Wavelet-Based Adaptive Computations of the Excitonic Eigenstates of Disordered Semiconductor Quantum Wires

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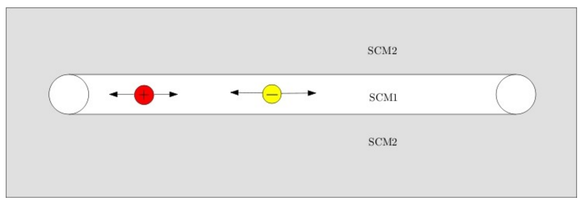
Quantum wire:



Model of a quantum wire; wire length *L*

Material SCM1
➡ Motion limited to 1-D

Roughness at the interface
➡ Disorder potential

Stationary Schrödinger equation:

$$E\,p(x_e,x_h) = (H_{kin} + H_{attr} + H_{dis})\,p(x_e,x_h) \quad (*)$$

Hamiltonian of two free particle: $H_{kin} = \frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial x_e^2} - \frac{\hbar^2}{2m_h}\frac{\partial^2}{\partial x_h^2}$

Electron-Hole attraction: $H_{attr} = \frac{-e^2}{4\pi\varepsilon_0\varepsilon_r(\min(|x_h - x_e|, |x_h - x_e| \pm L) + \gamma R)}$

Correlated Disorder: $H_{dis} = V_{dis,e}(x_e) + V_{dis,h}(x_h)$ with $V_{dis,e}(x_e) = \frac{m_h}{m_e}V_{dis,h}(x_h)$

Periodic boundary conditions

Stochastic influence:

Disorder modeled by step function: $V_{dis,e}(x_e) = \sum_{i=1}^{i=M} \mathrm{Ran}_{dis,e}(i)\mathbf{1}_{[(i-1)\frac{L}{M}, i\frac{L}{M}]}$

Assumption: Normally distributed stochastic influence: $\mathrm{Ran}_{dis,e}(i) \sim N(0,\sigma^2)$

Adaptive wavelet approach:

Based on the variational/weak formulation of (*)

Choosing a suitable wavelet basis

➡ **Well posed equivalent** reformulation on the sequence space ℓ_2 of square summable sequences

Using **adaptive** solution schemes

e.g. by T. Rohwedder, R. Schneider, A. Zeiser, Adv. Comp. Math. 34(1), 43-66 (2011)

Adaptivity: Employing degrees of freedom (dof) only where actually needed

➡ Using wavelet-based APPLY schemes of applying operators
e.g. by A. Cohen, W. Dahmen, R. DeVore, SIAM J. Math. Anal. 35(2), 279-303 (2003)

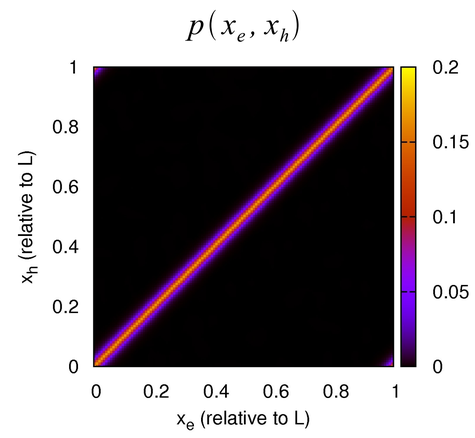
➡ Calculating on adaptive 'grids' depending on user-defined final accuracy

Optimal (computational) complexity

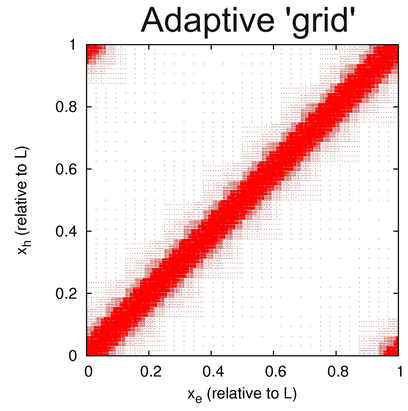
➡ Best possible work/accuracy balance

Numerical results (without disorder):

Adaptivity:



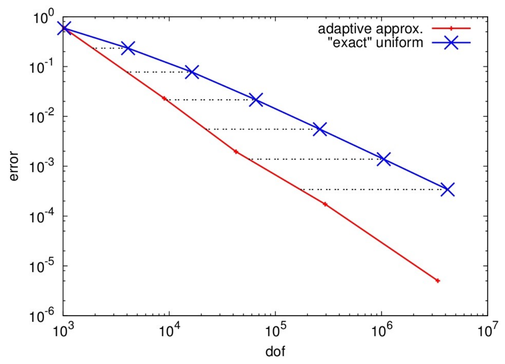
Contour-plot
L = 400nm



Distribution of degrees of freedom:
Each dot corresponds to a used wavelet

➡ Adaptive scheme resolves peak appropriately

Performance:

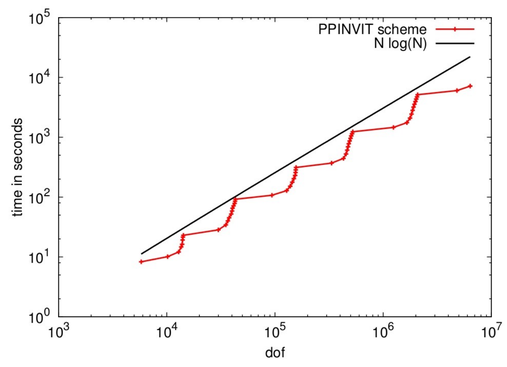


'Exact' eigenvalues on uniform grids
⬌ approximation on adaptive grid

Adaptive approximation much **more accurate** than best possible uniform approximation

➡ Much **less degrees of freedom** needed when using the adaptive wavelet method

Complexity:



Calculation time for approximation with N degrees of freedom

- Adaptive wavelet scheme requires sorting in APPLY

  ➡ complexity increases like $N\,log(N)$

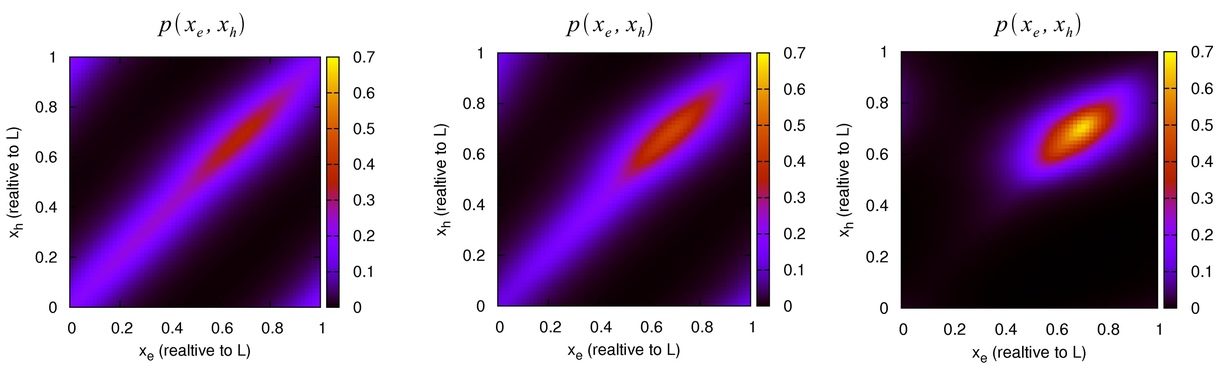
- Quasi-sorting avoids *log*-factor

Detailed information:

• Chr. Mollet, A. Kunoth, and T. Meier
Excitonic Eigenstates of Disordered Semiconductor Quantum Wires: *Adaptive Wavelet Computation of Eigenvalues for the Electron-Hole Schrödinger Equation*, IMA Preprint #2381, University of Minnesota, September 2011, submitted for publication, revised, April 2012, to appear in: Communications in Computational Physics (CiCP).

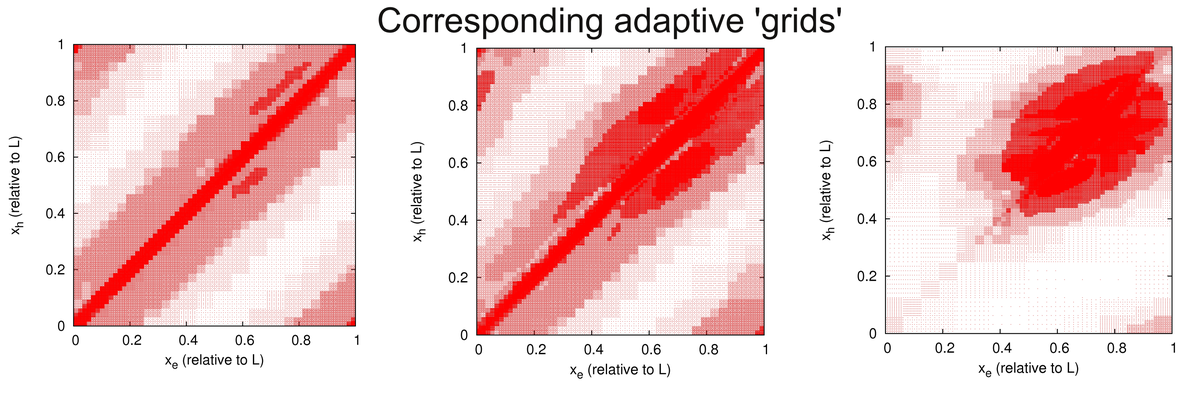
• H. Haug and S.W. Koch.
Quantum Theory of the Optical and Electronic Properties of Semiconductors. World Scientific Publishing, fourth edition, 2004.

Further results (with disorder):



L = 100nm, $\sigma = 0.015\,meV$ | *L = 100nm*, $\sigma = 0.03\,meV$ | *L = 100nm*, $\sigma = 0.14\,meV$

Corresponding adaptive 'grids'



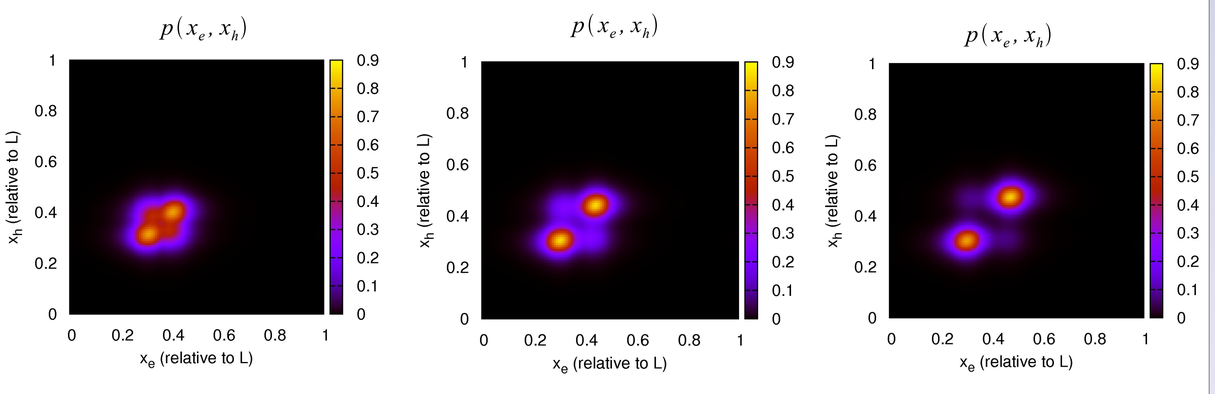
➡ Stronger disorder (controlled by variance σ^2) ➡ More localized peak

Adaptive grids well adapted to localization

Detailed information: T. Meier, P. Thomas, and S.W. Koch. *Coherent Semiconductor Optics*. Springer, 2007.

Further examples:

Coupled quantum dots:



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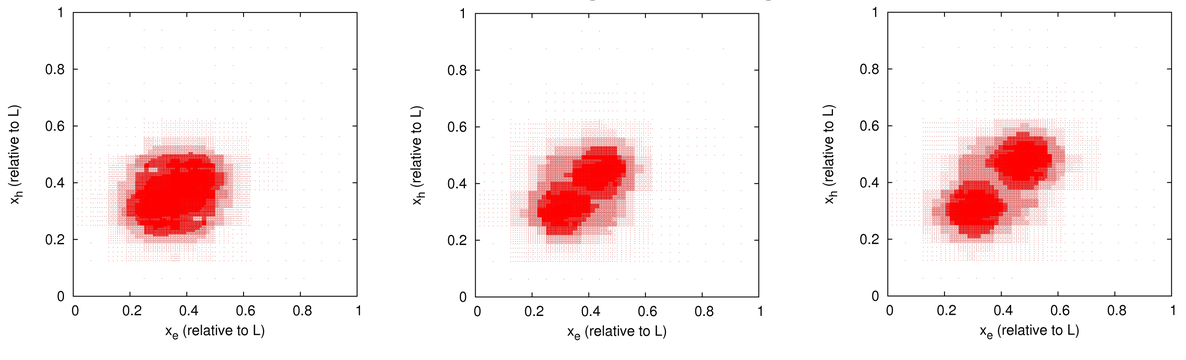

➡ Optimal adaptation of adaptive grids