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Quantum Transport Using Parallel Computing Techniques

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INTRODUCTION

In this contribution quantum transmission properties will be calculated using a parallel implementation of the recursive Green's function method.

COMPUTATIONAL METHOD

The computational method is based on an implementation of the recursive Green's function (RGF) method [1] on a parallel architecture of processors. The algorithm goes beyond the (straightforward) parallelization with respect to the external parameters of the scattering problem, such as e.g. Fermi energy or magnetic field, and proceeds with the scatterer's domain decomposition in internal independent domains which are linked via interface blocks. The latter are reordered and collected in a virtual block $\mathbf{A^{\Gamma\Gamma}}$. Fig. 1 shows the reordered matrix $\mathbf{A} = E\mathbf{I} - \mathbf{H_S} - \mathbf{\Sigma_R}(E) - \mathbf{\Sigma_L}(E)$ due to processor subdivision after row and column permutations. $\mathbf{H_S}$ is the tight-binding Hamiltonian matrix and $\mathbf{\Sigma_K}(E) = \mathbf{V_K^\dagger G_K}(E)\mathbf{V_K}$ the self-energy matrices due to the left ($\mathbf{K} = \mathbf{L}$) and right ($\mathbf{K} = \mathbf{R}$) reservoir. Then a parallel block Gaussian elimination is performed to calculate the Schur's complement $\mathbf{S} = \mathbf{A^{\Gamma\Gamma}} - \mathbf{A^{\Gamma I}}(\mathbf{A^{II}})^{-1}\mathbf{A^{I\Gamma}}$ and the final required Green's function is evaluated by using a cyclic reduction algorithm. In ref. [2] we formulate the parallel RGF algorithm.

PERFORMANCE ANALYSIS

In this section a performance analysis of our algorithm will be presented with respect to a rectangular billiard, as the one shown in Fig. 2. The efficiency F of the parallel algorithm will be the ratio of the cost of simulating the parallel algorithm on a single processor over the cost of the sequential algorithm, i.e.,

$$F = \frac{7NM^3}{p\left(7\frac{N}{p}M^3 + 5\,log_2(p)M^3\right)} \qquad (1)$$

The cost of the parallel algorithm is defined by the dominant numerical operations of matrix multiplications and inversions and is attributed to the algorithms of the parallel block Gaussian elimination and cyclic reduction. Fig. 3 shows the efficiency for the rectangular billiard of Fig. 2 discretized on a 400×250 lattice. To do the measurements we have kept the size of the lattice fixed and increase the number of processors. We observe that the measurements agree very well with the model of equation (1). At this point we would like to remark that the setup addressed here corresponds to a perfectly load balanced problem since the total numerical cost is distributed equally to each processor.

ACKNOWLEDGMENTS

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REFERENCES

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[2] P.S. Drouvelis, P. Schmelcher and P. Bastian, *Parallel implementation of the recursive Green's function method*, acc. f. publication to the Journal of Computational Physics, available from <*arXiv:cond-mat/0507415*>

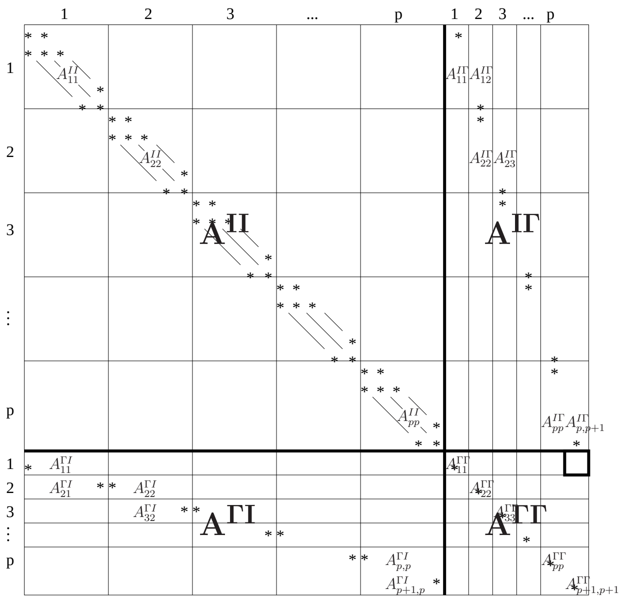

Fig. 1. Reordered matrix $\mathbf{A} = E\mathbf{I} - \mathbf{H_S} - \mathbf{\Sigma_R}(E) - \mathbf{\Sigma_L}(E)$ due to processor subdivision after row and column permutations.

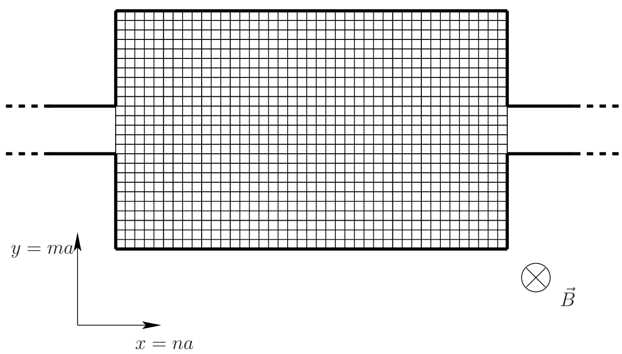

Fig. 2. Setup of a rectangular billiard attached to two reservoirs, discretized on a lattice with $n = 0, 1, \ldots, N-1$ slices of $m = 0, 1, \ldots, M-1$ sites each. The ratio of the two dimensions is $\frac{N}{M} = \frac{8}{5}$.

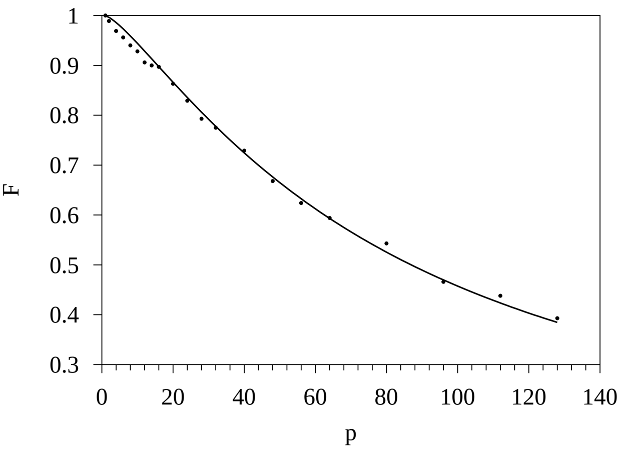

Fig. 3. Efficiency F as a function of the number p of processors. The dots correspond to the measured efficiency and the solid curve to the theoretical model employed by equation (1).