A 5th-Order Method for 1D-Device Solution

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Abstract. The so-called *Numerov process* provides a three-point interpolation with an $\sim \eta^5$ accuracy in grid's size η, much better than the standard finite-difference scheme that keeps the $\sim \eta^2$ terms. Such a substantial improvement is achieved with a minor increase in computational cost. As the method is applicable to second-order differential equations in one dimension, it is an ideal tool for solving, e.g., the Poisson and Schrödinger equations in ballistic electron devices, where the longitudinal (that is, along the channel) problem is typically separated from the lateral one and solved over a uniform grid. Despite its advantage, the Numerov process has found limited applications, due to the difficulty of keeping the same precision in the boundary conditions. A method to work out the boundary conditions consistently with the rest of the scheme is presented, and applications are shown.

Theory. Given a device whose channel extends from $x = 0$ to $x = s$, one needs to solve the 1D Schrödinger equation $\psi'' + q\psi = 0$ for a particle of effective mass m, with $q(x) = (2m/\hbar^2)\,(E - V)$, $E > 0$. The potential energy $V(x)$ is zero outside the channel, so that the wave vector is $k = \sqrt{2mE}/\hbar$ there. The transmission coefficient of the barrier formed by V in $0 \le x \le s$ is

$$T = \frac{4}{2 + (u_s)^2 + (u_s'/k)^2 + (v_s')^2 + (kv_s)^2}\,, \quad (1)$$

with u_s, v_s the fundamental solutions of $\psi'' + q\psi = 0$ at $x = s$ [1]; of them, u solves $u'' + qu = 0$ with the conditions $u(0) = 1$, $u'(0) = 0$, while v solves the same equation with $v(0) = 0$, $v'(0) = 1$. Therefore, an open integration is necessary, which may turn out to be inaccurate if V is not sufficiently smooth. The Numerov process for u over three consecutive nodes $i-1, i, i+1$ of a uniform grid reads [2]

$$(1 + r_{i+1})u_{i+1} + (1 + r_{i-1})u_{i-1} = 2(1 - 5r_i)u_i\,, \quad (2)$$

with $r_i = \eta^2 q_i/12$. While its structure and computational cost are similar to those of the finite-difference process $u_{i+1} + u_{i-1} = 2(1 - 6r_i)u_i$, its precision is higher by three orders in η. Unfortunately, while the finite-difference process readily provides a consistent starting point of the open integration, $u_0 = u(0) = 1$, $u_1 = 1$ and $v_0 = v(0) = 0$, $v_1 = \eta$, such a starting point would be too poor for the Numerov process and would spoil its accuracy. To calculate u_1, v_1 to the desired accuracy we Taylor expand u and v to the 5th-order at $x = 0$, and obtain the derivatives of order higher than 1 by differentiating the Schrödinger equation. This yields $u_1 = 1 + \eta^2\,\mu_0$, $v_1 = \eta\,(1 + \nu_0)$, with μ_0, ν_0 third- and fourth-order polynomials in η, respectively. Possible discontinuities in q are taken care of at this stage. The result shows the order of correction with respect to the less accurate approximations $u_1 = 1$, $v_1 = \eta$ mentioned above, and allows for a consistent application of (2) to calculate u, v over the barrier, and finally determine the values of u_s, v_s that appear in (1). Finally, the values of u_s', v_s' are calculated by the same token, taking one step backwards with respect to s.

Conclusions. The method has been tested on the double barrier of Fig. 1 because the exact solution is known (e.g., Fig. 2). For a fine grid the wave function obtained from the finite-difference method and Numerov process are close to each other and to the exact one (Fig. 3). At coarser grids the Numerov solution stays close to the exact one, while the finite-difference one substantially departs from it over the whole domain (Fig. 4). The largest error in an open integration is expected to occur at the end of the domain: Fig. 5 displays $|\psi|^2$ at $x = s$ as a function of the number of grid nodes. The relative error is not shown because energy E is off resonance, which makes $|\psi|^2$ small. An inexpensive, highly accurate discretization scheme for second-order equations has been made applicable to practical cases by working out a treatment of the boundary conditions of equal accuracy. Typical applications to electron devices are in the solution of the coupled Schrödinger-Poisson system in the device channel, as both equations are amenable to the same scheme.

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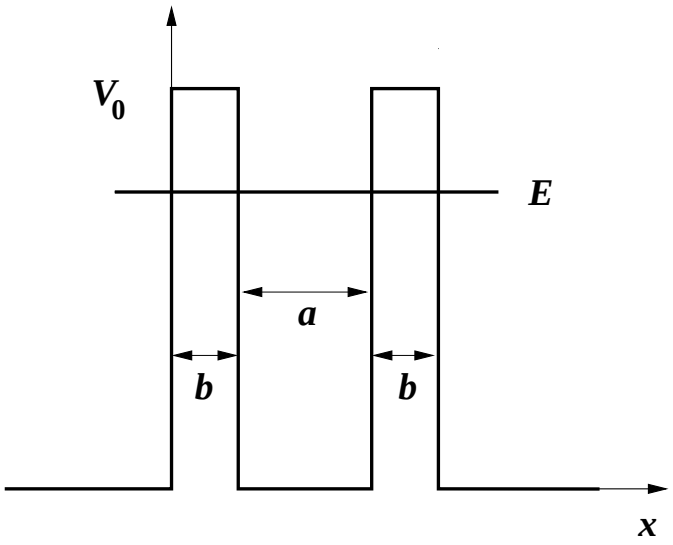

Fig. 1. Double-barrier profile.

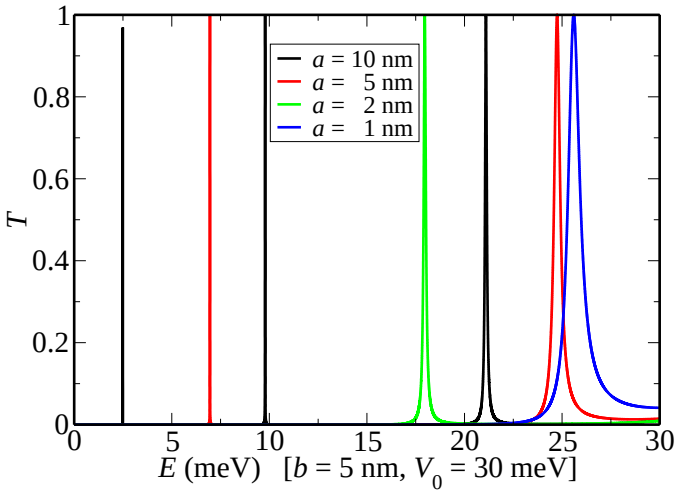

Fig. 2. Double barrier: transmission coefficient vs. electron energy (exact solution).

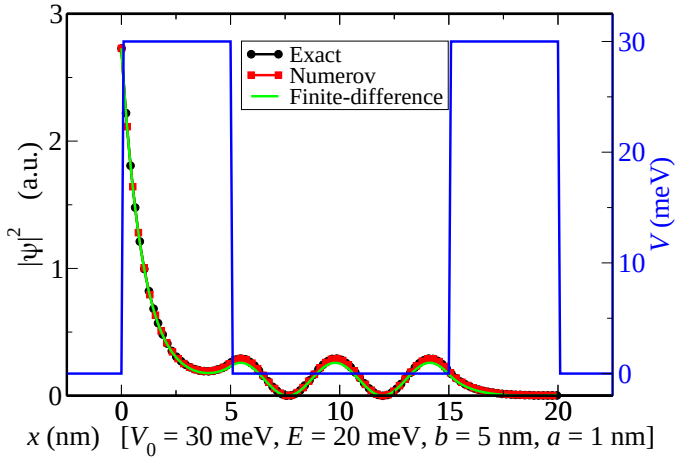

Fig. 3. Square modulus of the wave function vs. distance with a fine grid spacing ($\eta = 10^{-2}$ nm, 2000 nodes).

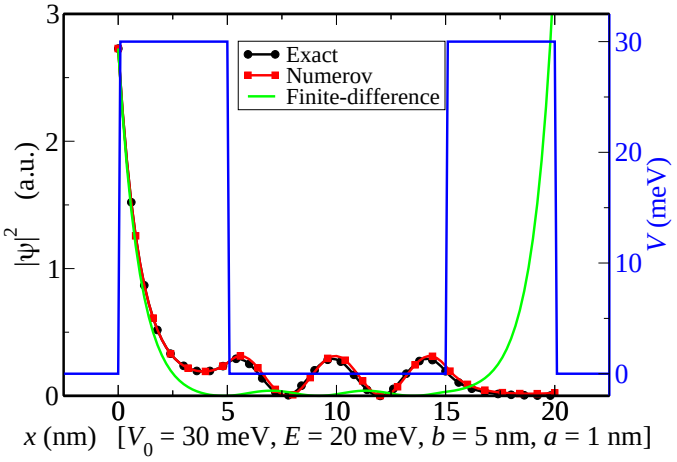

Fig. 4. Square modulus of the wave function vs. distance with a coarse grid spacing ($\eta = 2 \times 10^{-1}$ nm, 100 nodes).

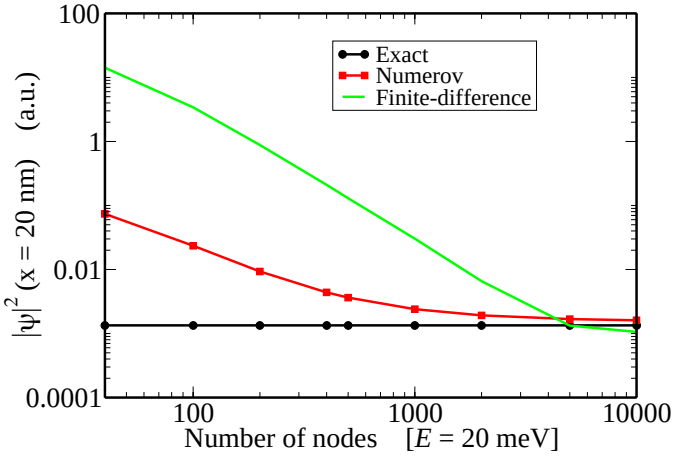

Fig. 5. Square modulus of the wave function at the end of the domain vs. the number of grid nodes.

References

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[2] B. Numerov, Publ. Obs. Central Astrophys. **2**, 188 (1933), cited in P. C. Chow, AJP **40**, 730 (1972).