On the stationary Schrödinger equation in the semi-classical limit: Asymptotic blow-up at a turning point

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We consider a model for the wave function of an electron, injected at a fixed energy E into an electronic device with stationary potential $V(x)$. This wave function is the solution of the stationary 1D Schrödinger equation. The scattering problem is modeled on an interval where the potential varies. Moreover, $V(x)$ is assumed constant in the exterior, i.e. in the leads of the device. Here we are interested in including turning points – points $\bar{x}$ where the potential and the energy of the particle coincide, i.e. $E = V(\bar{x})$. We show that including a turning point lets the wave function blow-up asymptotically as the scaled Planck constant $\varepsilon \to 0$. This is an essential difference to the uniformly bounded wave function if turning points are excluded.

1 Model

We consider a scattering problem for the stationary Schrödinger equation in 1D, which is a relevant quantum dynamical model for the electron transport in a diode. The diode covers the interval $[x_0, 1]$, having leads to both sides. Electrons are injected from the right lead in the form of a plane wave (of unit amplitude, e.g.).

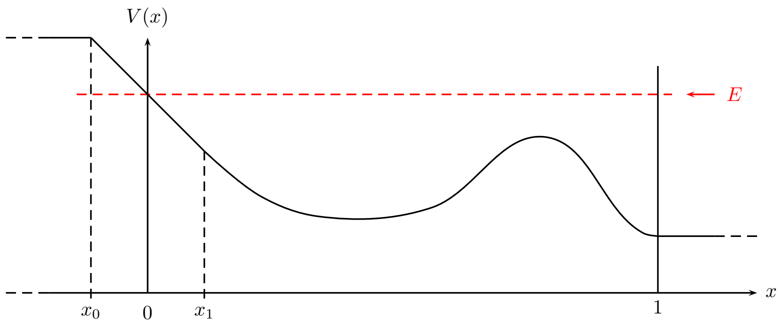

Fig. 1 Sketch of the model with linear potential in the vicinity of the turning point at $x = 0$, and constant continuation of the potential in the leads, i.e. outside $[x_0, 1]$. Electrons are injected at energy E from the right boundary at $x = 1$.

The scattering problem formulation for the wave function $\psi(x)$, with $a(x) := E - V(x)$, and the scaled Planck constant $\varepsilon := \frac{\hbar}{\sqrt{2m}}$ reads:

$$\begin{cases} \varepsilon^2 \psi''(x) + a(x)\psi(x) = 0\,, \quad x \in (x_0, 1)\,, \\ \varepsilon \psi'(x_0) - \sqrt{-x_0}\,\psi(x_0) = 0\,, \\ \varepsilon \psi'(1) - \mathrm{i}\sqrt{a(1)}\,\psi(1) = -2\mathrm{i}\sqrt{a(1)}\,, \end{cases} \tag{1}$$

where $0 < \varepsilon \ll 1$, $x_0 < 0 < x_1 < 1$, $a(x) = x$ on $[x_0, x_1]$, and $a(x) \geq \tau_1$ on $[x_1, 1]$ for some $\tau_1 > 0$. The two transparent boundary conditions correspond to constant potentials in the exterior problems, i.e. for $x \leq x_0$ and $x \geq 1$. The model includes a first order turning point (i.e. a zero of $a(x)$) at $x = 0$.

The goal of this note is to describe the asymptotic behavior of ψ_ε in the semi-classical limit – in particular close to the turning point. This is an important input information for the numerical treatment of (1). In [2] both of these questions were discussed for a very similar scattering problem, but having a linear potential $V(x) := E - x$ in the whole left lead. Here, we extend this to the more realistic case of constant potentials in both leads.

Away from the turning point, an efficient numerical treatment of the highly oscillatory problem (1) can be based on first eliminating analytically the dominant oscillations (using asymptotic WKB-approximations of the solution). Then, the resulting smoother problem can be solved numerically on a coarse grid [1, 2], with an error that is uniform in ε. Since this approach is not valid near a turning point, we assumed here and in [2], as a simplification, that the potential is linear in the vicinity of the turning point. ψ_ε can then be obtained as the numerical solution of (1) on $[x_1, 1]$, coupled to the explicit (analytic) solution on $[x_0, x_1]$:

$$\psi_\varepsilon(x) = \alpha_\varepsilon\, \hat{\psi}_\varepsilon(x)\,, \quad \hat{\psi}_\varepsilon(x) = \varepsilon^{-\frac{1}{6}} \left[\mathrm{Ai}\,(y(x)) - \tfrac{A_\varepsilon}{B_\varepsilon}\, \mathrm{Bi}\,(y(x)) \right], \tag{2}$$

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with some normalization constant α_ε, and $y(x) := -\frac{x}{\varepsilon^{2/3}}$, where

$$A_\varepsilon := \mathrm{Ai}'\big((y(x_0)\big) + \sqrt{y(x_0)}\,\mathrm{Ai}(y(x_0))\big)\,, \quad B_\varepsilon := \mathrm{Bi}'\big((y(x_0)\big) + \sqrt{y(x_0)}\,\mathrm{Bi}\,\big(y(x_0)\big)\,.$$

Here, Ai and Bi are the fundamental solutions to the Airy equation, i.e. Airy functions.

2 Asymptotic blow-up at a turning point

Example 2.1 Consider (1) with $x_0 = -0.3$ and $a(x) = x$ for $x \in [x_0, 1]$ and $0 < \varepsilon < 1$. Then the explicit solution is given by (2) on all of $[x_0, 1]$, and the normalization is chosen such that ψ_ε satisfies the right boundary condition:

$$\alpha_\varepsilon(\hat{\psi}_\varepsilon(1), \hat{\psi}'_\varepsilon(1)) := \frac{2\sqrt{a(1)}}{\hat{\psi}_\varepsilon(1)\sqrt{a(1)} + \mathrm{i}\varepsilon\hat{\psi}'_\varepsilon(1)}\,. \tag{3}$$

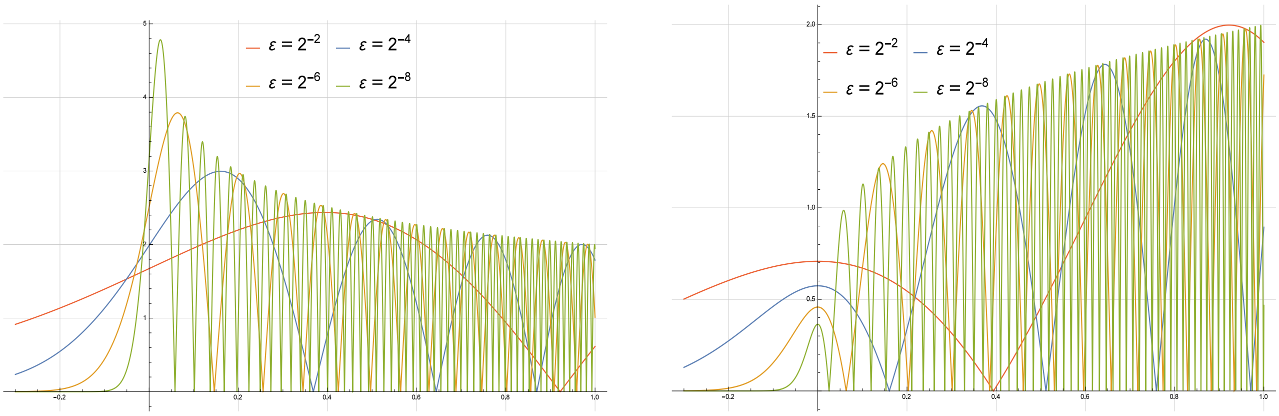

Fig. 2: $|\psi_\varepsilon(x)|$ (left) and $\varepsilon|\psi'_\varepsilon(x)|$ (right) for various values of ε. This example illustrates that $\varepsilon\|\psi'_\varepsilon\|_{L^\infty(x_0,1)}$ is uniformly bounded w.r.t. $0 < \varepsilon < 1$, but $\|\psi_\varepsilon\|_{L^\infty(x_0,1)}$ is *not* since $\{|\psi_\varepsilon(0)|\}$ becomes unbounded as $\varepsilon \to 0$.

In Figure 2, one can see that in the classically forbidden region (i.e. $a(x) = x < 0$) there is (approximately) exponential decay of ψ_ε, but in the classically allowed region (i.e. $a(x) > 0$) the solution is highly oscillatory with varying frequency of order $\mathcal{O}(\sqrt{a(x)}/\varepsilon)$. The asymptotic blow-up and, resp., boundedness of the solution in Example 2.1 extends to all potentials covered by the problem from (1):

Proposition 2.2 *Let* $0 < \varepsilon \ll 1$*, and* $x_0 < 0 < x_1 < 1$*. Further let* $a \in \mathcal{C}^2$ *on* $[x_0, 1]$ *with* $a(x) = x$ *on* $[x_0, x_1]$*, and* $a(x) \geq \tau_1 > 0$ *on* $[x_1, 1]$*. Then, the family of solutions* $\{\psi_\varepsilon(x)\}$ *to the boundary value problem* (1) *satisfies:*

a) $\|\psi_\varepsilon\|_{L^\infty(x_0,1)}$ *is of the (sharp) order* $\varepsilon^{-\frac{1}{6}}$*, i.e.* $\exists c_1, c_2 > 0$*, such that* $c_1\,\varepsilon^{-\frac{1}{6}} \leq \|\psi_\varepsilon\|_{L^\infty(x_0,1)} \leq c_2\,\varepsilon^{-\frac{1}{6}}$ *for* $\varepsilon \to 0$.

b) $\varepsilon\|\psi'_\varepsilon\|_{L^\infty(x_0,1)}$ *is uniformly bounded with respect to* $\varepsilon \to 0$.

Proof-idea. The blow-up of $|\psi_\varepsilon(0)|$ stems essentially from the $x^{-1/4}$–decay of the flipped Airy functions $\mathrm{Ai}(-x)$, $\mathrm{Bi}(-x)$ as $x \to \infty$. Moreover, since $A_\varepsilon/B_\varepsilon \overset{\varepsilon\to 0}{\longrightarrow} 0$, ψ_ε from (2) behaves like the scaled Airy function $\varepsilon^{-1/6}\,\mathrm{Ai}(-x\varepsilon^{-2/3})$ close to the turning point. This ε–scaling of the x variable compresses the Airy function decay to the (small) interval $[0, x_1]$. At the fixed point x_1, $\mathrm{Ai}(-x_1\varepsilon^{-2/3})$ is proportional to $\varepsilon^{1/6}$. This decay is compensated by the scaling factor $\varepsilon^{-1/6}$ of $\hat{\psi}_\varepsilon$ in (2). Since the resulting ε–uniformity of $|\psi_\varepsilon(x_1)|$ is not changed any more on the subsequent interval $[x_1, 1]$, this allows the solution to be matched at $x = 1$ to the incoming plane wave with amplitude 1 (independently of ε).

For the detailed proof see [3]; it is an adaption of the proof for Proposition 4.2 in [2]. □

With this information at hand, a hybrid analytical-numerical solution scheme for (1) can be formulated as in [2]. Since the analytical solution (2) is scaled by (3), it inherits an error from the numerical solution on $[x_1, 1]$. For obtaining an overall error that is uniform in ε, it is crucial that the numerical error on $[x_1, 1]$ decays faster than $\varepsilon^{1/6}$ (and this is possible with the WKB-based method from [1]). This way it can compensate the (inherited) error of the analytical, asymptotically unbounded solution ψ_ε on $[x_0, x_1]$. Let us remark here that the findings of this note are not limited to linear potentials around a turning point, but they apply with the same orders also to other first order turning points, i.e. zeros of $a(x)$ of first order, cf. [2, 3].

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