Applications of Smooth Absorbing Potentials on Mesoscopic Transport

J. M. Alendouro Pinho[1], H. Veiga[1], B. A. Amorim[1], J. M. V. Parente Lopes[1]

[1]Centro de Física da Universidade do Minho e do Porto, Faculdade de Ciências da Universidade do Porto, 4169-007, Porto, Portugal

1 Introduction

- Mesoscopic transport is described by the Caroli formula in terms of Green functions.
- Semi-infinite leads result in energy-dependent self-energies, demanding a new calculation for each energy.
- We propose a two-step approach:

1- Replace the leads by finite buffers with a smooth absorbing potential, yielding energy-independent self-energies

2 - Expand Green functions in a Faber polynomial series, allowing the evaluation of the transmission for many energies simultaneously.

Result: accurate transmission with a highly efficient, energy-separable algorithm

2 Model and Caroli Formula

We consider a 1D tight-binding chain with Hamiltonian

$$H = \sum_i \varepsilon_i |i\rangle\langle i| - t \sum_{\langle i,j \rangle} (|i\rangle\langle j| + |j\rangle\langle i|) \,.$$

Transmission is given by the Caroli formula

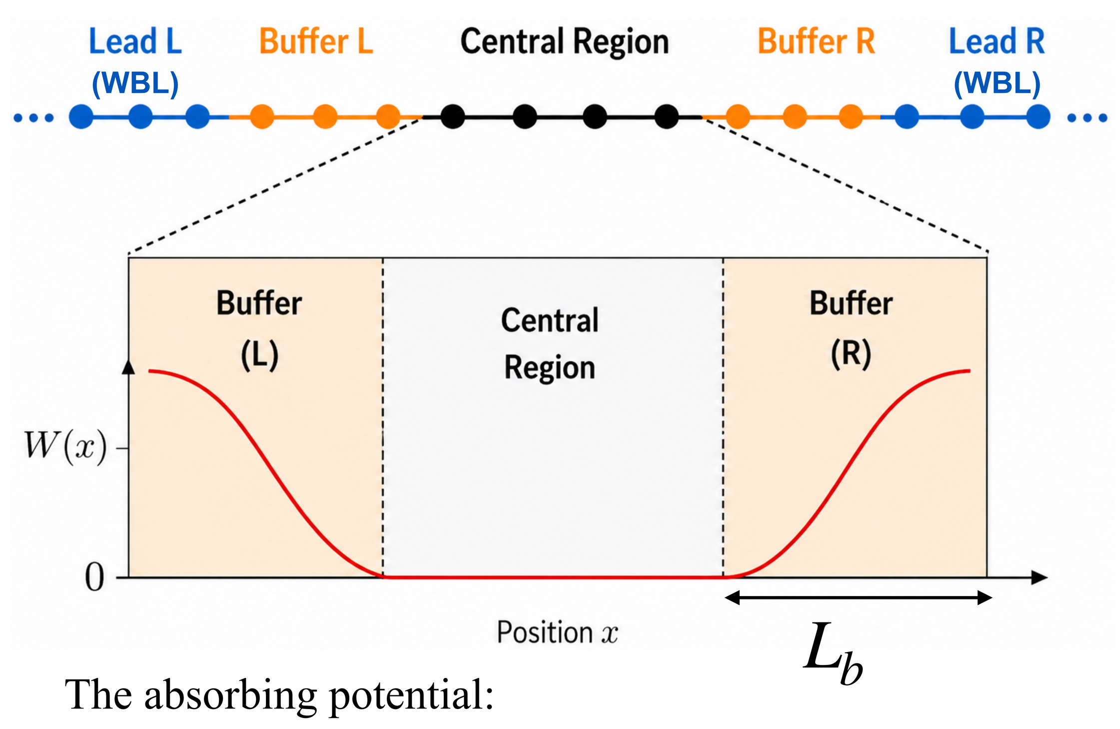
$$T(E) = \mathrm{Tr}\left[\Gamma_L(E) G^r(E) \Gamma_R(E) G^a(E)\right]$$

Where

- $G^r(E) = \left[EI - H - \Sigma_L(E) - \Sigma_R(E)\right]^{-1}$
- $\Gamma_{L/R}(E) = i\left[\Sigma^r_{L/R}(E) - \Sigma^a_{L/R}(E)\right]$

3 Step I - Smooth Absorbing Potential

Semi-infinite leads are replaced by finite buffers with a smooth absorbing potential



The absorbing potential:

$$W(x) = \begin{cases} \eta\left(\frac{x - x_0}{L_b}\right)^n, & x \in \text{ left buffer} \\ \eta\left(\frac{x - x_N}{L_b}\right)^n, & x \in \text{ right buffer} \end{cases}$$

The self-energies are

$$\Sigma^r_{L/R}(x) = -iW_n^{L/R}(x)$$

With sufficiently smooth potential (large L_b) the self-energies are energy independent:

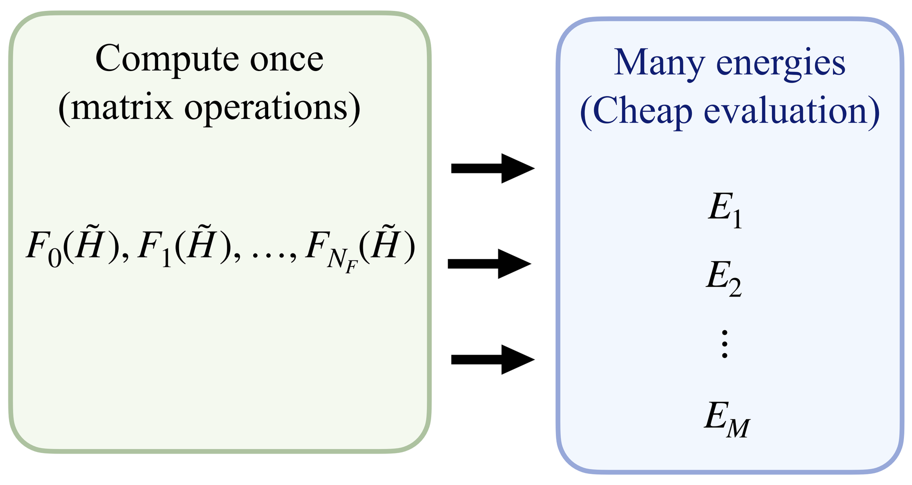
$$\Sigma_{L/R}(E) \approx \Sigma_{L/R} \text{ (constant)}$$

4 Step II - Faber Expansion

We expand the retarded (advanced) Green function in Faber polynomials

$$G^r(E) \approx \sum_{n=0}^{N_F} g_n(E) F_n(\tilde{H})$$

- Coefficients depend only on energy
- Matrices are computed once and reused for all energies



One expansion → transmission for many energies simultaneously!

5 Results

5.1 Step I - Smooth Absorbing Potential

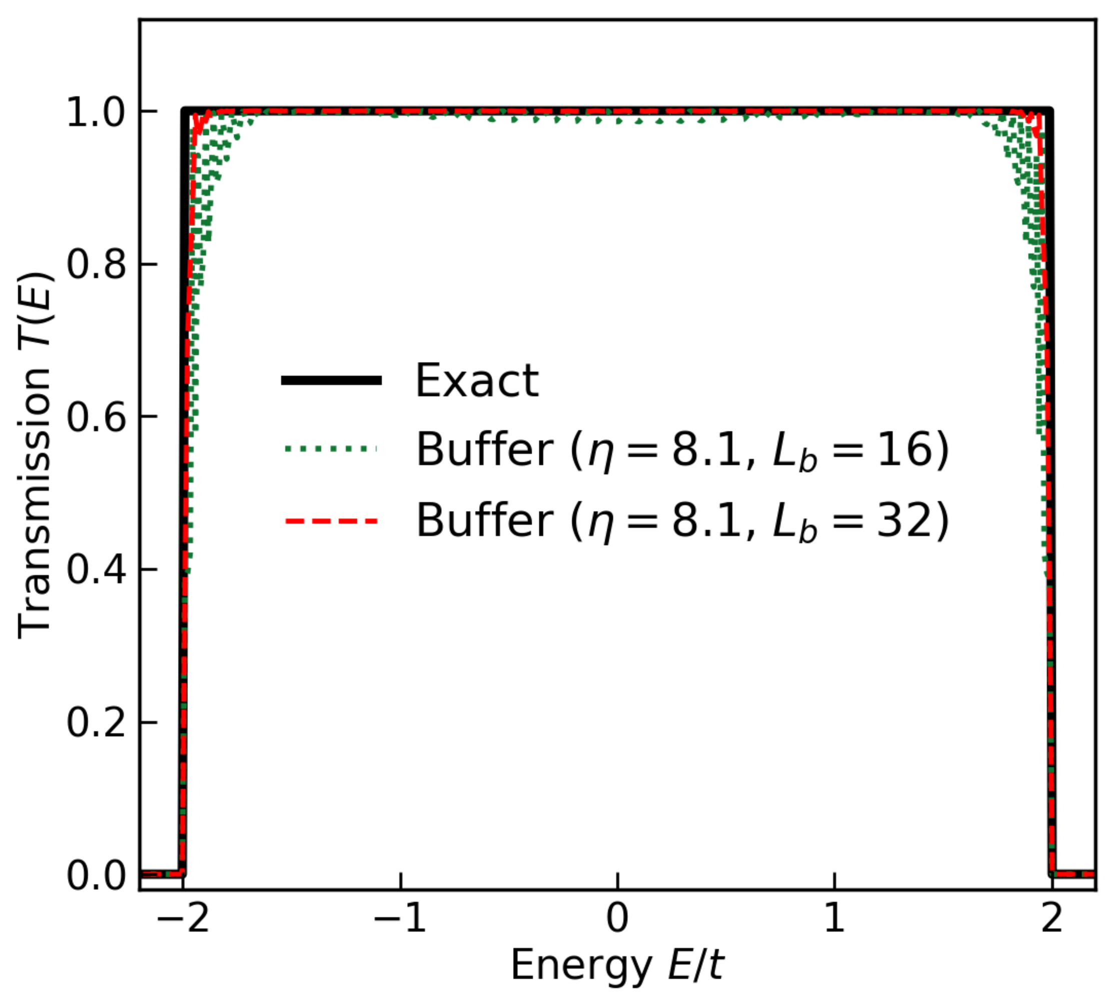


Fig. 2 - Transmission obtained with buffer zoen

The power law absorbing buffer reproduces the exact transmission with good accuracy.

5.2 Step II - Transmission with Faber expansion

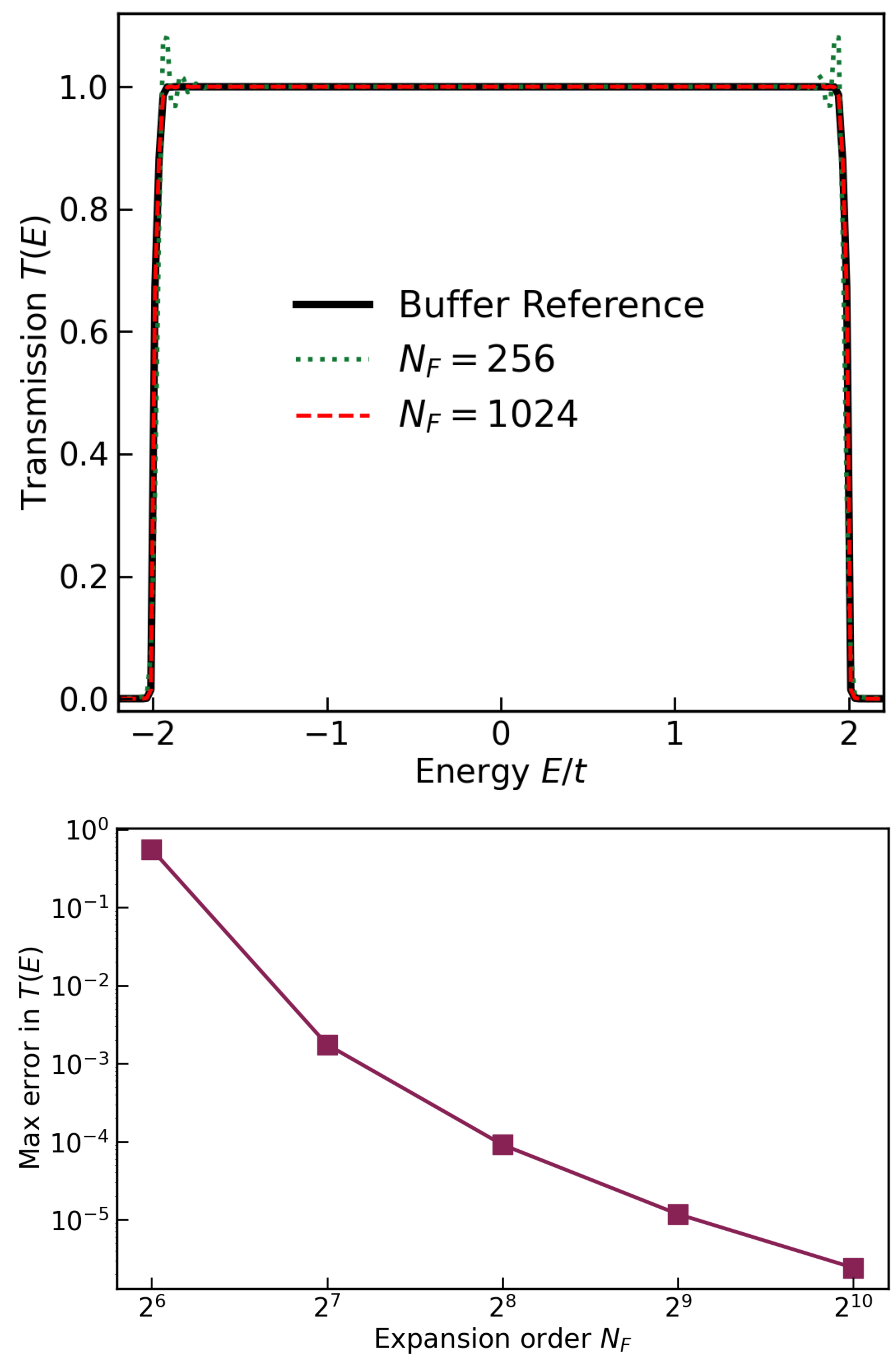


Fig. 4 - **Top** Transmission with finite buffers expanded for different polynomial numbers **Bottom** relative error with expansion order

Faber expansion converges rapidly and accurately reproduces the transmission over

6 Conclusions

- Energy-independent self-energies: no need to recompute $\Sigma_{L/R}(E)$ for each energy;
- Large speedup for dense energy grid;
- Controlled accuracy via buffer size L_b, power order n and expansion order N_F;

A scalable and reliable framework for quantum transport calculations

7 References

[1] C. Caroli, B. Roulet, and D. Saint-James, Phys. Rev. B **13**, 3884 (1976)

[2] Joseph Weston and Xavier Waintal, Phys. Rev. B **93**, 134506 (2016)

[3] Youhong Huang; Donald J. Kouri; David K. Hoffman, *J. Chem. Phys.* **101**, 10493–10506 (1994)

8 Acknowledgements

Work supported by Fundação para a Ciência e a Tecnologia (FCT, Portugal) in the framework of the Strategic Funding UID/04650/2025 - Centro de Física das Universidades do Minho e do Porto andthrough project No. EXPL/FISMAC/0953/2021 (B.A. and J.M.A.P.), and Grants. No. 2023.02155.BD (J.M.A.P), and No. CEECIND/02936/2017 (B.A.) is acknowledged. Further support by COST (European Cooperation in Science and Technology) in the framework of COST Action CA24109 – QOpen. COST is a funding agency for research and innovation networks. Our Actions help connect research initiatives across Europe and enable scientists to grow their ideas by sharing them with their peers. This boosts their research, career and innovation.

Funded by the European Union · cost https://cost.eu · QOpen https://qopen.eu/ · GOVERNO DE PORTUGAL · FCT Fundação para a Ciência e a Tecnologia

up201703751@up.pt