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THE SCHRÖDINGER WITH VARIABLE MASS MODEL: MATHEMATICAL ANALYSIS AND SEMI-CLASSICAL LIMIT

By

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Abstract. In this paper, we propose and analyze a one-dimensional stationary quantum-transport model: the Schrödinger with variable mass. In the first part, we prove the existence of a solution for this model, with a self-consistent potential determined by the Poisson problem, whereas, in the second part, we rigorously study its semi-classical limit which gives us the kinetic model limit. The rigorous limit was based on the analysis of the support of the Wigner transform.

1. Introduction. Electronic devices based on heterostructures are dominated by quantum-interference effects, such as tunneling effect or wave interference. These phenomena usually take place on active regions of the devices. One of the most representative devices in describing such physical phenomena is the Resonant Tunneling Diode (RTD). In general, semiconductor devices are three-dimensional structures. Here, the RTD is represented in one dimension because of its geometry and doping profiles. We assume that the quantum zone (Q) occupies an interval $[0, 1]$. In addition, when the length of the quantum zone (Q) is of the order of some nanometers, an electron submitted to the microscopic periodic potential behaves like an electron of an effective mass m depending on material. Therefore, we have to consider an effective mass approximation in studying such devices. The more appropriate approach to effective-mass theory is the use of the Daniel Ben Duke approach, which more conveniently includes the mass variation effects [1]. In one dimension, the associated Hamiltonian is written as

$$H = -\frac{\hbar^2}{2}\frac{d}{dx}\left(\frac{1}{m(x)}\frac{d}{dx}\right).$$

It corresponds to the Schrödinger Hamiltonian when the mass is constant. We know that the Schrödinger model has first been extensively analyzed in different contexts and settings (see [2], [3], [4], [5], and [6]$\cdots$). There is a solution when the potential is either prescribed or computed self-consistently. Its semi-classical limit has been analyzed in

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order to derive the interface conditions and to define the kinetic model limit (see [7], [8], [9], [10], [11], [12], [13]$\cdots$).

The mathematical analysis for the quantum and kinetic models developed up to now do not take into account the variation of mass. The purpose of the present paper is to study the quantum model Schrödinger with variable mass and to derive the associated kinetic model.

The paper is organized as follows: in Sec. 2, we set the problem and define the model. In Sec. 3, we prove the existence of a solution when the model is coupled to Poisson. Finally, in Sec. 4, the semi-classical limit is investigated when analyzing the support of Wigner transform and we conclude in Sec. 5.

2. Setting of the problem. As mentioned above and as treated in [7], the quantum region (Q) is represented by an interval $[0,1]$. We suppose that the electrons, with charge $-e$, are emitted at both sides of the region (Q). An external potential V is applied at the edges of the device. We suppose that each edge is connected with the same material, so for $x<0$, $V(x)=V_-$ and for $x>1$, $V(x)=V_+$. Furthermore, the effective mass depends on the variable x inside the Q zone and is constant outside. We denote by m_- its value for $x\le 0$ and m_+ its value for $x>1$. Then, let $\psi_q^\pm$ be the wave function associated to electrons injected at the left side $(-)$ and the right side $(+)$ of the Q zone according to the momentum q. It describes the transport of electron by the following equation:

$$-\frac{\hbar^2}{2}\frac{d}{dx}\left(\frac{1}{m(x)}\frac{d\psi_q^\pm}{dx}\right)-eV(x)\psi_q^\pm=\left[\frac{q^2}{2m_\pm}-eV_\pm+i\frac{\hbar\nu}{2}\right]\psi_q^\pm,\qquad q\ge 0,\ x\in[0,1].$$

We have added an absorption term $i\frac{\hbar\nu}{2}$ in the second term of the left-hand side of the previous equation, where ν is a non-negative constant and $\hbar$ is the reduced Planck constant. The absorption term is not needed in the analysis of the Schrödinger with variable mass-Poisson for a fixed $\hbar$. However, when passing to the limit $\hbar\to 0$, it will provide independent a priori estimates.

For the boundary conditions at $x=0$ and $x=1$, we assume that $\psi_q^\pm$ is a wave coming from $\pm\infty$ with an amplitude equal to 1. A part of it is reflected by the potential and goes back to $\pm\infty$, whereas the other part is transmitted and travels to $\mp\infty$.

Since V is defined on the intervals $]-\infty,0]$ and $[1,+\infty[$, the Schrödinger with variable mass can be solved explicitly and is given by

$$\psi_q^-(x)=e^{i\frac{q}{\hbar}x}+r_q^-e^{-i\frac{q}{\hbar}x},\ \psi_q^+(x)=t_q^+e^{-\frac{i}{\hbar}\sqrt[+]{q^2\frac{m_-}{m_+}+2em_-(V_--V_+)}x}\ \text{for } x<0 \tag{2.1}$$

$$\psi_q^-(x)=t_q^-e^{\frac{i}{\hbar}\sqrt[+]{q^2\frac{m_+}{m_-}+2em_+(V_+-V_-)}(x-1)},\ \psi_q^+(x)=e^{-i\frac{q}{\hbar}(x-1)}+r_q^+e^{i\frac{q}{\hbar}(x-1)}\ \text{for } x>1 \tag{2.2}$$

where $r_q^\pm$ and $t_q^\pm$ are respectively the reflection and the transmission coefficients and $\sqrt[+]{a}$ $(a\in\mathbb{R})$ the complex square root with non-negative imaginary part. The Schrödinger with variable mass can be reduced to the interval $[0,1]$. We eliminate the coefficients $r_q^\pm$

and $t_q^{\pm}$. Then we obtain Fourier type boundary conditions

$$\hbar\psi_q^{-\prime}(0) + iq\psi_q^-(0) = 2iq, \quad \hbar\psi_q^{+\prime}(0) = -i\sqrt[+]{\frac{m_-}{m_+}q^2 + 2em_-(V_- - V_+)}\psi_q^+(0)$$

$$\hbar\psi_q^{-\prime}(1) = i\sqrt[+]{\frac{m_+}{m_-}q^2 + 2em_+(V_+ - V_-)}\psi_q^-(1), \quad \hbar\psi_q^{+\prime}(1) - iq\psi_q^+(1) = -2iq.$$

In order to define the charge density, we assume that there exist sources at $-\infty$ and $+\infty$ sending the electrons according to a profile $G^-(q)$ and $G^+(q)$. Hence, the charge density is equal to

$$n(x) = \int_0^{+\infty} G^-(q)|\psi_q^-(x)|^2 dq + \int_0^{+\infty} G^+(q)|\psi_q^+(x)|^2 dq.$$

Once the charge density is defined, the potential V solves the Poisson equation

$$\frac{d^2V}{dx^2} = n(x),$$

with the following boundary conditions:

$$V(0) = V_-, \quad V(1) = V_+.$$

3. Existence of solutions. In this section, we use the Leray-Schauder fixed point theorem (see [14]) to prove the existence of a solution for the stationary Schrödinger with variable mass-Poisson problem. We follow the method given in [15]. Before stating the main theorem of this section, let us first recall the system

$$-\frac{\hbar^2}{2}\frac{d}{dx}\left(\frac{1}{m(x)}\frac{d\psi_q^{\pm}}{dx}\right) - eV(x)\psi_q^{\pm} = \left[\frac{q^2}{2m_{\pm}} - eV_{\pm} + i\frac{\hbar\nu}{2}\right]\psi_q^{\pm}, q \geq 0, x \in [0,1]. \tag{3.1}$$

$$\hbar\psi_q^{-\prime}(0) + iq\psi_q^-(0) = 2iq, \hbar\psi_q^{+\prime}(0) = -i\sqrt[+]{\frac{m_-}{m_+}q^2 + 2em_-(V_- - V_+)}\psi_q^+(0) \tag{3.2}$$

$$\hbar\psi_q^{-\prime}(1) = i\sqrt[+]{\frac{m_+}{m_-}q^2 + 2em_+(V_+ - V_-)}\psi_q^-(1), \hbar\psi_q^{+\prime}(1) - iq\psi_q^+(1) = -2iq \tag{3.3}$$

coupled with the Poisson problem

$$\frac{d^2V}{dx^2} = n(x), \tag{3.4}$$

$$V(0) = V_-, \quad V(1) = V_+. \tag{3.5}$$

The charge density n is given by

$$n(x) = \int_0^{+\infty} G^-(q)|\psi_q^-(x)|^2 dq + \int_0^{+\infty} G^+(q)|\psi_q^+(x)|^2 dq. \tag{3.6}$$

For the sake of clarity in the sequel, we will note

$$n(x) = n^-(x) + n^+(x), \quad \text{where } n^{\pm}(x) = \int_0^{+\infty} G^{\pm}(q)|\psi_q^{\pm}(x)|^2 dq. \tag{3.7}$$

Second, we assume that

- (H-1) There exist c and $C > 0$ such that $c \leq m(x) \leq C$.

- (H-2) G^- and G^+ are compactly supported functions and verify

$$G^\pm \geq 0 \text{ and } \int_0^{+\infty} G^\pm(q)dq < \infty.$$

THEOREM 3.1. Under hypotheses (H-1)–(H-2) and when $\nu \geq 0$, the system (3.1)–(3.5) admits a solution $(\psi_q^\pm, V)$ such that

$$\psi_q^\pm \in H^1(0,1) \text{ and } V \in W^{2,+\infty}(0,1).$$

In order to prove this theorem, we will construct the solution $(\psi_q^\pm, V)$ with a fixed point procedure. Starting with a potential $V \in L^\infty(0,1)$, we solve (3.1)–(3.3). We find a solution which we note by $\psi_q^\pm(V)$. Then, we define the charge density $n(V)$ associated to $\psi_q^\pm(V)$ to which we propose a new potential noted by V^*. It is computed by solving the Poisson equation

$$\frac{d^2V^*}{d^2x} = n(V)$$

and verifying the boundary conditions

$$V^*(0) = V_-, \quad V^*(1) = V_+.$$

In the sequel, we will note by T the operator transforming V into V^*:

$$\begin{aligned} T\colon L^\infty(0,1) &\to L^\infty(0,1) \\ V &\mapsto V^*. \end{aligned} \tag{3.8}$$

To prove that $(V, \psi_q^\pm(V))$ is a solution of the Schrödinger with variable mass-Poisson system, we need to prove that V is a fixed point of T. For this, we apply the Leray-Schauder fixed point theorem.

The proof of Theorem 3.1 is organized into several steps. At first, we prove that the Schrödinger with variable mass problem admits a solution for a fixed V. In fact, the problem (3.1)–(3.3) is equivalent to finding $\psi \in H^1(0,1)$ such that for all $\varphi \in H^1(0,1)$, we have, for $\psi = \psi_q^-$,

$$\begin{aligned} &\frac{\hbar^2}{2}\int_0^1 \frac{1}{m(x)}\psi_q^{-\prime}\overline{\varphi}'dx - \int_0^1\left[e(V - V_-) + \frac{q^2}{2m_-} + \frac{i\hbar\nu}{2}\right]\psi_q^-\overline{\varphi}dx \\ &\quad - \frac{i\hbar}{2m_+}\sqrt[+]{\frac{m_+}{m_-}q^2 + 2em_+(V_+ - V_-)}\psi_q^-(1)\overline{\varphi}(1) - \frac{i\hbar}{2m_-}q\psi_q^-(0)\overline{\varphi}(0) = -\frac{i\hbar}{m_-}q\overline{\varphi}(0). \end{aligned} \tag{3.9}$$

For $\psi = \psi_q^+$, we get

$$\begin{aligned} &\frac{\hbar^2}{2}\int_0^1 \frac{1}{m(x)}\psi_q^{+\prime}\overline{\varphi}'dx - \int_0^1\left[e(V - V_+) + \frac{q^2}{2m_+} + \frac{i\hbar\nu}{2}\right]\psi_q^+\overline{\varphi}dx \\ &\quad - \frac{i\hbar q}{2m_+}\psi_q^+(1)\overline{\varphi}(1) - \frac{i\hbar}{2m_-}\sqrt[+]{\frac{m_-}{m_+}q^2 + 2em_-(V_- - V_+)}\psi_q^+(0)\overline{\varphi}(0) = \frac{i\hbar}{m_+}q\overline{\varphi}(1). \end{aligned} \tag{3.10}$$

The method used to prove existence and uniqueness of ψ_q^- (and ψ_q^+) for a given V relies on the Fredholm alternative. The uniqueness is proven in the same spirit as in [15]. Namely, we use ψ_q^- as a test function in (3.9) with the homogeneous right-hand side. By taking the imaginary part, we deduce that $\psi_q^-(0) = 0$ which implies $\psi_q^{-\prime}(0) = 0$ in view of the homogeneous version of (3.2). Applying the Cauchy Lipschitz theorem to (3.1) leads to $\psi_q^- \equiv 0$. The same argument obviously holds for ψ_q^+.

Now, we give the following a priori estimates.

3.a. A priori estimates. First, let us give some bounds on $\psi_q^\pm$. Choosing $\psi_q^\pm$ as a test function in (3.9)–(3.10) and taking the imaginary part, we obtain

$$R^\nu_{q,\pm} + T^\nu_{q,\pm} + \frac{\nu m_\pm}{q}\int_0^1 |\psi_q^\pm(x)|^2 dx = 1 \tag{3.11}$$

with

$$R^\nu_{q,-} = |\psi_q^-(0) - 1|^2, T^\nu_{q,-} = \frac{m_-}{qm_+}\sqrt{\left[\frac{m_+}{m_-}q^2 + 2em_+(V_+ - V_-)\right]^+}\,|\psi_q^-(1)|^2 \tag{3.12}$$

$$R^\nu_{q,+} = |\psi_q^+(1) - 1|^2, T^\nu_{q,+} = \frac{m_+}{qm_-}\sqrt{\left[\frac{m_-}{m_+}q^2 + 2em_-(V_- - V_+)\right]^+}\,|\psi_q^+(0)|^2 \tag{3.13}$$

where, for a real number a, the relation $\sqrt{(a)^+} = \mathrm{Re}(\sqrt[+]{a})$ holds with $(a)^+ = \max(a, 0)$. Equation (3.11) with boundary conditions (3.2)–(3.3) implies

$$|\psi_q^-(0)| \le 2, \quad |\hbar\psi_q^{-\prime}(0)| \le 2q \tag{3.14}$$

$$|\psi_q^+(1)| \le 2, \quad |\hbar\psi_q^{+\prime}(1)| \le 2q. \tag{3.15}$$

Using the above estimates and a Gronwall type argument, Eq. (3.1) leads to

LEMMA 3.1. Let $V \in L^\infty(0,1)$ and let $\psi_q^\pm$ be the solution of ((3.1)–(3.3)); then there exists q_0 such that $\forall q \in [0, q_0]$ and there exists $C > 0$ independent of q such that

$$\|\psi_q^\pm\|_{L^\infty(0,1)} \le Ce^{C\sqrt{\|V\|_{L^\infty}}}. \tag{3.16}$$

In the following, we obtain a bound on V given by

LEMMA 3.2. There exists a constant $M > 0$ such that any $V \in L^\infty(0,1)$ solution of $V = \sigma TV$ with $\sigma \in [0,1]$ and where T is defined by (3.8) satisfies the inequality

$$\|V\|_{W^{2,\infty}(0,1)} \le M. \tag{3.17}$$

Proof. The proof of Lemma 3.2 follows in analogy with that of Theorem V.1 in [7]. We again use $\psi_q^\pm$ as a test function in (3.9)–(3.10), but now we take the real part. This leads to

$$\frac{\hbar^2}{2}\int_0^2 \frac{1}{m(x)}|\psi_q^{\pm\prime}(x)|^2 dx - \int_0^1 \left[e(V(x) - V_\pm) + \frac{q^2}{2m_\pm}\right]|\psi_q^\pm(x)|^2 dx \le Cq,$$

where C depends on $\hbar$. Multiplying this inequality by $G^\pm(q)$ and integrating with respect to q, we obtain

$$\begin{aligned}\frac{\hbar^2}{2}\int_0^{+\infty}\int_0^1 \frac{1}{m(x)}G^\pm(q)|\psi_q^{\pm\prime}(x)|^2 dx dq - e\int_0^1 V(x)\cdot n^\pm(x)dx \\ + eV_\pm\int_0^1 n^\pm(x)dx - \int_0^1\int_0^{+\infty}\frac{q^2}{2m_\pm}G^\pm(q)|\psi_q^\pm(x)|^2 dx dq \le C,\end{aligned} \tag{3.18}$$

where $n^{\pm}(x)$ is given by (3.7). Since $G^{\pm}$ is a compactly supported function, we have

$$\int_0^1 \int_0^{+\infty} \frac{q^2}{2m_{\pm}} G^{\pm}(q)|\psi_q^{\pm}(x)|^2 dx dq \leq C \int_0^1 n^{\pm}(x) dx.$$

Therefore, inequality (3.18) becomes

$$\frac{\hbar^2}{2} \int_0^{+\infty} \int_0^1 \frac{1}{m(x)} G^{\pm}(q)|\psi_q^{\pm\prime}(x)|^2 dx dq - e \int_0^1 V(x) \cdot n^{\pm}(x) dx \leq C + C \int_0^1 n^{\pm}(x) dx. \tag{3.19}$$

Introducing the kinetic energy density

$$K(x) = K^{-}(x) + K^{+}(x), \tag{3.20}$$

where

$$K^{\pm}(x) = \frac{\hbar^2}{2} \int_0^{+\infty} \frac{1}{m(x)} G^{\pm}(q)|\psi_q^{\pm\prime}(x)|^2 dq,$$

inequality (3.19) takes the following form:

$$\int_0^1 K(x) dx - e \int_0^1 V(x) \cdot n(x) dx \leq C + C \int_0^1 n(x) dx. \tag{3.21}$$

Using the identities

$$\frac{d^2 V_\sigma}{dx^2} = \sigma n(x), \quad V_\sigma(0) = \sigma V_-, \quad V_\sigma(1) = \sigma V_+, \tag{3.22}$$

we have

$$\int_0^1 K(x) dx + e \int_0^1 \frac{1}{\sigma} |V_\sigma'|^2 dx \leq C + \frac{C}{\sigma} |V_\sigma'(1) - V_\sigma'(0)| \leq C + 2\frac{C}{\sigma} \|V_\sigma'\|_{L^\infty(0,1)}. \tag{3.23}$$

The compactness of the support of $G^{\pm}$ and the bound of $\frac{1}{m}$ (see hypothesis (H-1)) leads to the following estimate:

$$\int_0^1 K^{\pm}(x) dx \geq C \int_0^{+\infty} G^{\pm}(q) \|\psi_q^{\pm\prime}(x)\|^2_{L^2(0,1)} dq. \tag{3.24}$$

Now, let us use estimates (3.14), (3.15) and the following relation between $\psi_q^{\pm}$ and $\psi_q^{\pm'}$:

$$\psi_q^{-2}(x) = \psi_q^{-2}(0) + 2\int_0^x \psi_q^{-\prime}(u)\psi_q^{-}(u) du, \psi_q^{+2}(x) = \psi_1^{+2}(1) - 2\int_x^1 \psi_q^{+\prime}(u)\psi_q^{+}(u) du.$$

Then, we obtain

$$\|\psi_q^{\pm'}\|^2_{L^2(0,1)} \geq C \|\psi_q^{\pm}\|^2_{L^\infty(0,1)} - C,$$

for which inequality (3.24) becomes

$$\int_0^1 K^{\pm}(x) dx \geq C \int_0^{+\infty} G^{\pm}(q) \|\psi_q^{\pm}\|^2_{L^\infty(0,1)} dq - C' \quad \left(C' = C \int_0^{+\infty} G^{\pm}(q) dq\right). \tag{3.25}$$

Moreover, as the charge density $n^{\pm}$ verify

$$\|n^{\pm}\|_{L^\infty(0,1)} \leq \int_0^{+\infty} G^{\pm}(q) \|\psi_q^{\pm}\|^2_{L^\infty(0,1)} dq,$$

inequality (3.25) gives

$$\int_0^1 K^{\pm}(x) dx \geq C \|n^{\pm}\|_{L^\infty(0,1)} - C'. \tag{3.26}$$

As V_σ is a solution of the Poisson problem, we have

$$\frac{1}{\sigma}\|V'_\sigma\|_{W^{1,\infty}(0,1)} \le \frac{C}{\sigma}\|V_\sigma\|_{W^{2,\infty}(0,1)} \le C\|n\|_{L^\infty(0,1)}.$$

Hence, for K, inequality (3.26) becomes

$$\int_0^1 K(x)dx \ge \frac{C}{\sigma}\|V'_\sigma\|_{W^{1,\infty}(0,1)} - C.$$

In view of (3.23), this leads to

$$\frac{C}{\sigma}\|V'_\sigma\|_{W^{1,\infty}(0,1)} + \frac{C}{\sigma}\|V'_\sigma\|^2_{L^2(0,1)} \le C + \frac{C}{\sigma}\|V'_\sigma\|_{L^\infty(0,1)}. \tag{3.27}$$

In the above estimate, we notice non-homogeneity between the left- and the right-hand sides. This is due to the nonlinear character of the system. Our purpose is to obtain a σ-independent bound. Indeed, a Gagliarolo-Nirenberg interpolation result (see [16]) leads to

$$\|V'_\sigma\|_{L^\infty(0,1)} \le C\|V'_\sigma\|^{2/3}_{L^2(0,1)}\|V'_\sigma\|^{1/3}_{W^{1,\infty}(0,1)}.$$

Applying Young inequality (see [16]), we have

$$\|V'_\sigma\|^{2/3}_{L^2(0,1)}\|V'_\sigma\|^{1/3}_{W^{1,\infty}(0,1)} \le C\|V'_\sigma\|^{4/3}_{L^2(0,1)} + C\|V'_\sigma\|^{2/3}_{W^{1,\infty}(0,1)}.$$

Hence, under these previous manipulations, estimate (3.27) becomes

$$\begin{aligned}&\frac{C}{\sigma}\|V'_\sigma\|_{W^{1,\infty}(0,1)} + \frac{C}{\sigma}\|V'_\sigma\|^2_{L^2(0,1)}\\ &\qquad \le C + \frac{C}{\sigma}\|V'_\sigma\|^{4/3}_{L^2(0,1)} + \frac{C}{\sigma}\|V'_\sigma\|^{2/3}_{W^{1,\infty}(0,1)}.\end{aligned}$$

Since the parameter σ is in $[0,1]$, we obtain a σ-independent bound

$$C\|V'\|_{W^{1,\infty}(0,1)} - C\|V'\|^{3/4}_{W^{1,\infty}(0,1)} + C\|V'\|^2_{L^2(0,1)} - C\|V'\|_{L^2(0,1)} - C\|V'\|^{3/2}_{L^2(0,1)} \le C.$$

Therefore, this estimate implies the bound of V in $W^{2,\infty}(0,1)$ and then Lemma 3.2 is proved.

As a consequence of this result, even $V^*(= TV)$ solution of the Poisson problem is bounded in $W^{2,\infty}(0,1)$. □

3.b. Compactness and continuity.

LEMMA 3.3. The operator T, defined by (3.8), is a continuous and compact operator on $L^\infty(0,1)$.

Proof. We first deduce from Lemma 3.1 regularities and properties of the Poisson equation that the image of a bounded set of $L^\infty(0,1)$ is a bounded set of $W^{2,\infty}(0,1)$. This proves compactness. To prove continuity, let V_j be a converging sequence in $L^\infty(0,1)$. Let V be its limit. Then, we denote by

$$(\psi_q^\pm)_j = \psi_q^\pm(V_j), \quad n_j = n((\psi_q^\pm)_j).$$

Since T is compact, we deduce after a possible extraction of a sequence that $V_j^*(= TV_j)$ converges strongly in $L^\infty(0,1)$ toward a limit V^*. Our purpose is to prove that $V^* = TV$. This incidentally will prove that there is no need to extract a sub-sequence. Since for any given q, $(\psi_q^{\pm})_j$ and n_j are respectively bounded in $H^1(0,1)$ and $L^\infty(0,1)$, we have after a possible extraction that

$$(\psi_q^{\pm})_j \to \psi_q^{\pm}\ H^1(0,1) \text{ strong},\ n_j \to n\ L^\infty(0,1) \text{ weak}*.$$

Passing to the limit in (3.1)–(3.3), we easily deduce that the limit $\psi_q^{\pm}$ of $(\psi_q^{\pm})_j$ is nothing but $\psi_q^{\pm}(V)$. The uniqueness of the limit implies that the entire sequence converges. Using the Lebesgue dominated convergence theorem, we deduce that

$$\lim_{j\to+\infty}\int_0^{+\infty} G^{\pm}(q)|(\psi_q^{\pm})_j|^2dq = \int_0^{+\infty} G^{\pm}(q)|\psi_q^{\pm}|^2dq.$$

We can now pass to the limit in

$$-V_j^{*\prime\prime} = n_j, \quad \text{with } V_j(0) = V_- \text{ and } V_j(1) = V_+,$$

which leads to

$$-V^{*\prime\prime} = n, \text{ with } V(0) = V_- \text{ and } V(1) = V_+.$$

This leads to the end of the proof.

Finally, using Lemma 3.2 and Lemma 3.3, we can apply the Leray-Schauder Fixed Point Theorem to T, which implies the existence of a solution. This ends the proof of Theorem 3.1. □

4. Semi-classical limit. Our purpose in this section is to pass to the limit $\hbar$ to zero in the Schrödinger with variable mass problem (3.1)–(3.3) and to obtain the kinetic model on the quantum region (Q). Due to the lack of estimates induced by turning points, here we shall prove the result only when the electric potential V is given and regular and when the absorption ν is strictly positive and fixed. This semi-classical limit is introduced and is formally studied in [17].

Before we start with the main theorem of this section, we define the Wigner transform (see [18]). In general case, for all $\psi \in L^2(\mathbb{R})$ and $\phi \in L^2(\mathbb{R})$, we denote by

$$W^\hbar[\psi,\phi] = \frac{1}{2\pi}\int_{\mathbb{R}} e^{i\eta p}\overline{\psi}\left(x+\frac{\hbar}{2}\eta\right)\phi\left(x-\frac{\hbar}{2}\eta\right)d\eta, \forall(x,p)\in\mathbb{R}^2, \tag{4.1}$$

where "$\bar{\cdot}$" denotes the complex conjugation. Moreover, when $\psi=\phi$, we note by $W^\hbar[\psi] = W^\hbar[\psi,\psi]$. Then, following [10], we introduce the space of test-functions

$$\mathcal{A} = \{\varphi = \varphi(x,p)/\mathcal{F}_p(\varphi)(x,\eta) \in L^1(\mathbb{R}_\eta; C([0,1]_x))\}, \tag{4.2}$$

where $\mathcal{F}_p$ is the Fourier transform with respect to p:

$$\mathcal{F}_p(\varphi(x,\eta)) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{i\eta p}\varphi(x,p)dp.$$

The norm on $\mathcal{A}$ is defined by

$$\|\varphi\|_{\mathcal{A}} = \int_{-\infty}^{+\infty}\sup_{x\in(0,1)}|\mathcal{F}(\varphi(x,\eta))|d\eta$$

and in the sequel we will denote by $\mathcal{A}'$ the dual space of $\mathcal{A}$.

As treated in [19], we shall assume the following nonresonance hypothesis on the electrostatic potential

Hypothesis (H)

- In case $V_- > V_+$, we suppose $V'(x) \leq 0$ in $[1-\delta_0, 1]$.
- In case $V_- < V_+$, we suppose $V'(x) \geq 0$ in $[0, \delta_0]$.

THEOREM 4.1. Let $\psi_q^\pm$, the solution of the problem (3.1)–(3.3), be bounded in $L^\infty(0,1)$ with $m \in C^2(0,1)$ and $V \in C^2(0,1)$ and satisfying Hypothesis (H). We assume $\nu > 0$ fixed. We also define $\mathcal{O}$ as a C^∞ compactly supported function identically equal to 1 in a neighborhood of $[0,1]$. Then, for $(n,p) \in [0,1] \times \mathbb{R}$, the Wigner function

$$\omega_\hbar(x,p) = \int_0^{+\infty} G^+(q) W^\hbar[\mathcal{O}\psi_q^+](x,p)dq + \int_0^{+\infty} G^-(q) W^\hbar[\mathcal{O}\psi_q^-](x,p)dq \tag{4.3}$$

converges in $\mathcal{A}'$ weakly $*$, when $\hbar$ goes to zero, toward the unique solution f of $(\mathcal{P}_{\text{Lim}})$

$$(\mathcal{P}_{\text{Lim}}) \begin{cases} \frac{\partial \mathcal{E}}{\partial p}\frac{\partial f}{\partial x} - \frac{\partial \mathcal{E}}{\partial x}\frac{\partial f}{\partial p} + \nu f = 0 \qquad \text{on } [0,1], \\ f(0,p) = G^-(p), \ f(1,-p) = G^+(p), \ p > 0, \end{cases}$$

where $\mathcal{E} = \frac{p^2}{2m(x)} - eV(x)$ is the total energy.

REMARK 4.1. The total energy $\mathcal{E}(x,p) = \frac{p^2}{2m(x)} - eV(x)$ is conserved along the characteristic curves defined by

$$\frac{dx}{dt} = \frac{p(t)}{m(x(t))}, \quad \frac{dp}{dt} = \frac{p^2}{2}\frac{m'(x(t))}{m^2(x(t))} + eV'(x(t)).$$

Before proving the theorem, let us first begin by showing some technical estimates.

4.a. Estimates.

LEMMA 4.1. Let V be in $C^2(0,1)$; then there exists a constant $C > 0$ independent of V, q, and $\hbar$ such that

$$\|\psi_q^\pm\|_{L^2(0,1)} \leq C\sqrt{q}, \ \|\psi_q^{\pm'}\|_{L^2(0,1)} \leq C\frac{\sqrt{q(q+1)}}{\hbar},$$
$$\|\psi_q^{\pm''}\|_{L^2(0,1)} \leq C\frac{\sqrt{q}(q+1)}{\hbar^2}, \quad \forall q \in \mathbb{R}_+.$$

Proof. Since $\psi_q^\pm$ is a solution of the Schrödinger with variable mass problem (3.1)–(3.3), it verifies the weak formulations (3.9)–(3.10). Considering $\psi_q^\pm$ as a test function and taking the imaginary part given by (3.11), we obtain for $\nu > 0$

$$\|\psi_q^\pm\|_{L^2(0,1)}^2 \leq Cq.$$

From the Schrödinger with variable mass and using the bound of m, we deduce that

$$\|\psi_q^{\pm''}\|_{L^2(0,1)} \leq C\frac{\sqrt{q}(q+1)}{\hbar^2}.$$

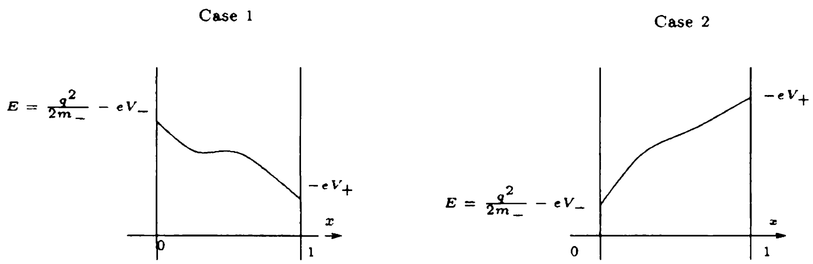

FIG. 1. The two cases

Now, we take the real part of the formulation (3.9)–(3.10):

$$\frac{\hbar^2}{2}\int_0^1 \frac{1}{m(x)}|\psi_q^{-'}(x)|^2 dx - \int_0^1 \left[e(V-V_-)+\frac{q^2}{2m_-}\right]|\psi_q^-(x)|^2 dx = -\frac{\hbar}{m_-} q\mathrm{Im}(\psi_q^-(0)), \tag{4.4}$$

$$\frac{\hbar^2}{2}\int_0^1 \frac{1}{m(x)}|\psi_q^{+'}(x)|^2 dx - \int_0^1 \left[e(V-V_+)+\frac{q^2}{2m_+}\right]|\psi_q^+(x)|^2 dx = -\frac{\hbar}{m_+} q\mathrm{Im}(\psi_q^+(1)). \tag{4.5}$$

Then, using the estimates on $\psi_q^-(0)$ and $\psi_q^+(1)$ given by (3.14)–(3.15), we obtain

$$\|\psi_q^{\pm'}\|_{L^2(0,1)} \le C\frac{\sqrt{q(q+1)}}{\hbar}.$$

In the following, let us give some L^∞-bound on ψ_q^+ and ψ_q^-. □

LEMMA 4.2. Let V be in $C^2(0,1)$ and satisfy Hypothesis (H). Then the following estimates hold:

$$|\psi_q^-(1)|^2 \le \frac{Cq}{\sqrt{|q^2+2em_-(V_+-V_-)|}}, \quad \hbar^2\|\psi_q^{-'}\|^2_{L^\infty} \le Cq(1+q)$$
$$|\psi_q^+(0)|^2 \le \frac{Cq}{\sqrt{|q^2+2em_+(V_--V_+)|}}, \quad \hbar^2\|\psi_q^{+'}\|^2_{L^\infty} \le Cq(1+q).$$

Proof. For the sake of simplicity, we will only prove the estimate for ψ_q^-. We first recall that in view of the boundary condition (3.2) and expression (3.11), we have

$$|\psi_q^-(0)| \le 2, \quad |\hbar\psi_q^{-'}(0)| \le 2q.$$

To look for the bound of ψ_q^- and $\psi_q^{-'}$ at $x=1$, we distinguish two cases. This is illustrated in Figure 1.

CASE 1. The term $\sqrt[+]{q^2+2em_-(V_+-V_-)} \in \mathbb{R}^+$. In view of the boundary condition (3.3) and expressions (3.11), (3.12), and (3.13), we have

$$|\psi_q^-(1)|^2 \le \frac{Cq}{\sqrt{q^2+2em_-(V_+-V_-)}}, \quad \hbar^2|\psi_q^{-'}(1)|^2 \le Cq\sqrt{q^2+2em_-(V_+-V_-)}.$$

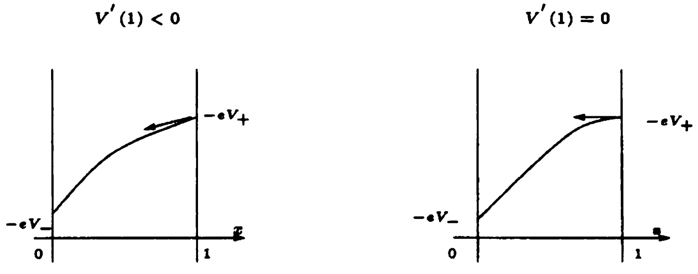

FIG. 2. Behavior of potential in neighborhood of $x = 1$

CASE 2. The term $\sqrt[+]{q^2 + 2em_-(V_+ - V_-)} \in i\mathbb{R}^+$. We multiply (3.1) by $\overline{\psi_q^-}$ and we take the real part. After some algebra, we obtain the following equation on $|\psi_q^-|^2$:

$$\frac{\hbar^2}{2}\frac{d}{dx}\left(\frac{1}{m(x)}\frac{d|\psi_q^-|^2}{dx}\right) = 2\left[-\frac{q^2}{2m_-} + e(V_- - V(x))\right]|\psi_q^-|^2 + \frac{\hbar^2}{m(x)}|\psi_q^{-\prime}|^2.$$

Due to the fact that the second term of the right-hand side is non-negative and that $1/m(x)$ is bounded, we get the following inequality:

$$C\hbar^2(|\psi_q^-|^2)'' \geq \left(eV_- - eV(x) - \frac{q^2}{2m_-}\right)|\psi_q^-|^2. \tag{4.6}$$

Let us denote by

$$l = -q^2 + 2em_-(V_- - V_+) > 0.$$

Inequality (4.6) becomes

$$(|\psi_q^-|^2)'' \geq \frac{C}{\hbar^2}(l + 2em_-(V_+ - V(x)))|\psi_q^-|^2. \tag{4.7}$$

Besides, the boundary condition (3.2) at $x = 1$ yields

$$(|\psi_q^-|^2)'(1) = -\frac{2}{\hbar}\sqrt{\frac{-m_+}{m_-}q^2 - 2em_+(V_+ - V_-)}|\psi_q^-|^2(1) \leq 0. \tag{4.8}$$

In order to solve (4.7)–(4.8), we have to bound the right-hand side of inequality (4.7). Under Hypothesis (H), we distinguish the case where $V'(1) < 0$ and the case where $V'(1) = 0$. This can be illustrated in Figure 2.

In the case when $V'(1) < 0$, there exists $\delta_0 > 0$ such that $\forall x \in [1 - \delta_0]$, (4.7) verifies

$$(|\psi_q^-|^2)'' \geq C\frac{l}{\hbar^2}|\psi_q^-|^2. \tag{4.9}$$

Solving the above differential inequality with condition (4.8), we obtain

$$|\psi_q^-(x)|^2 \geq |\psi_q^-(1)|^2 e^{-C\frac{\sqrt{l}}{\hbar}(x-1)}, \quad \text{on } [1 - \delta_0, 1].$$

Now, integrating with respect to x in $[1 - \delta_0, 1]$, we get

$$\delta_0|\psi_q^-(1)|^2 \leq |\psi_q^-(1)|^2 \int_{1-\delta_0}^1 e^{-C\frac{\sqrt{l}}{\hbar}(x-1)}dx \leq \int_0^1 |\psi_q^-(x)|^2 dx \leq Cq.$$

Consequently, the estimate for $|\psi_q^-(1)|^2$ holds in this case.

In case $V'(1) = 0$, as V is continuous, we have

$$\forall \epsilon > o, \exists \eta > 0 \text{ s.t. } |x-1| < \eta \text{ and } |eV_+ - eV(x)| \leq \epsilon.$$

Using Taylor series expansion, we have the following estimate:

$$|eV_+ - eV(x)| \leq \frac{e\|V''\|_{L^\infty}}{2}(x-1)^2.$$

It suffices then that $\frac{e\|V''\|_{L^\infty}}{2}|x-1|^2 \leq \frac{l}{2}$, to get $|x-1| \leq C\sqrt{l}$. Then, there exists an interval of length $\sqrt{l}$, for which the estimate holds.

We group the results and get the following estimate on $\psi_q^-(1), \psi_q^{-'}(1)$:

$$|\psi_q^-(1)|^2 \leq \frac{Cq}{\sqrt{|q^2 + 2em_-(V_+ - V_-)|}}, \hbar^2|\psi_q^{-'}(1)|^2 \leq Cq\sqrt{|q^2 + 2em_-(V_+ - V_-)|}, \tag{4.10}$$

where C does not depend on either q or $\hbar$. Then, the first estimate of the lemma holds.

Let us now introduce the function

$$G(x) = \frac{\hbar^2}{2m(x)}|\mathrm{Re}\psi_q^{-'}(x)|^2 + \left(\frac{q^2}{2m_-} - eV_- + eV(x)\right)|\mathrm{Re}\psi_q^-(x)|^2.$$

Using the Schrödinger with variable mass equation (3.1), we have

$$G'(x) = eV'(x)|\mathrm{Re}\,\psi_q^-(x)|^2 + \frac{\hbar^2 m'(x)}{2m^2(x)}|\mathrm{Re}\,\psi_q^{-'}(x)|^2 + \hbar\nu\mathrm{Re}\,\psi_q^{-'}(x)\mathrm{Im}\,\psi_q^-(x).$$

Since $\|\psi_q^-\|_{L^2(0,1)} \leq C\sqrt{q}$ and $\hbar^2\|\psi_q^{-'}\|^2_{L^2(0,1)} \leq Cq(q+1)$ (see Lemma 4.1), then

$$\|G'\|_{L^1(0,1)} \leq Cq(q+1).$$

Moreover, (4.10) implies the estimate

$$|G(1)| \leq Cq(1+q).$$

Consequently, $G(x)(= -\int_x^1 G'(t)dt + G(1))$ is bounded in L^∞ by $Cq(1+q)$. Let now, a point $x_M \in [0,1]$ on which $|\mathrm{Re}\,\psi_q^{-'}(x)|$ achieves its maximum. If $x_M = 0$ or $x_M = 1$, then

$$\hbar^2|\mathrm{Re}\,\psi_q^{-'}(x_M)|^2 \leq Cq(1+q).$$

If $x_M \in [0,1]$, then $\mathrm{Re}\,\psi_q^{-''}(x_M) = 0$. Using the Schrödinger with variable mass equation (3.1), we deduce that

$$\left(\frac{q^2}{2m_-} - eV_- + eV(x_M)\right)|\mathrm{Re}\,\psi_q^-(x_M)|^2 \leq Cq(1+q),$$

which implies in view of the bound on G that

$$\hbar^2|\mathrm{Re}\,\psi_q^{-'}(x_M)|^2 \leq Cq(1+q).$$

Hence in all cases we have

$$\sup_{x\in[0,1]} \hbar^2|\mathrm{Re}\,\psi_q^{-'}(x)|^2 \leq Cq(1+q).$$

The same manipulation can be done by considering the imaginary part and this finally yields

$$\hbar^2\|\psi_q^{-'}\|^2_{L^\infty} \leq Cq(1+q).$$

This ends the proof.

□

4.b. Property of Wigner transform. In the sequel, we shall denote the Wigner transform $W^\hbar$ associated to $\psi_q^\pm$ by different expressions:

$$W_\hbar^\pm = W_\hbar^\pm(q,x,p) = W_q^{\hbar,\pm}(x,p) = W^\hbar[O\psi_q^\pm](x,p)$$

and its limit by

$$W^\pm = W^\pm(q,x,p) = W_q^\pm(x,p).$$

LEMMA 4.3. There exists $W^\pm \geq 0$ in $L^\infty_{\mathrm{Loc}}(\mathbb{R}_q^+;\mathcal{A}')$ such that $\frac{W^\pm}{(1+q)} \in L^\infty(\mathbb{R}_q^+;\mathcal{A}')$ and after a possible extraction, we have

$$\frac{W_\hbar^\pm}{(1+q)} \underset{\hbar\to 0}{\rightharpoonup} \frac{W^\pm}{(1+q)} \quad \text{in} \quad L^\infty(\mathbb{R}_q^+;\mathcal{A}') \text{ weak}^*.$$

Proof. Let Q be a test function in $\mathcal{A}$. We have

$$\left|\int_0^1\int_{-\infty}^{+\infty} Q(x,p)W_q^{\hbar,\pm}(x,p)dxdp\right|$$
$$\leq \int_0^1\int_{-\infty}^{+\infty}\left|\mathcal{F}_p(Q(x,\eta))\overline{O\psi_q^\pm}\left(x+\frac{\hbar}{2}\eta\right)O\psi_q^\pm\left(x-\frac{\hbar}{2}\eta\right)\right|dxd\eta \quad \leq \|Q\|_{\mathcal{A}}\|\psi_q^\pm\|_{L^2}^2.$$

As $\psi_q^\pm$ is bounded in $L^2(0,1)$, $W_q^{\hbar,\pm}$ is bounded in $\mathcal{A}'$. A direct consequence is that $\frac{W_\hbar^\pm}{(1+q)}$ is bounded in $L^\infty(\mathbb{R}_q^+;\mathcal{A}')$ and there exists a sub-sequence (also denoted by $\hbar$) which converges to $\frac{W^\pm}{(1+q)}$ in $L^\infty(\mathbb{R}_q^+;\mathcal{A}')$ weak*. □

REMARK 4.2. In order to lighten the already heavy notation, we note $\psi_q^\pm(\pm) = \psi_q^\pm(x\pm\frac{\hbar}{2}\eta)$ and analogously for $O(\pm)$ and $m(\pm)$.

4.c. Proof of Theorem 4.1. To pass to the semiclassical limit in problem (3.1)–(3.2), we proceed analogously to [19]. We shall see that new difficulties arise because the effective mass is not constant. A long but straightforward computation leads to the following identity:

$$\begin{aligned}\frac{p}{m(x)}\frac{\partial W_q^{\hbar,\pm}}{\partial x}(x,p) &= \sum_{i=1}^3 r_\hbar^i(x,p) + \left[p\frac{m'(x)}{m^2(x)} - \nu\right]W_q^{\hbar,\pm}(x,p)\\ &\quad - \frac{i}{2\pi m(x)}\left(\frac{q^2}{2m_\pm} - eV_\pm\right)\int_{-\infty}^{+\infty} e^{i\eta p}\delta_\hbar(m)\overline{O\psi_q^\pm}(+)O\psi_q^\pm(-)d\eta\\ &\quad + \frac{i}{2\pi m(x)}\int_{-\infty}^{+\infty} e^{i\eta p}\delta_\hbar(m\mathcal{V})\overline{O\psi_q^\pm}(+)O\psi_q^\pm(-)d\eta,\end{aligned} \tag{4.11}$$

where

$$r_\hbar^1(x,p) = \frac{-\hbar}{m(x)}\,\mathrm{Im}(W^\hbar[O''\psi_q^\pm, O\psi_q^\pm]),\ r_\hbar^2(x,p) = \frac{-2\hbar}{m(x)}\,\mathrm{Im}(W^\hbar[O'\psi_q^{\pm\prime}, O\psi_q^\pm])$$
$$r_\hbar^3(x,p) = -\hbar\frac{m'(x)}{m^2(x)}\,\mathrm{Im}(W^\hbar[O'\psi_q^\pm, O\psi_q^\pm])$$

and

$$\delta_\hbar(m\mathcal{V}) = \frac{m(+)\mathcal{V}(+) - m(-)\mathcal{V}(-)}{\hbar}, \text{ with } \mathcal{V}(x) = -eV(x)$$
$$\delta_\hbar(m) = \frac{m(+) - m(-)}{\hbar}.$$

Let $Q(x,p)$ be a function test in $\mathcal{A}$. Multiplying (4.11) by Q and integrating with respect to (x,p) in $[0,1] \times \mathbb{R}$, we obtain

$$\begin{aligned}
&\int_0^1 \int_{-\infty}^{+\infty} Q(x,p)\frac{p}{m(x)}\frac{\partial W_q^{\hbar,\pm}}{\partial x}(x,p)dxdp \\
&\quad = \int_0^1 \int_{-\infty}^{+\infty} \sum_{i=1}^5 r_\hbar^i(x,p)Q(x,p)dxdp \\
&\quad + \int_0^1 \int_{-\infty}^{+\infty} Q(x,p)\left(p\frac{m'(x)}{m(x)} - \nu\right) W_q^{\hbar,\pm}(x,p)d\eta dxdp \\
&\quad - \frac{i}{2\pi}\left(\frac{q^2}{2m_\pm} - eV_\pm\right)\int_0^1\int_{-\infty}^{+\infty}\frac{Q(x,p)}{m(x)}\int_{-\infty}^{+\infty} e^{i\eta p}\eta m'(x)\overline{O\psi_q^\pm}(+)O\psi_q^\pm(-)d\eta dxdp \\
&\quad + \frac{i}{2\pi}\int_0^1\int_{-\infty}^{+\infty}\frac{Q(x,p)}{m(x)}\int_{-\infty}^{+\infty} e^{i\eta p}\eta(m\mathcal{V})'(x)\overline{O\psi_q^\pm}(+)O\psi_q^\pm(-)d\eta dxdp,
\end{aligned} \tag{4.12}$$

where

$$r_\hbar^4(x,p) = \frac{i}{2\pi m(x)}\int_{-\infty}^{+\infty} e^{i\eta p}[\delta_\hbar(m\mathcal{V}) - \eta(m\mathcal{V})']\overline{O\psi_q^\pm}(+)O\psi_q^\pm(-)d\eta$$
$$r_\hbar^5(x,p) = -\frac{i}{2\pi m(x)}\left(\frac{q^2}{2m_\pm} - eV_\pm\right)\int_{-\infty}^{+\infty} e^{i\eta p}[\delta_\hbar(m) - \eta m'(x)]\overline{O\psi_q^\pm}(+)O\psi_q^\pm(-)d\eta.$$

Afterward, we integrate by parts the first member of Eq. (4.12) and we multiply the resulting identity by a second function test $S(q) \in L^1(\mathbb{R}_q^+, (1+q)dq)$. Once more, we integrate with respect to q. This leads to the following identity:

$$\begin{aligned}
&\int_0^{+\infty}\Bigg(\left[\int_{-\infty}^{+\infty}\frac{p}{m(x)}Q(x,p)W_q^{\hbar,\pm}(x,p)dp\right]_0^1 - \int_0^1\int_{-\infty}^{+\infty} W_q^{\hbar,\pm}(x,p)\Bigg(\frac{p}{m(x)}\frac{\partial}{\partial x} \\
&\quad + \left(\left(\frac{q^2}{2m_\pm} - eV_\pm + eV(x)\right)\frac{m'(x)}{m(x)} + eV'(x)\right)\frac{\partial}{\partial p} - \nu\Bigg)Q(x,p)dxdp\Bigg)S(q)dq \\
&\quad = \int_0^{+\infty}\left(\int_0^1\int_{-\infty}^{+\infty}\left(\sum_{i=1}^5 r_\hbar^i(x,p)\right)Q(x,p)dxdp\right)S(q)dq.
\end{aligned} \tag{4.13}$$

Now we pass to the limit in each member of (4.13). For the first term of the left-hand side of (4.13), we use the following lemma:

LEMMA 4.4. Let $\psi_q^\pm$ be a solution of (3.1)–(3.3); then the following asymptotics hold in the strong L^∞ topology:

1) i) $\psi_q^-(\hbar\eta) = e^{iq\eta} + r_q^- e^{-iq\eta} + o(1)$,

ii) $\psi_q^-(1+\hbar\eta) = t_q^-(e^{i\sqrt{\frac{m_+}{m_-}q^2+2em_+(V_+-V_-)}\eta} + o(1))$,

(2) i) $\psi_q^+(\hbar\eta) = t_q^+(e^{-i\sqrt{\frac{m_-}{m_+}q^2+2em_-(V_--V_+)}\eta} + o(1))$,

ii) $\psi_q^+(1+\hbar\eta) = e^{-iq\eta} + r_q^+ e^{+iq\eta} + o(1)$,

where $o(1)$ is uniform when (q,η) lie in a bounded set.

Proof. We shall just give the details of 1-i). The other expansions follow in analogy. The proof relies on stability results for differential equations. First, we note

$$\phi_\hbar(\eta) = \psi_q^-(\hbar\eta), U_\hbar(\eta) = V(\hbar\eta) \text{ and } M_\hbar(\eta) = m(\hbar\eta).$$

Then, let

$$\delta_\hbar(\eta) = \psi_q^-(\hbar\eta) - e^{iq\eta} - r_q^- e^{-iq\eta}.$$

Using (3.2), it verifies

$$\delta_\hbar(0) - \delta_\hbar'(0) = 0.$$

Straightforward algebra leads to

$$-\frac{1}{2m_1}\delta_\hbar'' = \frac{q^2}{2m_1}\delta_\hbar + \left(\frac{1}{2M_\hbar} - \frac{1}{2m_1}\right)\phi_\hbar'' - \frac{M_\hbar'}{2M_\hbar}\phi_\hbar' + e(U_\hbar - V_1).$$

Since $U_\hbar$ (resp. $M_\hbar$) converges uniformly to V_1 (resp. m_1) on bounded intervals and since $M_\hbar'(\eta) = \hbar m'(\hbar\eta)$, then $\delta_\hbar$ converges in L^∞ weak* to the unique solution of

$$\begin{cases} -\frac{1}{2m_1}\delta'' = \frac{q^2}{2m_1}\delta \\ \delta(0) = \delta'(0) = 0. \end{cases}$$

$\delta = 0$. Moreover, $\delta_\hbar''$ is bounded in L^∞ which proves that the convergence to zero of $\delta_\hbar$ holds in L^∞ strong. Then the proof ends. □

Now, let us give the following result:

LEMMA 4.5. Let $S(q)$ be a test function in $L^1(\mathbb{R}_q^+, (1+q)dq)$. We assume that $Q(0,p)$ vanishes for non-positive p's and $Q(1,p)$ vanishes for positive p's. Then, when $\hbar$ tends to zero, we have

i) $\mathrm{Lim}_{\hbar\to 0}\int_0^{+\infty}\int_{\mathbb{R}} \frac{p}{m_-}Q(0,p)W_q^{\hbar,-}(0,p)S(q)dpdq = \int_0^{+\infty}\frac{q}{m_-}Q(0,q)S(q)dq$,

ii) $\mathrm{Lim}_{\hbar\to 0}\int_0^{+\infty}\int_{\mathbb{R}} \frac{p}{m_+}Q(1,p)W_q^{\hbar,-}(1,p)S(q)dpdq = 0$,

iii) $\mathrm{Lim}_{\hbar\to 0}\int_0^{+\infty}\int_{\mathbb{R}} \frac{p}{m_-}Q(0,p)W_q^{\hbar,+}(0,p)S(q)dpdq = 0$,

iv) $\mathrm{Lim}_{\hbar\to 0}\int_0^{+\infty}\int_{\mathbb{R}} \frac{p}{m_+}Q(1,p)W_q^{\hbar,+}(1,p)S(q)dpdq = -\int_0^{+\infty}\frac{q}{m_+}Q(1,-q)S(q)dq$.

Proof. We use the same technique that is shown to prove Lemma B.1 in [19]. We just prove i). The proof of the other terms is similar. We start from

$$\int_0^{+\infty}\int_{-\infty}^{+\infty}\frac{p}{m_-}Q(0,p)W_q^{\hbar,-}(0,p)S(q)dpdq$$
$$= \frac{1}{2\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_0^{+\infty}\frac{p}{m_-}Q(0,p)e^{i\eta p}\mathcal{O}\overline{\psi_q^-}\left(\frac{\hbar}{2}\eta\right)\mathcal{O}\psi_q^-\left(-\frac{\hbar}{2}\eta\right)S(q)d\eta dpdq,$$

and replace $\psi_q^-(\frac{\hbar}{2}\eta)$ by its asymptotic expression $e^{i\frac{q}{2}\eta}+r_q^-e^{-i\frac{q}{2}\eta}+o(1)$ for $\eta<0$. This leads to

$$\mathcal{O}\overline{\psi_q^-}\left(\frac{\hbar}{2}\eta\right)\mathcal{O}\psi_q^-\left(-\frac{\hbar}{2}\eta\right)=e^{-iq\eta}+2\operatorname{Re}(r_q^-)+|r_q^-|^2e^{iq\eta}+o(1).$$

Hence

$$\begin{aligned}&\operatorname{Lim}_{\hbar\to0}\int_0^{+\infty}\int_{-\infty}^{+\infty}\frac{p}{m_-}Q(0,p)W_q^{\hbar,-}(0,p)S(q)dpdq\\&=\operatorname{Lim}_{\hbar\to0}\frac{1}{2\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_0^{+\infty}\frac{p}{m_-}Q(0,p)e^{i\eta p}[e^{-iq\eta}+2\operatorname{Re}(r_q^-)+|r_q^-|^2e^{iq\eta}]S(q)d\eta dpdq.\end{aligned}\tag{4.14}$$

To rigorously prove this equality, we use the Lebesgue dominated convergence theorem. Indeed, Lemma 4.2 implies that the integrand of the left-hand side of (4.14) is bounded. Using the back Fourier transform with respect to η and noticing that $Q(0,p)$ vanishes for non-positive p's, we get

$$\begin{aligned}&\operatorname{Lim}_{\hbar\to0}\int_0^{+\infty}\int_{-\infty}^{+\infty}\frac{p}{m_-}Q(0,p)W_q^{\hbar,-}(0,p)S(q)dpdq\\&=\operatorname{Lim}_{\hbar\to0}\int_0^{+\infty}S(q)\frac{q}{m_-}[Q(0,q)-|r_q^-|^2Q(0,-q)]dq=\int_0^{+\infty}\frac{q}{m_-}Q(0,q)S(q)dq.\end{aligned}$$

This ends the proof of Lemma 4.5. □

For the second integral term of the left-hand side of (4.13), we use Lemma 4.3, where $W_\hbar^\pm$ converges to $W^\pm$, $L^\infty_{\mathrm{Loc}}(\mathbb{R}_q^+;\mathcal{A}')$ weak*. We obtain

$$\begin{aligned}&\operatorname{Lim}_{\hbar\to0}\int_{\mathbb{R}+}\int_{[0,1]\times\mathbb{R}}(W_q^{\hbar,\pm}(x,p)-W_q^\pm(x,p))\left(\frac{p}{m(x)}\frac{\partial}{\partial x}\right.\\&\left.+\left(\left(\frac{q^2}{2m_\pm}-eV_\pm+eV(x)\right)\frac{m'(x)}{m(x)}+eV'(x)\right)\frac{\partial}{\partial p}-\nu\right)Q(x,p)S(q)dxdpdq=0.\end{aligned}$$

But for the right-hand side of (4.13), we use the following lemma:

LEMMA 4.6.

$$\int_0^1\int_{-\infty}^{+\infty}r_\hbar^i(x,p)Q(x,p)dxdp\underset{\hbar\to0}{\longrightarrow}0\qquad\text{for all } i=1,2,3,4,5.$$

Proof. Since $\|\psi_q^\pm\|^2_{L^2(0,1)}\le Cq,\hbar^2\|\psi_q^{\pm'}\|^2_{L^2(0,1)}\le Cq(q+1)$ and $\mathcal{O}\equiv1$ on $[0,1]$, we have

$$\int_0^1\int_{\mathbb{R}}r_\hbar^i(x,p)Q(x,p)dxdp\underset{\hbar\to0}{\longrightarrow}0\qquad i=1,3.$$

Then for $i=4,5$, we write

$$\int_0^1\int_{\mathbb{R}}r_\hbar^i(x,p)Q(x,p)dxdp=\int_0^1\int_{\mathbb{R}}\mathcal{F}_p(Q(x,\eta))S_\hbar^i(x,\eta,q)dxdp$$

where we set by

$$S_\hbar^4(x,\eta,q) = \frac{i}{m(x)}[\delta_\hbar(m\mathcal{V}) - \eta(m\mathcal{V})']O\overline{\psi}_q^{\pm}(+)O\psi_q^{\pm}(-),$$

$$S_\hbar^5(x,\eta,q) = -\frac{iE}{m(x)}[\delta_\hbar(m) - \eta m'(x)]O\overline{\psi}_q^{\pm}(+)O\psi_q^{\pm}(-).$$

Using the bound of $\psi_q^{\pm}$ in $L^2(0,1)$ and that

$$\delta_\hbar(m\mathcal{V}) - \eta(m\mathcal{V})' \underset{\hbar\to 0}{\longrightarrow} 0, \quad \delta_\hbar(m) - \eta m'(x) \underset{\hbar\to 0}{\longrightarrow} 0,$$

we apply Lemma A.1 in [19] to $r_\hbar^i$ $(i=4,5)$. We obtain

$$\int_0^1\int_{-\infty}^{+\infty} r_\hbar^i(x,p)Q(x,p)dxdp \underset{\hbar\to 0}{\longrightarrow} 0, \quad \forall Q\in C_0^\infty(\mathbb{R},\mathbb{R}) \text{ for } i=4,5.$$

Consequently, simultaneous for ψ_q^- and ψ_q^+, (4.13) converges to the following formulations:

$$\int_0^{+\infty}\frac{q}{m_-}Q(0,q)S(q)dq + \int_0^1\int_{-\infty}^{+\infty} W_q^-(x,p)\left(\frac{p}{m(x)}\frac{\partial}{\partial x}\right.$$
$$\left.+\left(\left(\frac{q^2}{2m_-} - eV_- + eV(x)\right)\frac{m'(x)}{m(x)} + eV'(x)\right)\frac{\partial}{\partial p} - \nu\right)Q(x,p)S(q)dxdpdq = 0, \tag{4.15}$$

$$\int_0^{+\infty}\frac{q}{m_+}Q(1,-q)S(q)dq + \int_0^1\int_{-\infty}^{+\infty} W_q^+(x,p)\left(\frac{p}{m(x)}\frac{\partial}{\partial x}\right.$$
$$\left.+\left(\left(\frac{q^2}{2m_+} - eV_+ + eV(x)\right)\frac{m'(x)}{m(x)} + eV'(x)\right)\frac{\partial}{\partial p} - \nu\right)Q(x,p)S(q)dxdpdq = 0. \tag{4.16}$$

We remark that these formulations are nothing but the weak expression of the following problem

$$\frac{\partial}{\partial x}\left(\frac{p}{m(x)}W_q^{\pm}\right) + \left(\left(\frac{q^2}{2m_\pm} - e(V_\pm - V(x)\right)\frac{m'(x)}{m(x)} + eV'(x)\right)\frac{\partial W_q^{\pm}}{\partial p} + \nu W_q^{\pm} = 0, \tag{4.17}$$

$$W_q^-(0,p) = \delta(p-q), \quad W_q^-(1,-p) = 0, \quad p>0, \tag{4.18}$$

$$W_q^+(0,p) = 0, \quad W_q^+(1,-p) = \delta(-p+q), \quad p>0. \tag{4.19}$$

The purpose is to get the problem $(\mathcal{P}_{\text{Lim}})$. So, first of all, we must remove dependence on q by analyzing the support of $W_q^{\pm}$. This will be done using the following lemma: □

LEMMA 4.7. The support of $W_q^{\pm}$ associated to $\psi_q^{\pm}$ is included in $\mathcal{C}^{\pm}$, where

$$\mathcal{C}^{\pm} = \left\{(x,p)\in\,]0,1[\, \times\mathbb{R} \text{ such that } \frac{p^2}{2m(x)} - eV(x) = \frac{q^2}{2m_\pm} - eV_\pm\right\}.$$

Before we state the proof, we define the operator $T^{*,\pm}$

$$T^{*,\pm} = T_0^{*,\pm} - \nu, \tag{4.20}$$

with

$$T_0^{*,\pm} = \frac{p}{m(x)}\frac{\partial}{\partial x} + \left(\left(\frac{q^2}{2m_\pm} - eV_\pm + eV(x)\right)\frac{m'(x)}{m(x)} + eV'(x)\right)\frac{\partial}{\partial p}.$$

Proof. As mentioned above, here we prove only the inclusion for W_q^-. Our purpose is to prove that $\operatorname{supp} W_q^- \subset \mathcal{C}^-$, which is equivalent to showing for all $\Psi \in \mathcal{D}([0,1],\mathbb{R})$ such that $\Psi \equiv 0$ in the neighborhood of $\mathcal{C}^-$, we have

$$\langle W_q^-, \Psi\rangle_{\mathcal{D}',\mathcal{D}} = 0.$$

For this, let us denote by φ the solution of the following equation

$$T^{*,-}(\varphi) = \Psi \tag{4.21}$$

with the boundary conditions

$$\varphi(0,p) = 0, \quad \text{for } p < 0, \quad \varphi(1,p) = 0, \quad \text{for } p > 0. \tag{4.22}$$

We recall that $T^{*,-}$ is defined by (4.20). But, as W_q^- is a solution of (4.17)–(4.18), then in the sense of duality, where φ is considered as a test function, we get

$$\langle W_q^-, T^{*,-}\varphi\rangle - \frac{q}{m_-}\varphi(0,q) = 0. \tag{4.23}$$

In this formulation, it is readily seen that it suffices to prove $\varphi(0,p) = 0$ in the neighborhood of $p = q$. However, (4.23) cannot be used immediately because φ is not in $C^1([0,1]\times\mathbb{R})$. To overcome this difficulty, we regularize φ by a convolution procedure $\varphi_\epsilon = \varrho_\epsilon \star \varphi$, where ϱ_ϵ is a non-negative C^∞ approximation of the Dirac measure. For ϵ small, φ_ϵ satisfy (4.23) and

$$T^{*,-}\varphi_\epsilon \underset{\epsilon\to 0}{\longrightarrow} \Psi, \text{ in } C^0_{\mathrm{Loc}}.$$

Now, we prove $\varphi(0,p) \equiv 0$ in neighborhood of the point $p = q$. Let

$$G(x,p) = g\left(m(x)\left(\frac{p^2}{2m(x)} - eV(x) - \frac{q^2}{2m_-} + eV_-\right)\right),$$

where g is a function in C^∞ such that $g(t) = 1$ in the neighborhood of the point $t = 0$ and $\operatorname{supp} g \subset [-\alpha,\alpha]$, for a small $\alpha > 0$. The function G verifies $G\Psi = 0$. It satisfies $T_0^{*,-}G = 0$. Then $G\varphi$ is a solution of the following system:

$$\begin{cases} T^{*,-}(G\varphi) = 0 \\ G\varphi(0,p) = 0, \ p < 0 \\ G\varphi(1,p) = 0, \ p > 0 \end{cases}$$

and the $G\varphi \equiv 0$. Using that $G(0,p) \equiv 1$ in the neighborhood of the point $p = q$, we have $\varphi(0,p) = 0$ in the neighborhood of the point $p = q$.

As a consequence of the previous lemma, we replace the term

$$\left(\left(\frac{q^2}{2m_\pm} - e(V_\pm - V(x))\right)\frac{m'(x)}{m(x)} + eV'(x)\right) \quad \text{by} \quad \left(\frac{p^2}{2m(x)}\frac{m'(x)}{m(x)} + eV'(x)\right).$$

Formulations (4.15) and (4.16) become

$$\int_0^{+\infty} \frac{q}{m_-} Q(0,q)S(q)dq + \int_0^1 \int_{-\infty}^{+\infty} W_q^-(x,p) \left(\frac{p}{m(x)} \frac{\partial}{\partial x} + \left(\frac{p^2}{2} \frac{m'(x)}{m^2(x)} + eV'(x) \right) \frac{\partial}{\partial p} - \nu \right) Q(x,p)S(q)dxdpdq = 0 \quad (4.24)$$

$$\int_0^{+\infty} \frac{q}{m_+} Q(1,-q)S(q)dq + \int_0^1 \int_{-\infty}^{+\infty} W_q^+(x,p) \left(\frac{p}{m(x)} \frac{\partial}{\partial x} + \left(\frac{p^2}{2} \frac{m'(x)}{m^2(x)} + eV'(x) \right) \frac{\partial}{\partial p} - \nu \right) Q(x,p)S(q)dxdpdq = 0. \quad (4.25)$$

Rewritten in terms of the energy $\mathcal{E} = \frac{p^2}{2m(x)} - eV(x)$ and removing the derivation on $W_q^\pm$, these formulations are nothing but the weak formulation of the following problem:

$$\frac{\partial \mathcal{E}}{\partial p} \frac{\partial W_q^\pm}{\partial x} - \frac{\partial \mathcal{E}}{\partial x} \frac{\partial W_q^\pm}{\partial p} + \nu W_q^\pm = 0,$$
$$W_q^-(0,p) = \delta(p-q), \quad W_q^-(1,-p) = 0, \quad p > 0$$
$$W_q^+(0,p) = 0, \quad W_q^+(1,-p) = \delta(-p+q), \quad p > 0.$$

Since $G^\pm(q)$ defined by (H-2) satisfies the hypothesis of Lemma 4.5, we can take it as a function test in formulations (4.24) and (4.25), which implies, using the result of Lemma 4.3, that f defined by

$$f(x,p) = \int_0^{+\infty} G^+(q)W_q^+(x,p)dq + \int_0^{+\infty} G^-(q)W_q^-(x,p)dq$$

is noting but the limit of the Wigner function $\omega_\hbar$ (defined by (4.3)) in $\mathcal{A}'$ weak*. Moreover, it verifies

$$\frac{\partial \mathcal{E}}{\partial p} \frac{\partial f}{\partial x} - \frac{\partial \mathcal{E}}{\partial x} \frac{\partial f}{\partial p} + \nu f = 0$$

with the standard inflow boundary conditions

$$f(0,p) = \int_0^{+\infty} G^+(q)W_q^+(0,p)dq + \int_0^{+\infty} G^-(q)W_q^-(0,p)dq = G^-(p)$$

and

$$f(1,-p) = \int_0^{+\infty} G^+(q)W_q^+(1,p)dq + \int_0^{+\infty} G^-(q)W_q^-(1,-p)dq = G^+(p).$$

This completes the proof of the main theorem of this paper. □

5. Conclusion. The purpose of the present paper was to investigate the properties of an effective electron mass in a semiconductor device where quantum effects cannot be neglected. In a quantum region of such device, we require a more sophisticated model to take into account the variation of effective mass. For this, we have described such a suitable mathematical model: the Schrödinger with variable mass. A natural work was a mathematical analysis of this model in the case where the electric potential is self-consistent. Finally, we have studied the semiclassical limit of this model which leads to its corresponding kinetic model. Both of these models, the quantum and the kinetic one, will probably constitute significant models to describe a far-from equilibrium transport in a resonant tunneling diode, particularly when we couple them under appropriate interface conditions.

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