mathcal{M}\boldsymbol{\psi}^\varepsilon_{\mathsf{q}}\,\mathrm{d}q\ . \tag{52}$$

Furthermore, we denote the solution of Eq. (18) by $\boldsymbol{\psi}^0_{\mathsf{q}}$. We decompose the density $n^\varepsilon \equiv n^\varepsilon_{\mathbb{R}+}$ as $n^\varepsilon = n^\varepsilon_{\Omega_\delta} + n^\varepsilon_{\mho_\delta}$ and we study separately the limit $(\varepsilon, \delta) \to 0$ for $n^\varepsilon_{\Omega_\delta}$ and $n^\varepsilon_{\mho_\delta}$.

1. $\lim_{\delta\to 0}\lim_{\varepsilon\to 0} n^\varepsilon_{\Omega_\delta}$

We write $\boldsymbol{\psi}^\varepsilon_{\mathsf{q}} = (\mathcal{P}_j + \mathcal{Q}_j)\,\boldsymbol{\psi}^\varepsilon_{\mathsf{q}}$, where

$$\mathcal{P}_j = \left(\boldsymbol{w}^j, \boldsymbol{\psi}^\varepsilon_{\mathsf{q}}\right)_{\mathbf{L}^2\times\mathbf{L}^2} \boldsymbol{w}^j$$

is the projector on the $j-$th eigenvector and $\mathcal{Q}_j = \mathcal{I} - \mathcal{P}_j$ where $\mathcal{I}$ denotes the identity. We have

$$\mathcal{M}\left[\left(\mathcal{P}_j + \mathcal{Q}_j\right)\boldsymbol{\psi}_{\mathsf{q}}(x)\right] = \sum_{s=c,v} \left|\left[\mathcal{P}_j \psi_{\mathsf{q}}\right]_s\right|^2 + \left|\left[\mathcal{Q}_j \psi_{\mathsf{q}}\right]_s\right|^2 + 2\Re\left(\left[\left(\mathcal{P}_j \psi_{\mathsf{q}}\right)\left(\mathcal{Q}_j \psi_{\mathsf{q}}\right)\right]_s\right)$$
$$+2\gamma\,\Re\frac{\mathrm{d}}{\mathrm{d}x}\left[\overline{\left(\left[\mathcal{P}_j\psi_{\mathsf{q}}\right]_c + \left[\mathcal{Q}_j\psi_{\mathsf{q}}\right]_c\right)}\left(\left[\mathcal{P}_j\psi_{\mathsf{q}}\right]_v + \left[\mathcal{Q}_j\psi_{\mathsf{q}}\right]_v\right)\right] .$$

The operator $\mathcal{M}$ is related to the particle density via Eq. (17). In particular, we write $\mathcal{M}\left[\left(\mathcal{P}_j + \mathcal{Q}_j\right)\boldsymbol{\psi}_{\mathsf{q}}(x)\right] = \mathcal{M}\left[\mathcal{P}_j\boldsymbol{\psi}_{\mathsf{q}}(x)\right] + \mathcal{M}_{\mathcal{Q}_j}$. We obtain the following bound

$$2\left|\mathcal{M}_{\mathcal{Q}_j}\right| \le \gamma\left(\left|\frac{\mathrm{d}}{\mathrm{d}x}\mathcal{Q}_j\psi_{\mathsf{q}}\right|_{\ell^2}\left|\mathcal{Q}_j\psi_{\mathsf{q}}\right|_{\ell^2} + \left|\frac{\mathrm{d}}{\mathrm{d}x}\mathcal{P}_j\psi_{\mathsf{q}}\right|_{\ell^2}\left|\mathcal{Q}_j\psi_{\mathsf{q}}\right|_{\ell^2} + \left|\mathcal{P}_j\psi_{\mathsf{q}}\right|_{\ell^2}\left|\frac{\mathrm{d}}{\mathrm{d}x}\mathcal{Q}_j\psi_{\mathsf{q}}\right|_{\ell^2}\right)$$
$$+\left|\mathcal{Q}_j\psi_{\mathsf{q}}\right|^2_{\ell^2} + \left|\mathcal{P}_j\psi_{\mathsf{q}}\right|_{\ell^2}\left|\mathcal{Q}_j\psi_{\mathsf{q}}\right|_{\ell^2}$$
$$\le C\sum_{\nu=0,1}\left(\left|\frac{\mathrm{d}^\nu}{\mathrm{d}x^\nu}\psi_{\mathsf{q}}\right|_{\ell^2}\left|\frac{\mathrm{d}^{(1-\nu)}}{\mathrm{d}x^\nu}\mathcal{Q}_j\psi_{\mathsf{q}}\right|_{\ell^2}\right).$$

We have

$$n^\varepsilon_{\Omega_\delta} = \sum_j n^\varepsilon_{\varpi_j} = \sum_j \int_{\varpi_j} G(q)\mathcal{M}\left[\mathcal{P}_j\boldsymbol{\psi}_{\mathsf{q}}(x)\right]\,\mathrm{d}q + \int_{\varpi_j} G(q)\mathcal{M}_{\mathcal{Q}}\,\mathrm{d}q\,. \tag{53}$$

We prove that the second term goes to zero in the limit $(\delta,\varepsilon)\to 0$. We obtain

$$\int\int_{\varpi_j} G(q)\left|\mathcal{M}_{\mathcal{Q}}\right|\,\mathrm{d}q\,\mathrm{d}x$$
$$\le C\sum_{\nu=0,1}\int_{\varpi_j} G(q)\left(\sum_{k\neq j}\left|\left(\boldsymbol{w}^k,\boldsymbol{\psi}^{\boldsymbol{\varepsilon}}_{\mathsf{q}}\right)_{\mathbf{L}^2\times\mathbf{L}^2}\right|\left\|\frac{\mathrm{d}^\nu}{\mathrm{d}x^\nu}\boldsymbol{\psi}_{\mathsf{q}}\right\|_{\mathbf{L}^2\times\mathbf{L}^2}\left\|\boldsymbol{w}^k\right\|_{\mathbf{H}^1\times\mathbf{H}^1}\right)\,\mathrm{d}q$$
$$\le C\sum_{\nu=0,1}\int_{\varpi_j} G(q)\left(\sum_{k'}\sum_{k\neq j}\left|\left(\boldsymbol{w}^k,\boldsymbol{\rho}^\varepsilon_{\mathsf{q}}\right)_{\mathbf{L}^2\times\mathbf{L}^2}\right|\left|\left(\boldsymbol{w}^{k'},\boldsymbol{\rho}^\varepsilon_{\mathsf{q}}\right)_{\mathbf{L}^2\times\mathbf{L}^2}\right|\left\|\boldsymbol{w}^k\right\|^2_{\mathbf{H}^1\times\mathbf{H}^1}\left\|\boldsymbol{\psi}_{\mathsf{q}}\right\|^2_{\mathbf{L}^2\times\mathbf{L}^2}\right)\,\mathrm{d}q, \tag{54}$$

where we defined

$$\boldsymbol{\varrho}^j_{\mathsf{q}} = \frac{\boldsymbol{\psi}^{\varepsilon_j}_{\mathsf{q}}}{\left\|\boldsymbol{\psi}^{\varepsilon_j}_{\mathsf{q}}\right\|_{\mathbf{L}^2\times\mathbf{L}^2}} \tag{55}$$

and we used the Cauchy-Schwartz inequality together with Eq. (53). In the hypothesis that $\lim_{\varepsilon\to 0}\left\|\boldsymbol{\psi}^\varepsilon_{\mathsf{q}}\right\|^2_{\mathbf{L}^2\times\mathbf{L}^2} < \infty$, all the functions inside the integral are bounded and the integral goes to zero when $\delta\to 0$. On the contrary, when $\lim_{\varepsilon\to 0}\left\|\boldsymbol{\psi}^\varepsilon_{\mathsf{q}}\right\|^2_{\mathbf{L}^2\times\mathbf{L}^2} = \infty$, it is easy to see that $\lim_{\varepsilon\to 0}\left(\boldsymbol{w}^k,\boldsymbol{\psi}^\varepsilon_{\mathsf{q}}\right)_{\mathbf{L}^2\times\mathbf{L}^2}\left\|\boldsymbol{\psi}^\varepsilon_{\mathsf{q}}\right\|^{-2}_{\mathbf{L}^2\times\mathbf{L}^2} = 0$ with $k\neq j$. The integral in Eq. (54) has the following form

$$\int_{E_j-\delta}^{E_j+\delta} g^\varepsilon(q) f^\varepsilon(q)\,\mathrm{d}q\,, \tag{56}$$

where the g^ε, f^ε are two sequences of functions such that $\lim_{\varepsilon\to 0} g_\varepsilon = 0$, $\lim_{\varepsilon\to 0}\sup f_\varepsilon = \infty$ and $\int_{E_j-\delta}^{E_j+\delta} f^\varepsilon(q)\,\mathrm{d}q < C$ for every ε (the last property follows from theorem 6). Under these conditions, $\lim_{\delta\to 0}\lim_{\varepsilon\to 0}\int_{E_j-\delta}^{E_j+\delta} g^\varepsilon(q) f^\varepsilon(q)\,\mathrm{d}q = 0$. Concerning the first terms of Eq. (53) we get

$$\begin{aligned}\mathcal{M}\left[\mathcal{P}_j\boldsymbol{\psi}_{\mathfrak{q}}(x)\right] &= \left|\mathcal{P}_j\boldsymbol{\psi}_{\mathfrak{q}}\right|_{\ell^2}^2 + 2\gamma\,\frac{\mathrm{d}\,\Re\left(\overline{[\mathcal{P}_j\boldsymbol{\psi}_{\mathfrak{q}}]_c}\,[\mathcal{P}_j\boldsymbol{\psi}_{\mathfrak{q}}]_v\right)}{\mathrm{d}x} \\ &= \left(\left|\boldsymbol{w}^j\right|_{\ell^2}^2 + 2\gamma\,\frac{\mathrm{d}\,\Re\left(\overline{\boldsymbol{w}_c^j}\boldsymbol{w}_v^j\right)}{\mathrm{d}x}\right)\left|\left(\boldsymbol{w}^j,\boldsymbol{\rho}_{\mathfrak{q}}^{\boldsymbol{\varepsilon}}\right)_{\mathbf{L}^2\times\mathbf{L}^2}\right|^2\left\|\boldsymbol{\psi}_{\mathfrak{q}}^{\boldsymbol{\varepsilon}}\right\|_{\mathbf{L}^2\times\mathbf{L}^2}^2 .\end{aligned}$$

Furthermore,

$$\begin{aligned}\int_{\varpi_j} G(q)\mathcal{M}\left[\mathcal{P}_j\boldsymbol{\psi}_{\mathfrak{q}}(x)\right]\,\mathrm{d}q = \int_{\varpi_j} G(q)&\left(\left|\boldsymbol{w}^j\right|_{\ell^2}^2 + 2\gamma\,\frac{\mathrm{d}\,\Re\left(\overline{\boldsymbol{w}_c^j}\boldsymbol{w}_v^j\right)}{\mathrm{d}x}\right)\times \\ &\left|\left(\boldsymbol{w}^j,\boldsymbol{\rho}_{\mathfrak{q}}^{\boldsymbol{\varepsilon}}\right)_{\mathbf{L}^2\times\mathbf{L}^2}\right|^2\left\|\boldsymbol{\psi}_{\mathfrak{q}}^{\boldsymbol{\varepsilon}}\right\|_{\mathbf{L}^2\times\mathbf{L}^2}^2\,\mathrm{d}q .\end{aligned} \tag{57}$$

The uniform bound of n^ε and the regularity of the $\boldsymbol{w}^j$ ensure that

$$\lim_{\delta\to 0}\lim_{\varepsilon\to 0}\int_{\varpi_j} G(q)\mathcal{M}\left[\mathcal{P}_j\boldsymbol{\psi}_{\mathfrak{q}}(x)\right]\,\mathrm{d}q = \Delta_j\left(\left|\boldsymbol{w}^j\right|_{\ell^2}^2 + 2\gamma\,\frac{\mathrm{d}\,\Re\left(\overline{\boldsymbol{w}_c^j}\boldsymbol{w}_v^j\right)}{\mathrm{d}x}\right), \tag{58}$$

where

$$\Delta_j = \lim_{\delta\to 0}\int_{\varpi_j} G(q)\left|\left(\boldsymbol{w}^j,\boldsymbol{\rho}_{\mathfrak{q}}^{\boldsymbol{\varepsilon}}\right)_{\mathbf{L}^2\times\mathbf{L}^2}\right|^2\left\|\boldsymbol{\psi}_{\mathfrak{q}}^{\boldsymbol{\varepsilon}}\right\|_{\mathbf{L}^2\times\mathbf{L}^2}^2\,\mathrm{d}q < \infty . \tag{59}$$

2. $\lim_{\delta\to 0}\lim_{\varepsilon\to 0} n_{\mho_\delta}^\varepsilon$

The study of the limit $\varepsilon\to 0$ of $n_{\mho_\delta}^\varepsilon$ proceed straightforwardly. It is sufficient to note that the parameter $\mathfrak{q}_\varepsilon$ converges to a value that belongs to $\mho_\delta$. Here, the limit of $\psi_{\mathfrak{q}}^\varepsilon$ is easily found. Since the density is uniformly bounded, we obtain

$$\lim_{\delta\to 0}\lim_{\varepsilon\to 0} n_{\mho_\delta}^\varepsilon = n_{\Re+}^0. \tag{60}$$

This end the proof of the theorem 8. ∎

VII. NUMERICAL TESTS: RESONANT DIODE

One of the most interesting point that emerges from the analysis of the MEF problem, is the presence of resonant states whose energies are embedded in the continuous spectrum of the Hamiltonian operator. This is also the source of the major problems for establishing well-posedness of the stationary problem and the convergence towards the asymptotic solution. We present some numerical tests performed on the MEF system that illustrate the behavior of the system around these critical values. The interband resonant tunneling diode (IRDT) provides a ideal electronic configuration for the study of the interaction between delocalized

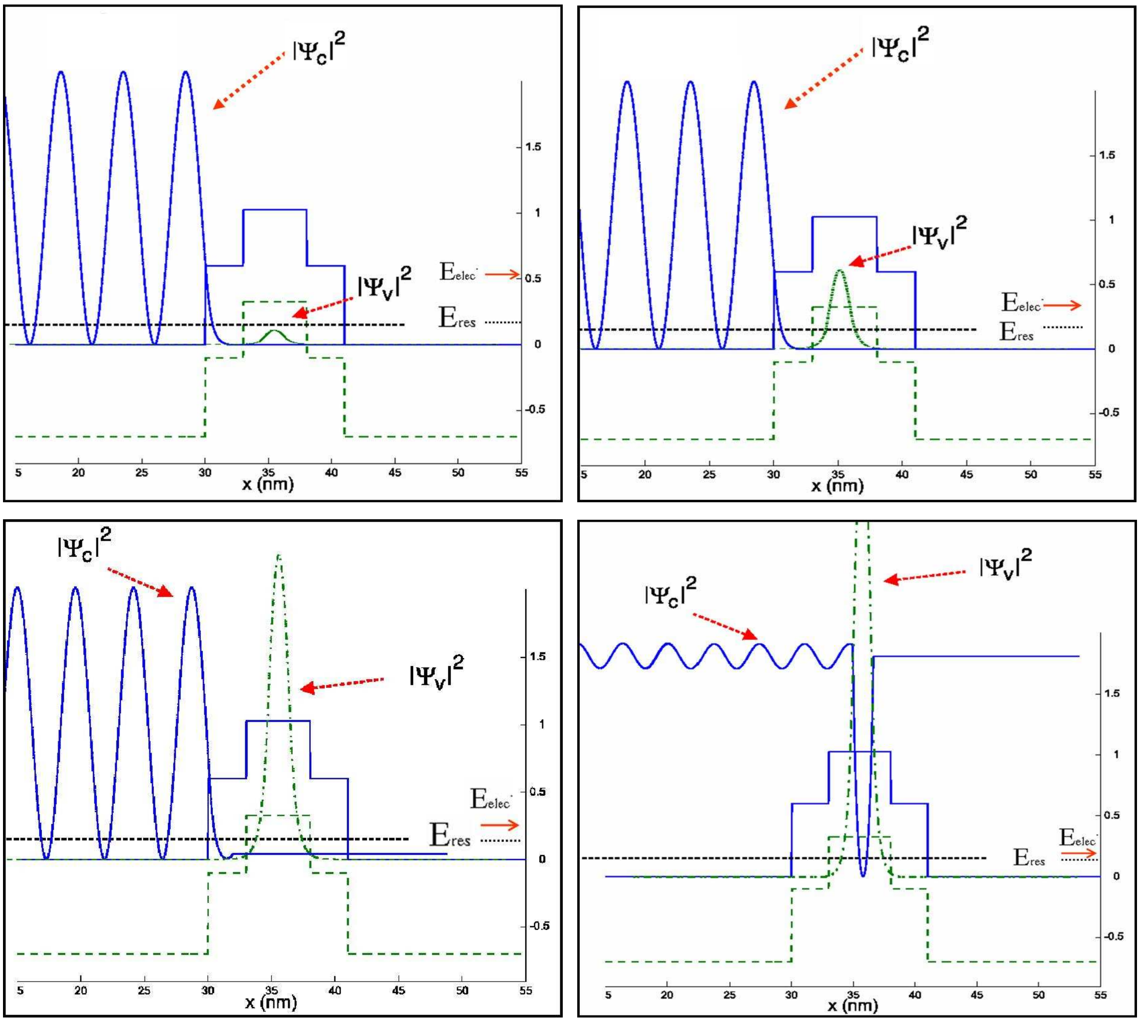

FIG. 1. Excitation of the bounded state via plane waves. Solution of the MEF system for decreasing values of $|E_{el} - E_{ris}|$ (from top to the bottom). Continuous blue line: $|\psi_c|$, dashed green line: $|\psi_v|$.

and resonant states. The use of multiband models for reproducing the current voltage characteristics of a resonant diode has been deeply investigated, (see for example [35–39]). We consider the simple diode described in Ref. [31]. It consists of a single quantum trap of 5 nm width, sandwiched between two potential barriers of 3 nm thickness.

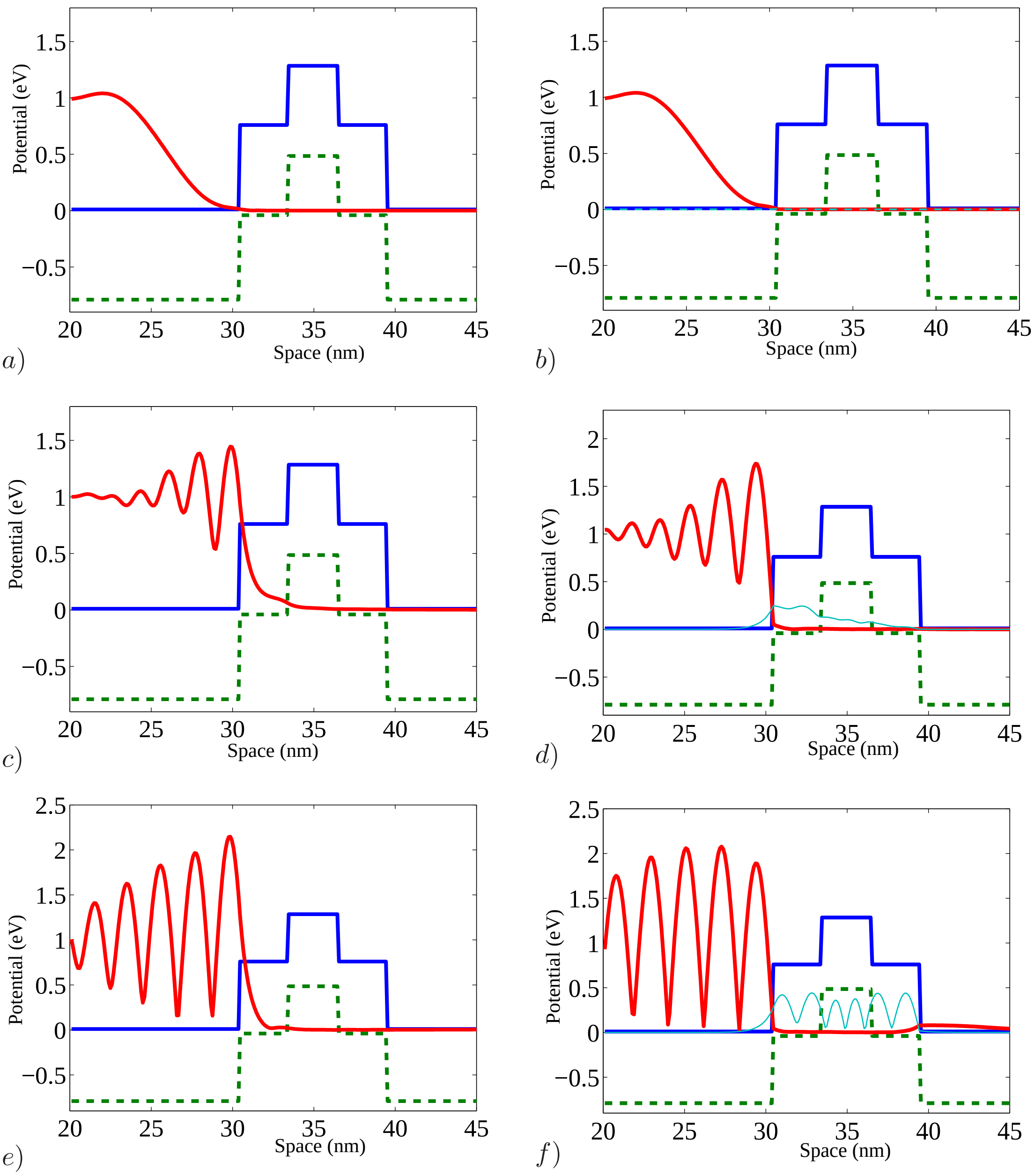

FIG. 2. Time dependent solution of the MEF problem for different times: (a,b) $t = 1$ ps, (c,d) $t = 5$ ps, (e,f) $t = 10$ ps. Continuous red line: $|\psi_c|$, thin blue line: $|\psi_v|$. In the left panels, we depict the solution in the single band approximation.

At the boundaries, we consider traveling waves in the conduction band. They are characterized by the energy E_{el}. The band structure of the diode represents an electrostatic trap for the electrons in the valence band containing resonant states with energy E_{res}. In fig. 1 we show that, when E_{el} approaches to E_{res}, a strong enhancement of the charge localized in the center of the device is observed. In the physical literature this behavior is referred to as "excitation of the resonant state". The oscillations of the solution (thin blue line in fig. 1) outside the trap indicate the partial reflection of the wave. In particular, they are pronounced in the off-resonant regime and disappear when $|E_{el} - E_{res}| \to 0$. This indicates that when the scattering wave is resonant with the bound state, the particles pass through the entire device without reflection. They use the localized state as a "bridge" state. This is illustrated in fig. 1. In particular, the plot shows that, when the energy of the plane wave approaches the resonant values ($|E_{el} - E_{res}| \sim 0$), the $\mathbf{L}^\infty$ norm of the ψ_v component diverges. Similar results are obtained by studying the time-dependent solution. In fig. 2 we depict the time dependent solution of the MEF problem for the same device. The numerical code is based on a Crank-Nicolson scheme and the stationary transparent boundary conditions are substituted by the time-dependent versions (see i. e. [28] for a complete description of the time-dependent problem). We plot the solution for different times (from the top to the bottom). In particular, in the fig. 2 we depict the modulus of ψ_c (red continuous line) and of ψ_v (blue dashed line) and in the left panels, we show the same situation for the single band approximation (i. e. when $\gamma = 0$ in Eqs. (1)-(2)). The simulations show that in the single-band approximation the wave is reflected by the potential barrier (fig.1-d), whereas in the two band case, the particles tunnel in the valence band.

VIII. CONCLUSION

The present work is focused on the mathematical analysis of a self-consistent two-band model containing high-order corrections to the effective mass approximation for the valence band. Transparent boundary conditions are derived for the multi-band envelope Schrödinger model and the existence of a solution to the nonlinear problem is provided by an asymptotic procedure. Some numerical tests illustrate the presence of resonant states in a simple interband resonant diode.

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Appendix A: Density of charge and conservation laws

The definition of the particle density plays a key role for the well-posedness of the non-linear Schrödinger-Poisson problem. For the sake of completeness, we derive the expression of the particle density of the MEF envelope function model used in the present work. As we show in the following, the non-standard definition of the particle density given in Eqs. (16)-(17), follows directly from the conservation of the total energy of the time-dependent MEF system.

We expand the full crystal lattice wave function Ψ (i. e. the solution of the Schrödinger equation for a particle in the presence of the periodic lattice potential) on the Bloch-Wannier basis

$$\Psi(\mathbf{x}) = \sum_n \int_{\mathcal{B}_r \times \mathbb{R}^3_{\mathbf{x'}}} \psi_n(\mathbf{x'})\, \mathfrak{u}_n(\mathbf{k}, \mathbf{x'})\, e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x'})}\, \mathrm{d}\mathbf{k}\, \mathrm{d}\mathbf{x'} \,. \tag{A1}$$

Where the $\mathbf{k}$, $\mathbf{x'}$ integrations are performed, respectively, on the first Brillouin zone and $\mathbb{R}^3$. Here $\psi_n(\mathbf{x})$ are the expansion coefficients and $\mathfrak{u}_n(\mathbf{k}, \mathbf{x})$ are a basis set of periodic functions [40]. According to Ref. [31], the particle density $n(\mathbf{x})$ is the mean value of the modulus of Ψ on a lattice cell. At the first order on the quasi-momentum $\mathbf{k}$, we obtain the following estimate of $n(\mathbf{x})$

$$n(\mathbf{x}) = \sum_n |\psi_n(\mathbf{x})|^2 + \sum_{n \neq n'} \frac{2\hbar^2}{m} \frac{\mathbf{P}_{n',n}}{E_n(\mathbf{k}) - E_{n'}(\mathbf{k})} \cdot \Re\left[\psi_n(\mathbf{x}) \nabla \overline{\psi_{n'}}(\mathbf{x})\right] + o(\mathbf{k}) \tag{A2}$$

where $\mathbf{P}_{n',n}$ is the Kane crystal momentum and $E_n(\mathbf{k})$ denotes the energy of the particles with momentum $\mathbf{k}$ in the n-th band. For a two band system in a one-dimensional crystal, we obtain

$$n(x) \simeq |\psi_c|^2 + |\psi_v|^2 + \frac{2P\hbar^2}{m_0 E_g} \frac{\mathrm{d}\,\Re\left\{\overline{\psi_c}\psi_v\right\}}{\mathrm{d}x} \,. \tag{A3}$$

We check the consistency of this definition by considering the energy conservation low. We make the substitution $E \to i\hbar\frac{\partial}{\partial t}$ in Eqs. (1)-(2), we multiply by $\overline{\psi_c}$, $\overline{\psi_v}$ and we integrate over $\mathbb{R}$. We obtain

$$\frac{\partial}{\partial t}\int_{\mathbb{R}}\left(E_c|\psi_c|^2+E_v|\psi_v|^2+a\left|\frac{\mathrm{d}^2\,\psi_v}{\mathrm{d}x^2}\right|^2+b_c\left|\frac{\mathrm{d}\,\psi_c}{\mathrm{d}x}\right|^2-b_v\left|\frac{\mathrm{d}\,\psi_v}{\mathrm{d}x}\right|^2+\frac{1}{2}V\,n\right)\,\mathrm{d}x=0\,. \qquad \text{(A4)}$$

We used

$$\int_{\mathbb{R}}V\,\frac{\partial n}{\partial t}\,\mathrm{d}x=\frac{1}{2}\frac{\partial}{\partial t}\int_{\mathbb{R}}V\,n\,\mathrm{d}x\,,$$

that follows from the Poisson equation.

Appendix B: Variational form of the MEF-ε problem: boundary conditions

The weak formulation of the MEF-ε problem is

$$(\mathcal{H}\boldsymbol{\psi},\boldsymbol{\varphi})_{\mathbf{L}^2\times\mathbf{L}^2}-\left(\overline{E}(\mathfrak{q})+i\varepsilon\right)(\boldsymbol{\psi},\boldsymbol{\varphi})_{\mathbf{L}^2\times\mathbf{L}^2}+\mathrm{TBC}_c+\mathrm{TBC}_v=0\quad\forall\boldsymbol{\varphi}\in\mathbf{H}^1(\Omega)\times\mathbf{H}^2(\Omega)\quad, \qquad \text{(B1)}$$

where $(\boldsymbol{\psi},\boldsymbol{\varphi})_{\mathbf{L}^2\times\mathbf{L}^2}=\sum_{i=c,v}(\psi_i,\varphi_i)_{\mathbf{L}^2}$ denotes the standard scalar product in $\mathbf{L}^2\times\mathbf{L}^2$. The boundary terms TBC_c, TBC_v are given by

$$\mathrm{TBC}_c=-b_c\frac{\mathrm{d}\,\psi_c}{\mathrm{d}x}\varphi_c\Big|_{x_l}^{x_r} \qquad \text{(B2)}$$

$$\mathrm{TBC}_v=\mathcal{F}(x_r)-\mathcal{F}(x_r) \qquad \text{(B3)}$$

with

$$\mathcal{F}(x)=a\,\overline{\varphi_v}\frac{\mathrm{d}^3\,\psi_v}{\mathrm{d}x^3}-a\,\frac{\mathrm{d}\overline{\varphi_v}}{\mathrm{d}x}\frac{\mathrm{d}^2\psi_v}{\mathrm{d}x^2}+b_v\,\overline{\varphi_v}\frac{\mathrm{d}\psi_v}{\mathrm{d}x}\,, \qquad \text{(B4)}$$

where we used integration by parts. We have

$$\mathcal{F}(x)=\widetilde{\boldsymbol{\varphi}_v}^{\,t}\,\mathcal{B}\,\widetilde{\boldsymbol{\psi}_v}+\mathbf{I}^s\widetilde{\boldsymbol{\varphi}_v}^{\,t}\,, \qquad \text{(B5)}$$

where we defined $\widetilde{\boldsymbol{\psi}_v}=\begin{pmatrix}\psi_v\\ \frac{\mathrm{d}\psi_v}{\mathrm{d}x}\end{pmatrix}$ (and analogous for $\widetilde{\boldsymbol{\varphi}_v}$), the suffix t denotes transpose conjugation and

$$\mathcal{B}=\left\{a\begin{pmatrix}0&1\\-1&0\end{pmatrix}\mathcal{A}^s+\begin{pmatrix}0&b\\0&0\end{pmatrix}\right\}\,. \qquad \text{(B6)}$$

In order to simplify the mathematical analysis of the problem, it is convenient to separate the real part of $\mathcal{B}$ ($\mathcal{B}^r$) from the imaginary one ($\mathcal{B}^i$). We write $\mathcal{B}=\mathcal{B}^r+i\mathcal{B}^i$. We denote by Θ^j ($j=r,i$) the matrix that diagonalizes $\mathcal{B}^j$, i. e. $(\Theta^j)^t\mathcal{B}^j\Theta^j=\Lambda^j$ where Λ^j is a diagonal matrix. We denote the eigenvalues of $\mathcal{B}^r$ and $\mathcal{B}^i$ in $x = x_s$ (with $s = l, r$) by λ^s and ζ^s, respectively. Their explicit expressions are given in table I. We remark that for $x = x_l$ ($x = x_r$) we obtain $\zeta_j \le 0$ ($\zeta_j \ge 0$). Equation (B5) becomes

$$\mathcal{F}(x) = (\Theta^i \widetilde{\boldsymbol{\varphi}_v})^t \Lambda^i \Theta^i \widetilde{\boldsymbol{\psi}_v} + (\Theta^r \widetilde{\boldsymbol{\varphi}_v})^t \Lambda^r \Theta^r \widetilde{\boldsymbol{\psi}_v} + \mathbf{I}^s \widetilde{\boldsymbol{\varphi}_v}^t \tag{B7}$$

$$= \sum_{j=1,2} i\zeta_j \left[\overline{\Theta^i \widetilde{\boldsymbol{\varphi}_v}}\right]_j \left[\Theta^i \widetilde{\boldsymbol{\psi}_v}\right]_j + \lambda_j \left[\overline{\Theta^r \widetilde{\boldsymbol{\varphi}_v}}\right]_j \left[\Theta^r \widetilde{\boldsymbol{\psi}_v}\right]_j + \mathbf{I}^s \widetilde{\boldsymbol{\varphi}_v}^t \,, \tag{B8}$$

where $\left[\Theta^r \widetilde{\boldsymbol{\psi}}\right]_j$ denotes the j-th component of the column vector $\Theta^r \widetilde{\boldsymbol{\psi}_v}$. In particular, for $\boldsymbol{\varphi} = \boldsymbol{\psi}$ the previous equation gives

$$\mathcal{F}(x) = \sum_{j=1,2} i\zeta_j(x) \left|\left[\Theta^i \widetilde{\boldsymbol{\psi}}\right]_j\right|^2 + \lambda_j(x) \left|\left[\Theta^r \widetilde{\boldsymbol{\psi}}\right]_j\right|^2 + \mathbf{I}^s \widetilde{\boldsymbol{\varphi}_v}^t \,. \tag{B9}$$

When $\varepsilon = 0$, the solution of the homogeneous problem (26) is characterized by $\psi_c(x_l) = \psi_c(x_r) = 0$. We write the analogous of (26) for the non-homogeneous problem MEF-ε (when the term $\mathcal{L}(\boldsymbol{\varphi})$ is included). The imaginary part of Eq. (21) for $\boldsymbol{\varphi} = \boldsymbol{\psi}$ is

$$\begin{aligned} &\sum_{j=1,2;k=l,r} \sigma^k \zeta_j^k \left|\left[\Theta^i \widetilde{\boldsymbol{\psi}}\right]_j\right|^2 + \Im\left(\mathbf{I}^s \widetilde{\boldsymbol{\psi}}^t\right) \\ &- \sum_{s=l,r} \sigma^s \left(2b_c \iota^s \Re\left(q_c^s \overline{\psi_c}(x_s)\right) + b_c \Re\left(q_c^s\right) |\psi_c(x_s)|^2\right) - \varepsilon \|\boldsymbol{\psi}\|^2_{\mathbf{L}^2 \times \mathbf{L}^2} = 0 \,. \end{aligned} \tag{B10}$$

$s = l, r$	λ_1^s	λ_2^s	ζ_1^s	ζ_2^s
$\overline{E} > E_v + V(x_s)$	$aq_+^s q_-^s$	$-aq_+^s q_-^s$	$aq_+^s q_-^s (q_+^s + q_-^s)$	$-a(q_+^s + q_-^s)$
$V(x_s) - \frac{b_v^2}{4a} < \overline{E} < E_v + V(x_s)$	$-a\left\|q_+^s\right\|^2 \left\|q_-^s\right\|$	aq_-^s	0	$-aq_+^s(1 + \left\|q_-^s\right\|^2)$

TABLE I. Eigenvalues of the real and imaginary part of $\mathcal{B}$.

$s = l, r$	χ_c^s	$s = l, r$	χ_+^s	χ_-^s
$\overline{E} > E_c + V(x_s)$	1	$\overline{E} > E_v + V(x_s)$	1	$-i$
$\overline{E} < E_c + V(x_s)$	i	$V(x_s) - \frac{b_v^2}{4a} < \overline{E} < E_v + V(x_s)$	1	-1

TABLE II. Value of coefficients χ classified in terms of the position of the injection energy $\overline{E}$.

In order to obtain some ε-independent estimates it is convenient to write the previous expression as (for $\varepsilon = 0$)

$$\sum_{j=1,2;s=l,r} \sigma^s \zeta_j^s \left| \left[\Theta^i \left(\widetilde{\boldsymbol{\psi}} - i \frac{\widetilde{\boldsymbol{\psi}}}{\sigma^s \zeta_j^s} \right) \right]_j \right|^2 - \frac{\sigma^s \zeta_j^s}{2|\sigma^s \zeta_j^s|} \left| \left[\Theta^i \mathbf{I}^s \right]_j \right|^2 \tag{B11}$$

$$- \sum_{s=l,r} \sigma^s \left(b_c \Re \left(q_c^s \right) |\psi_c(x_s) - \iota^s|^2 - b_c \Re \left(q_c^s \right) \right) = 0 \ ,$$

where we used that when $\Im \left(q_c^s \right) \neq 0$ we have $\iota^s = 0$, and that $\sum_{i,j} a_j \left| \Theta_{ji} \mathbf{x}_i \right|^2 + \sum_j \Im \left(\mathbf{v}_j \overline{\mathbf{x}_j} \right) = \sum_{i,j} a_j \left| \Theta_{ij} \left(\mathbf{x}_j - i \frac{\mathbf{v}_j}{2a_i} \right) \right|^2 - \sum_{ij} \frac{a_i}{2|a_i|} \left| \Theta_{ij} \mathbf{v}_j \right|^2$. Here $\mathbf{x}$, $\mathbf{v}$ are vectors, Θ is a unitary matrix and a is a constant. Equation (B11) shows that, at the boundary, $\psi_c(x)$ is bounded

$$\sum_{s=l,r} |\psi_c(x_s)|^2 < C \ . \tag{B12}$$

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