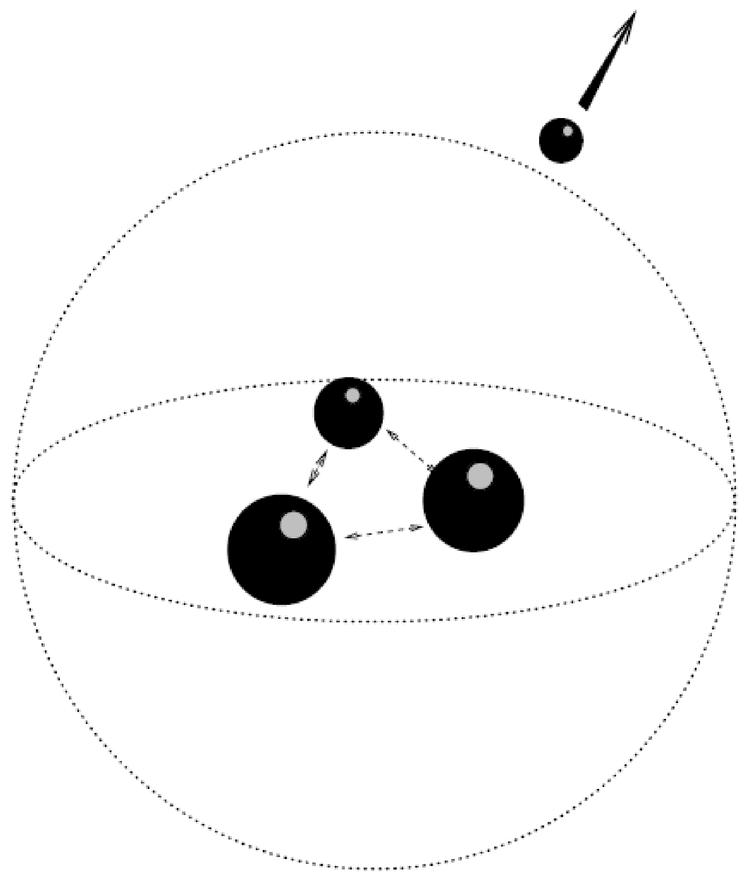
To throw away some particles – and yet keep the rest



Sølve Selstø , Oslo and Akershurs University College of Applied Sciences, Norway

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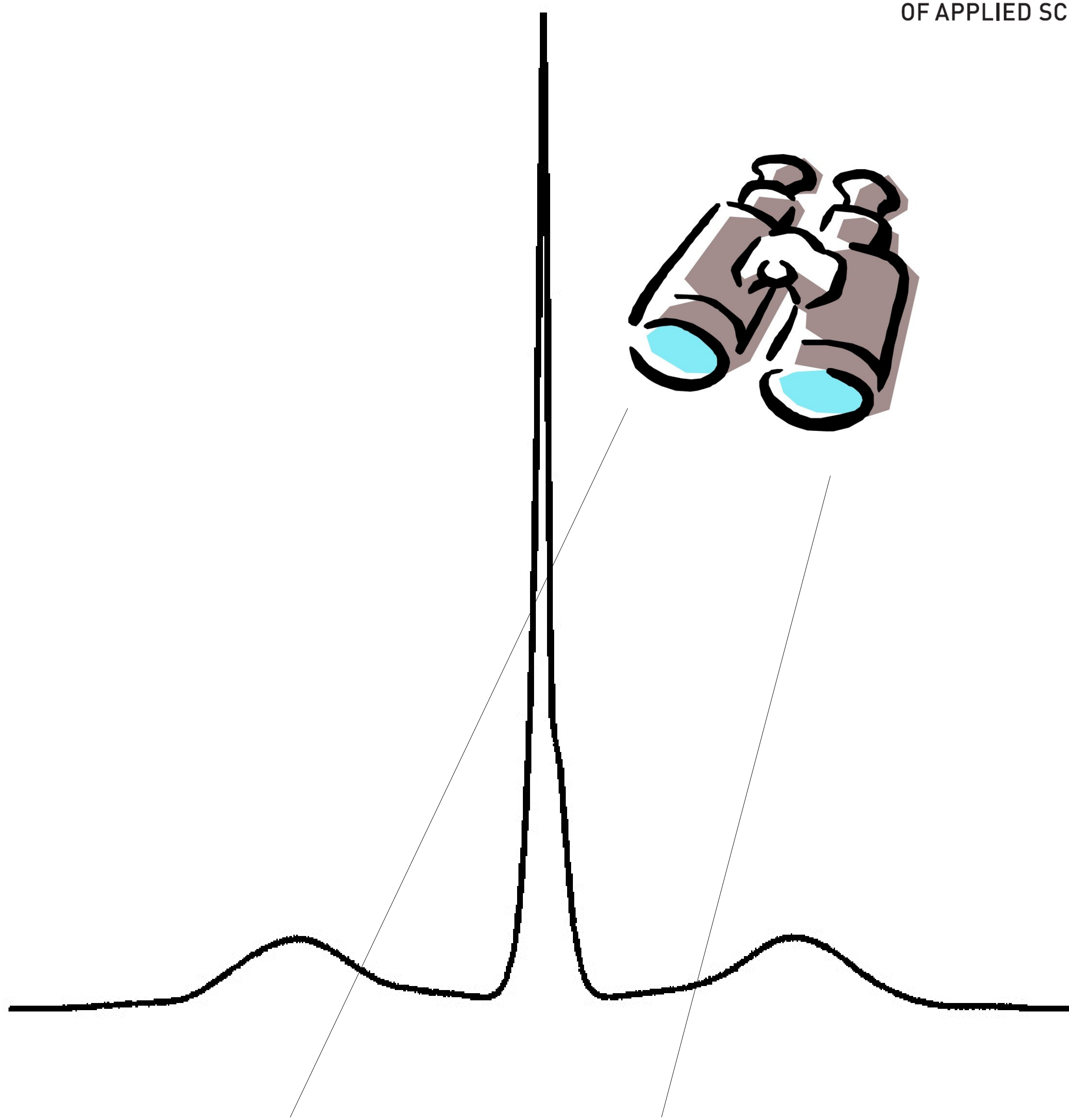
Suppose we are only interested in the wave function in a limited region



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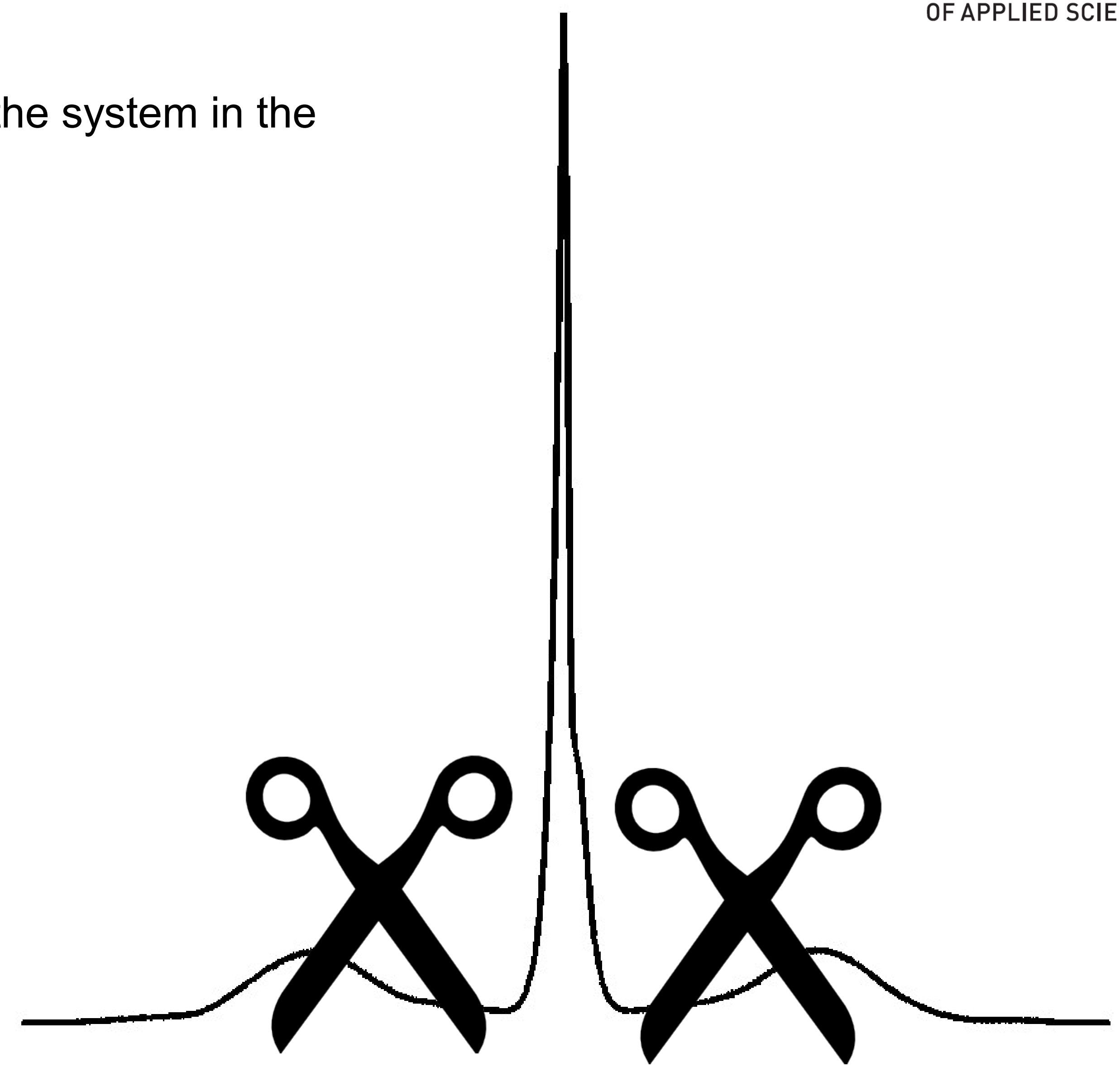
Suppose we are only interested in the wave function in a limited region

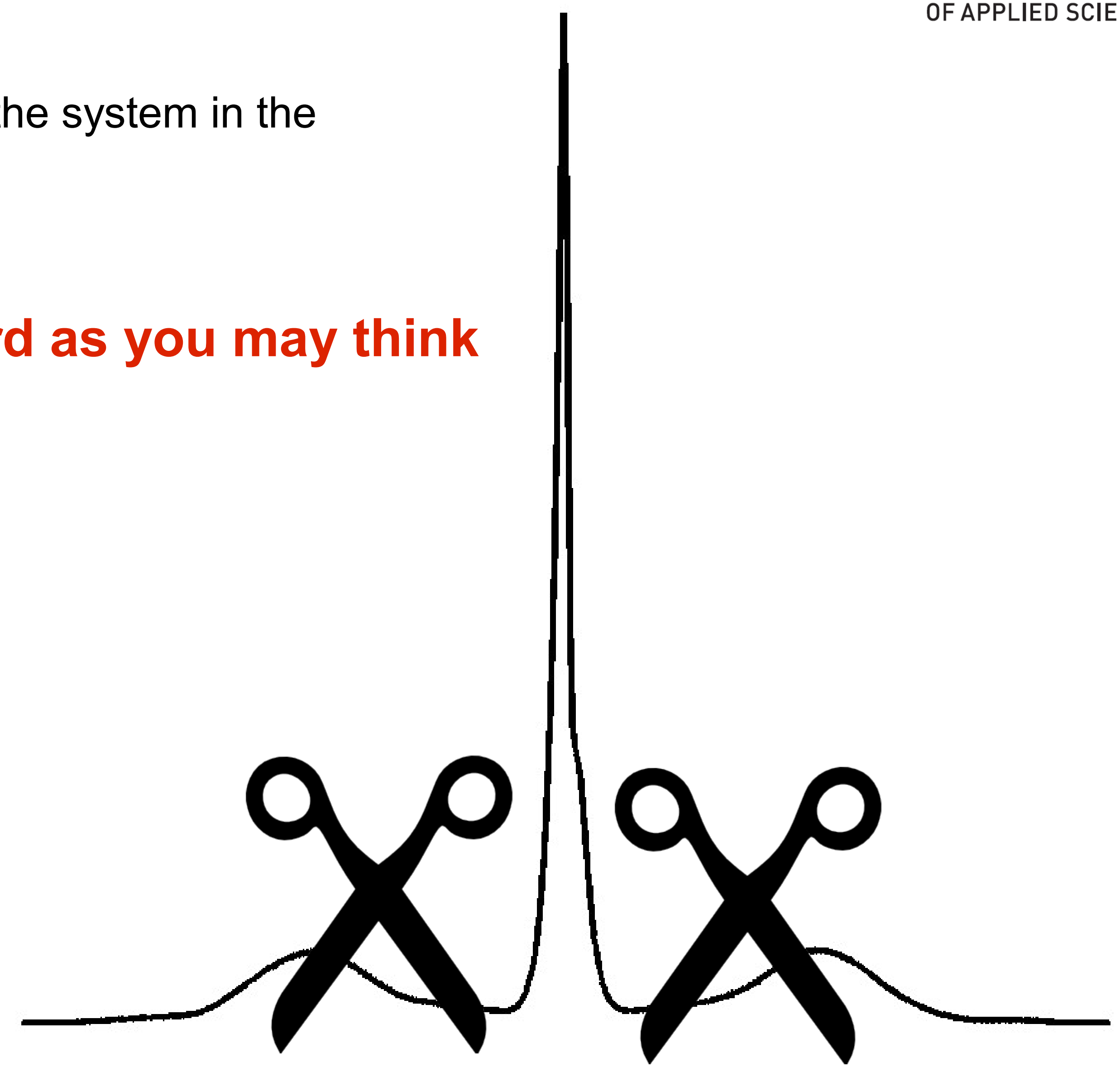
Remove information about the system in the asymptotic region



Suppose we are only interested in the wave function in a limited region

Remove information about the system in the asymptotic region

Not as straightforward as you may think



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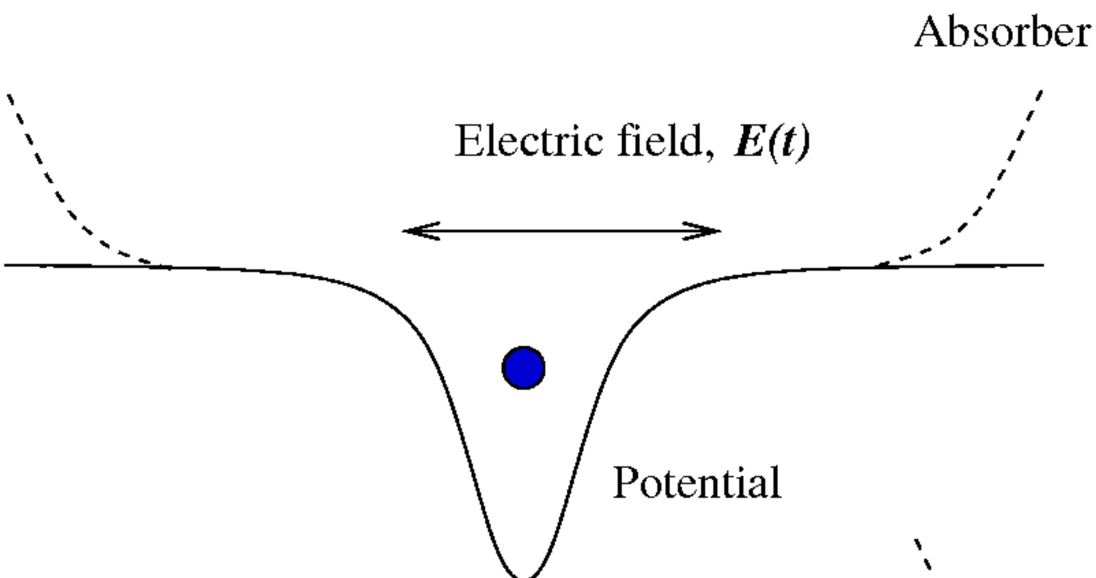
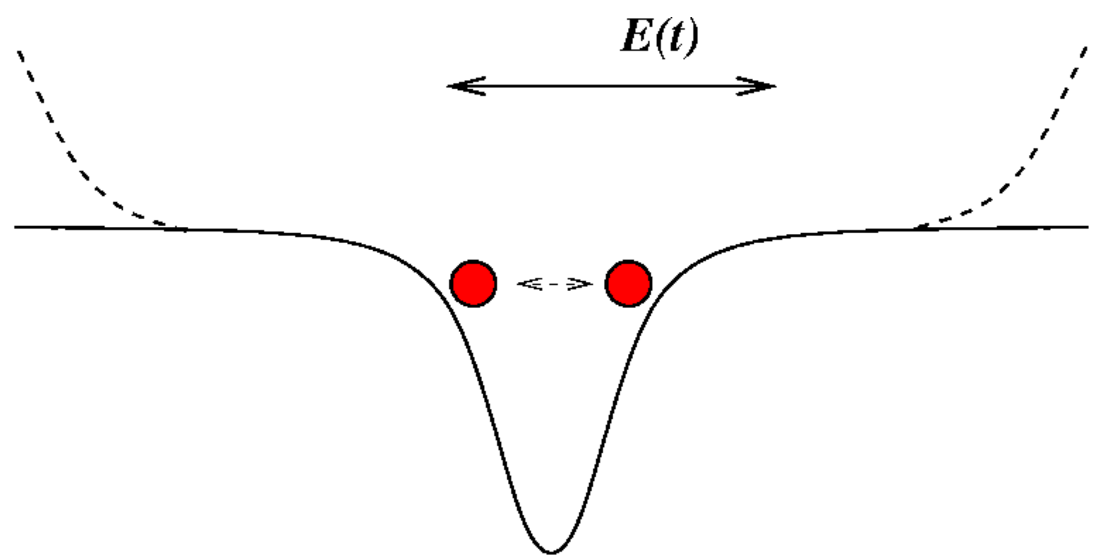
One particle



Two particles



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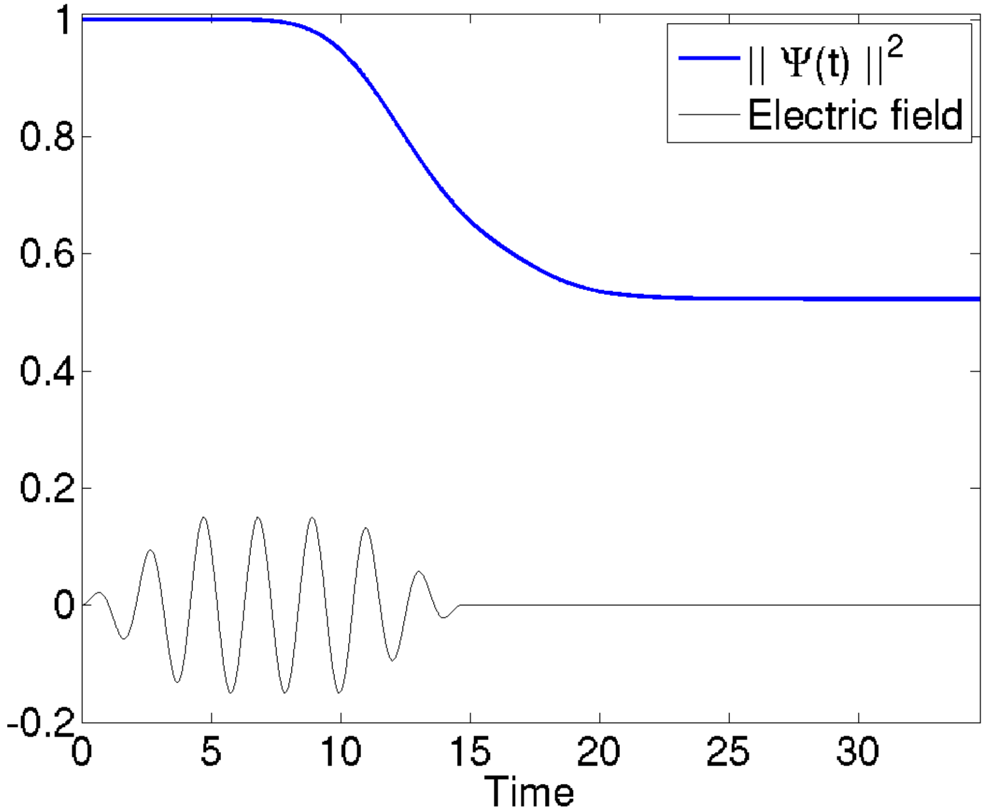
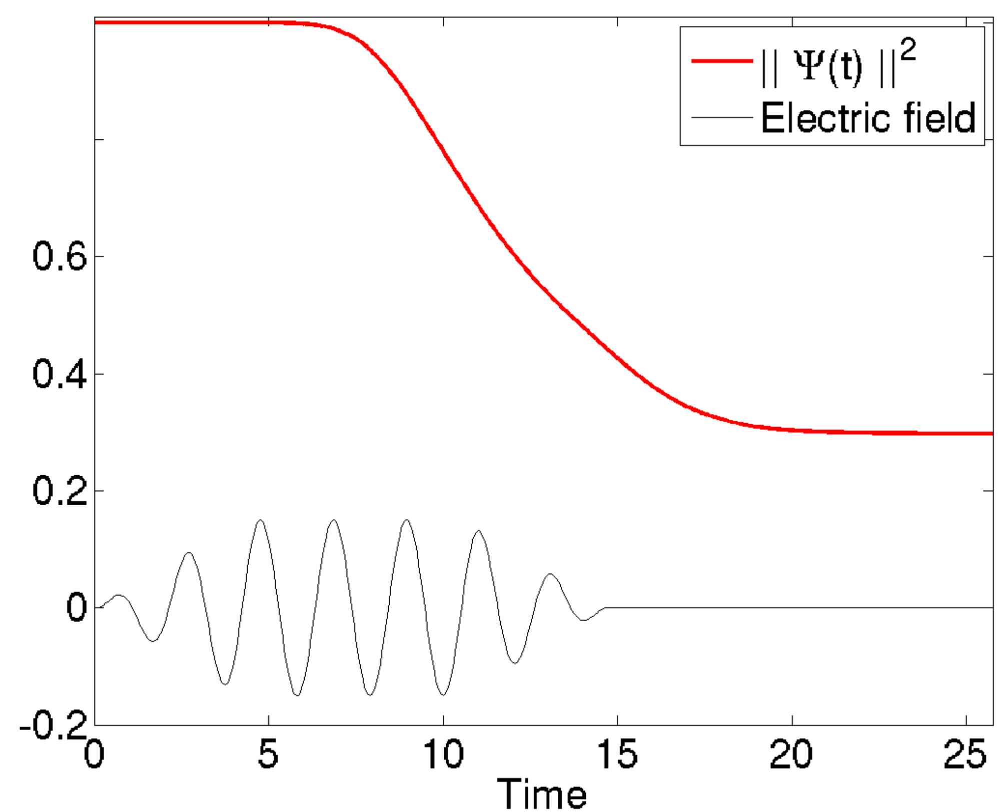
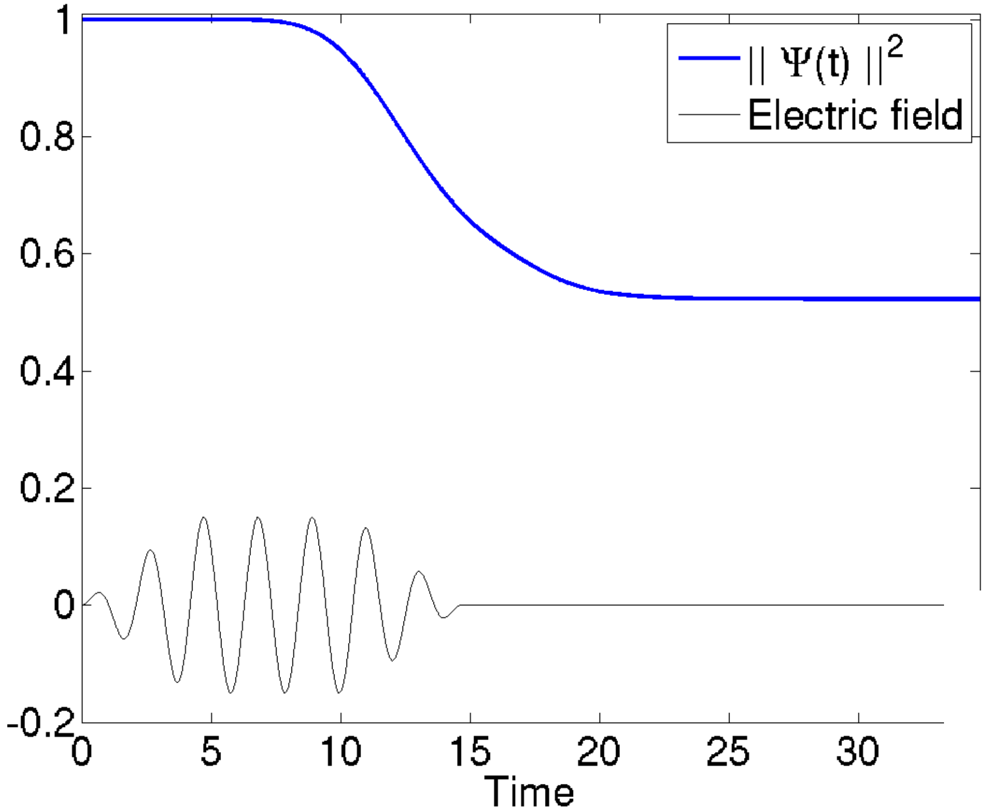
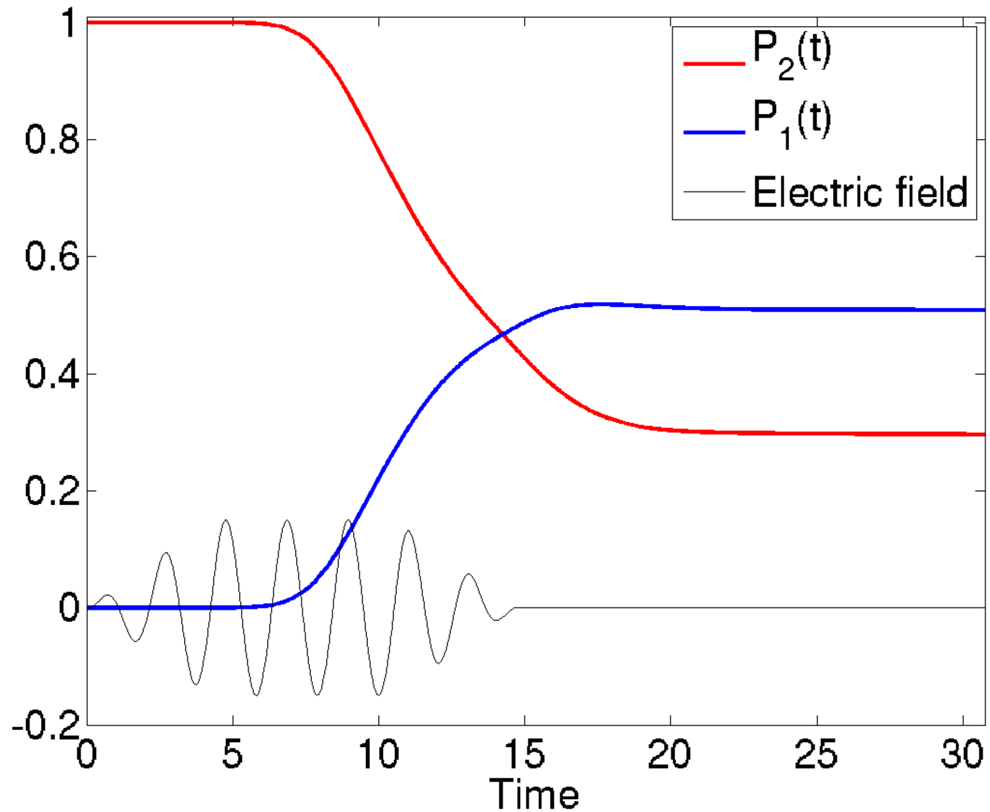






Aim:



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The time-dependent Schrödinger equation – with a complex absorbing potential (CAP):

$$i\hbar\dot{\Psi} = \left(\hat{H} - i\hat{\Gamma}\right)\Psi$$

The corresponding von Neumann equation:

$$i\hbar\dot{\rho} = \left[\hat{H}, \rho\right] - i\left\{\hat{\Gamma}, \rho\right\}$$

If one or more particles are fully absorbed:

$$|\Psi(t)|^2 = \langle\Psi_0|\, e^{-2\hat{\Gamma}t/\hbar}\, |\Psi_0\rangle \to 0$$

Absorption is a Markovian process

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Any Markovian process which preserves trace and positivity:

$$i\hbar\dot{\rho} = \left[\hat{H}, \rho\right] - i\sum_{k,l}\gamma_{k,l}\left(\left\{A_k^\dagger A_l, \rho\right\} + 2A_l\rho A_k^\dagger\right)$$

-G. Lindblad, Commun. Math. Phys. ***48****, 119 (1976)*
-V. Gorini, A. Kossakowski and E. Sudarshan, J. Math. Phys. ***17****, 821–5 (1976)*

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$$i\hbar\dot{\rho} = \left[\hat{H}, \rho\right] - i \left\{ \hat{\Gamma}, \rho \right\}$$

$$\hat{\Gamma} = \sum_{k,l} \gamma_{k,l} A_k^\dagger A_l$$

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Second quantizatoin (grid):

$$\hat{\Gamma} = \sum_n \Gamma(x_n) c_n^\dagger c_n$$

n-particle sub-system:

$$i\hbar \dot{\rho}_n = [\hat{H}, \rho_n] - i\{\hat{\Gamma}, \rho_n\} + 2i \sum_n \Gamma(x_n) c_n \rho_{n+1} c_n^\dagger$$

*-S. S. and S. Kvaal, J. Phys. B **43**, 065004 (2010)*

*-P. Caban et al., Phys. Rev. A **72**, 032106 (2005)*
*-R. Bertlmann et al., Phys. Rev. A **73**, 054101 (2006)*
*-U. Harbola et al., Phys. Rev. B **78**, 235309 (2006)*

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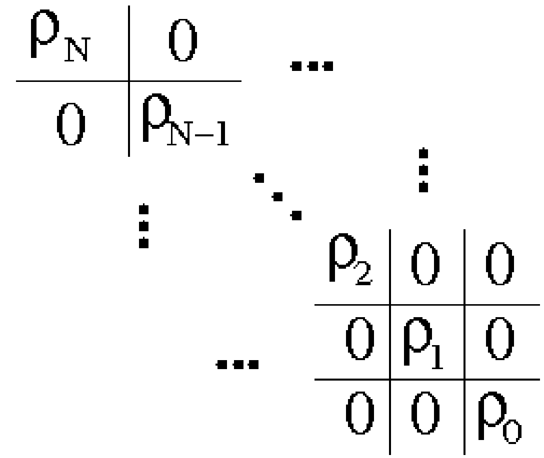
$$\hat{\Gamma} = \sum_n \Gamma(x_n) c_n^\dagger c_n$$



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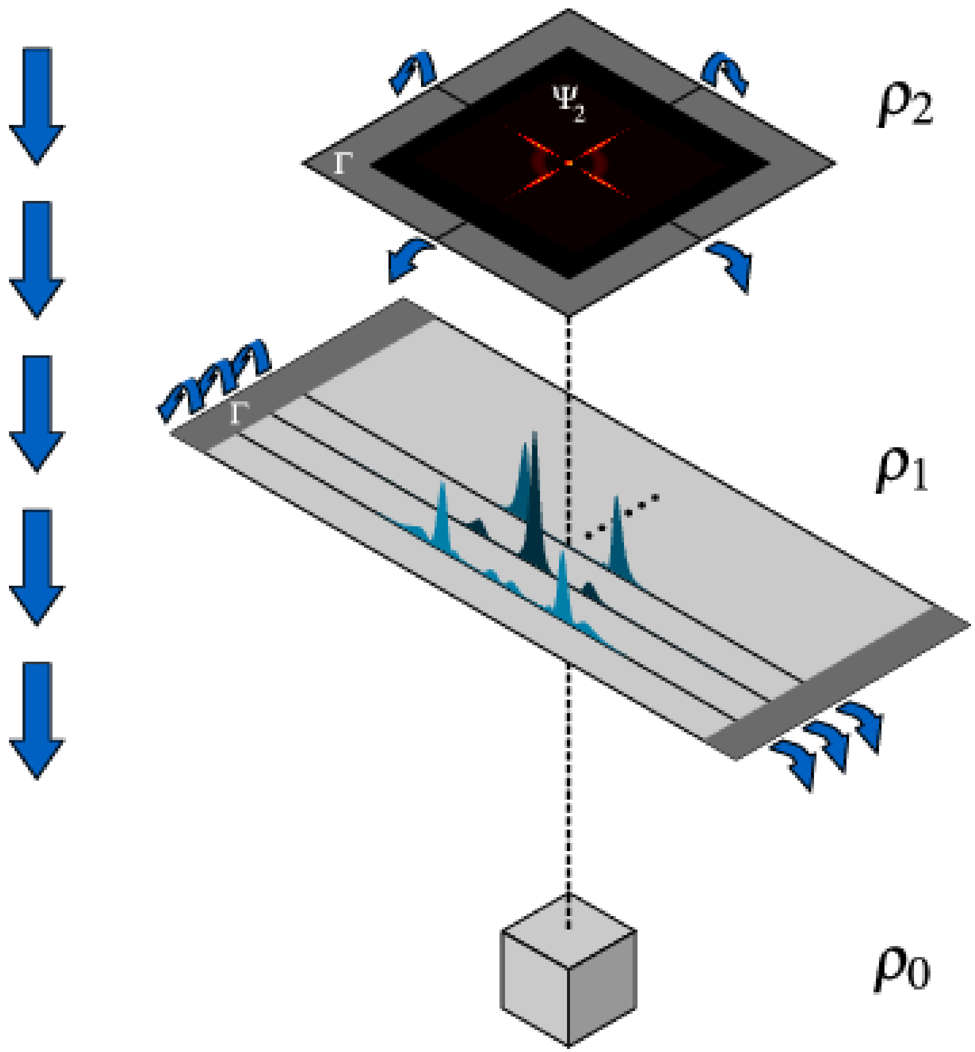
Unitary evolution

Absorption

Source term

$$\mathrm{Tr}\rho = \sum_{n=0}^{N} \mathrm{Tr}\rho_n = 1, \quad \forall t$$

Application:
Two-photon non-sequential double ionization of helium (1D model)



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Ionization probabilities via the Lindblad equation

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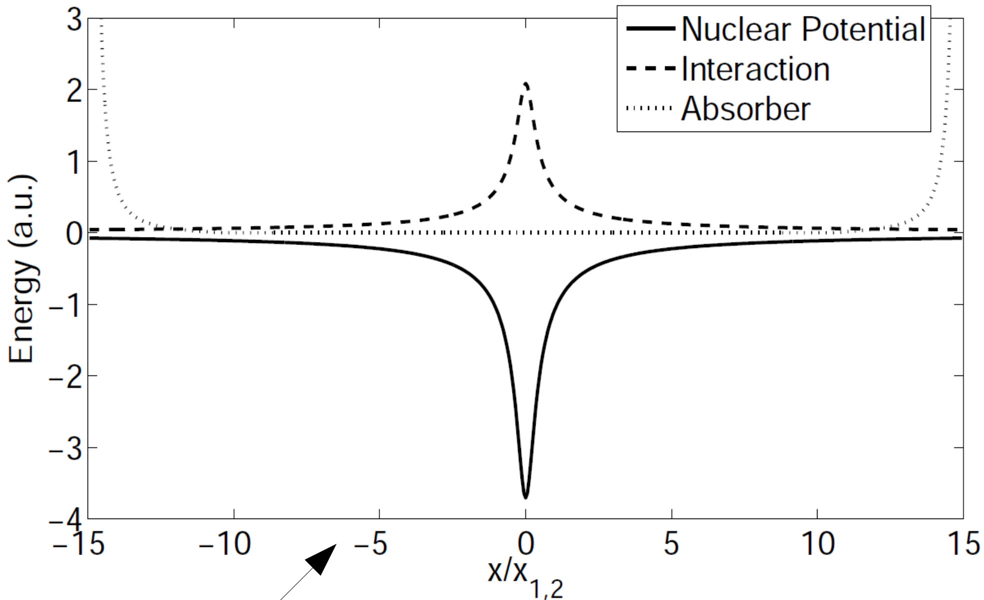
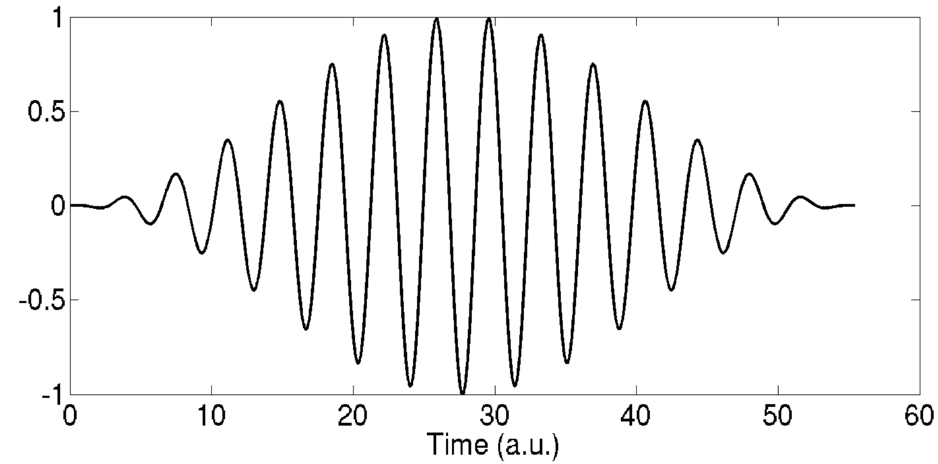
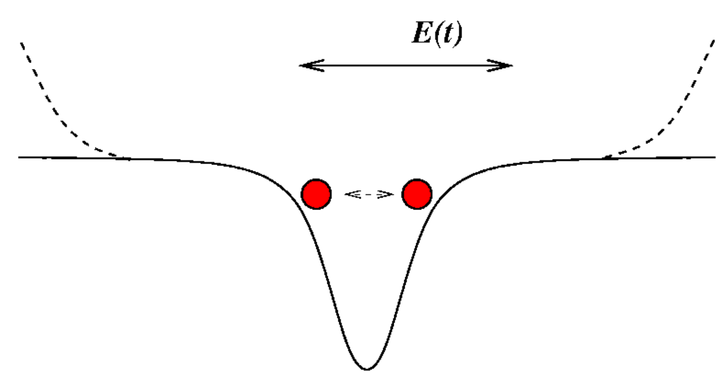


$$E(t) = E_0 \sin^2\left(\frac{\pi t}{T}\right)\sin(\omega t + \varphi)$$



$$V_{\mathrm{Nucl}}(x) = -\frac{eZ_{\mathrm{Nucl}}}{\sqrt{x^2+\delta^2}}$$

$$V_{\mathrm{Int}}(x_{1,2}) = \frac{eZ_{\mathrm{Int}}}{\sqrt{x_{1,2}^2+\delta^2}}, \quad x_{1,2} \equiv |x_1 - x_2|$$



Absorber, $\Gamma(x)$: Manolopoulos-type,
D. E. Manolopoulos, J. Chem. Phys. ***117****, 9552 (2002)*

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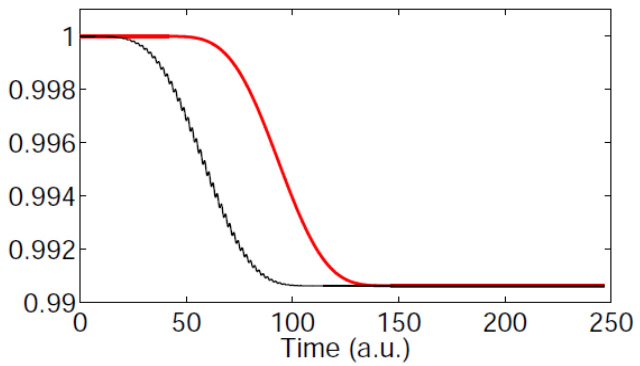
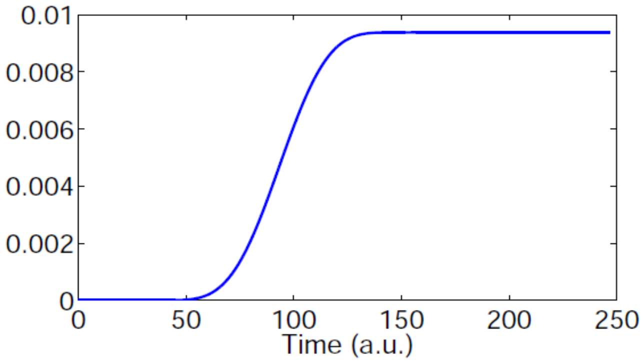
$$
\begin{aligned}
i\hbar\dot{\Psi}_2 &= (\hat{H} - i\hat{\Gamma})\Psi_2 \\
i\hbar\dot{\rho}_1 &= [h, \rho_1] - i\{\Gamma, \rho_1\} + 2i\mathcal{S}[\Psi_2] \\
\hbar\dot{\rho}_0 &= 2\sum_n \Gamma(x_n) c_n \rho_1 c_n^\dagger
\end{aligned}
$$

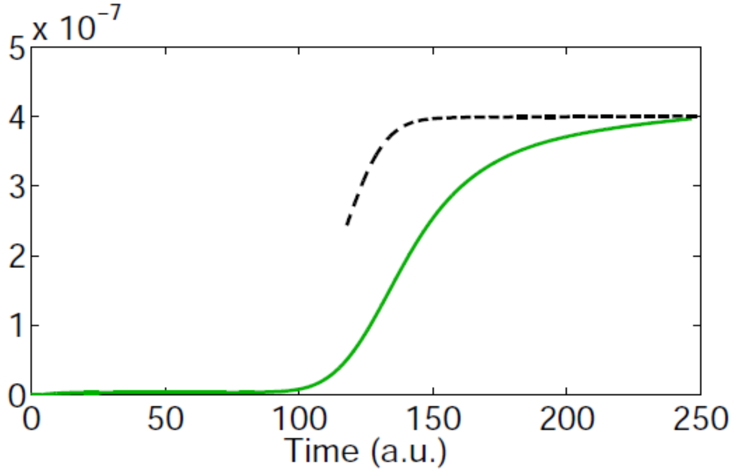
$$
\mathcal{S}[\Psi_2] = \sum_n \Gamma(x_n) c_n |\Psi_2\rangle\langle\Psi_2| c_n^\dagger
$$



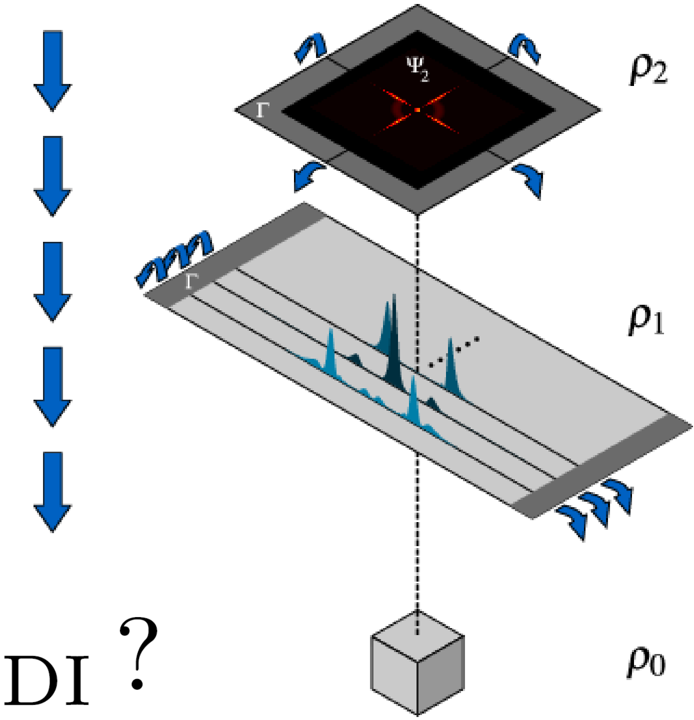
$$p_2(t) = |\Psi_2|$$



$$p_1(t) = \mathrm{Tr}(\rho_1)$$



$$p_0(t) \rightarrow p_{\mathrm{DI}}\,?$$



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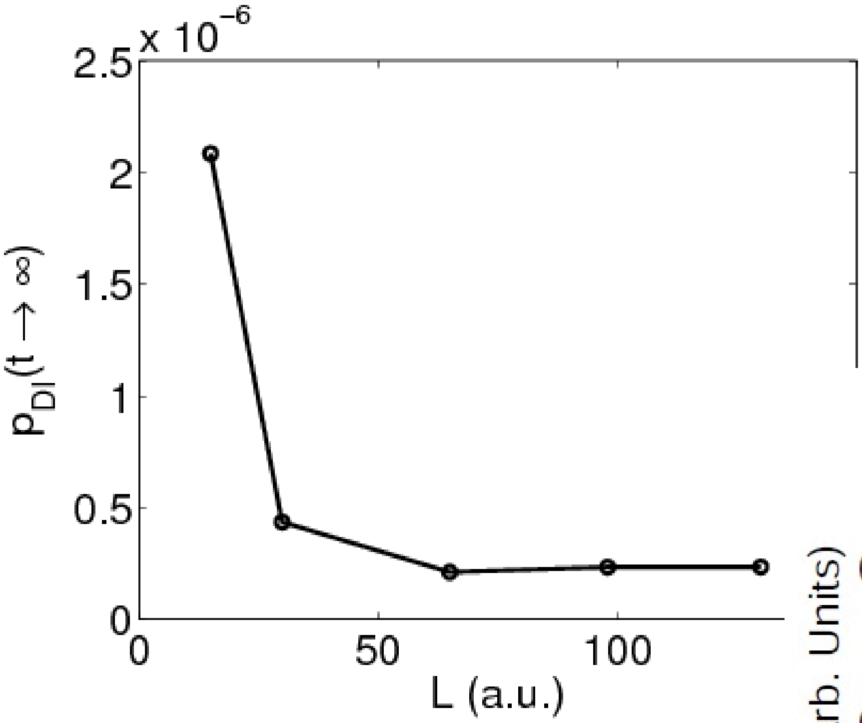
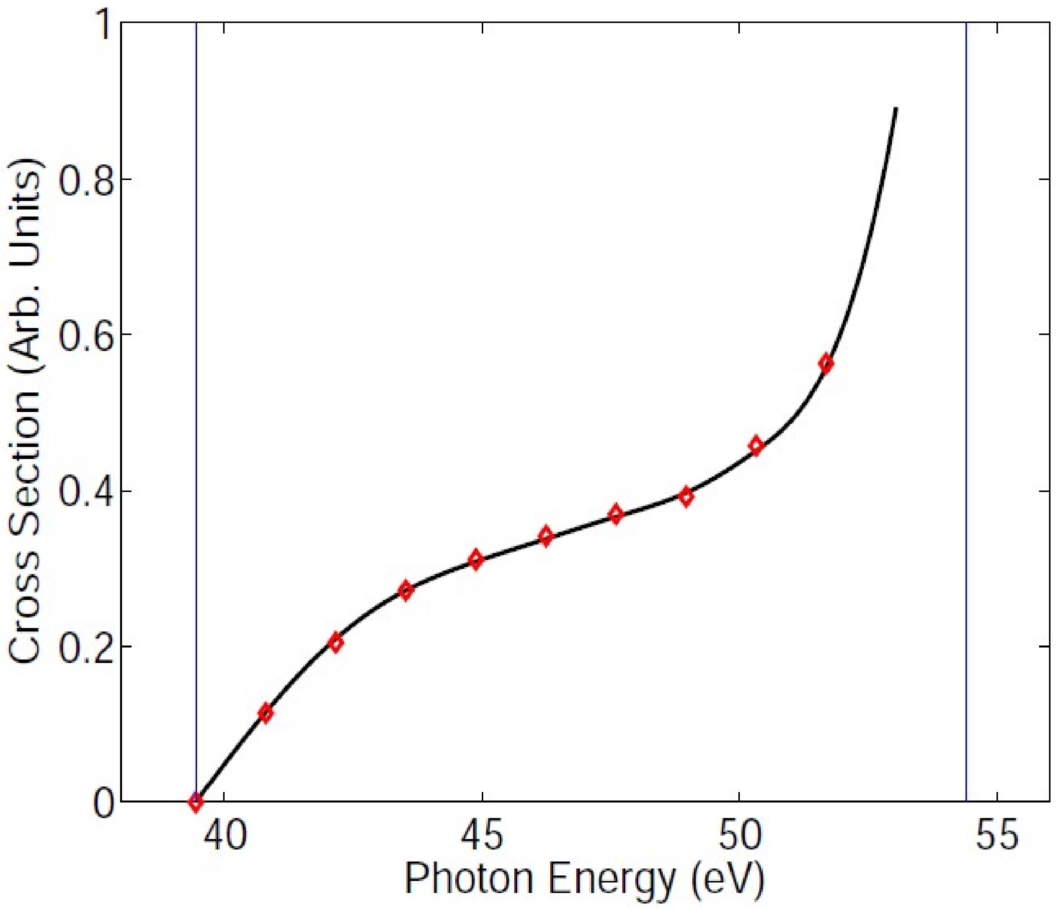
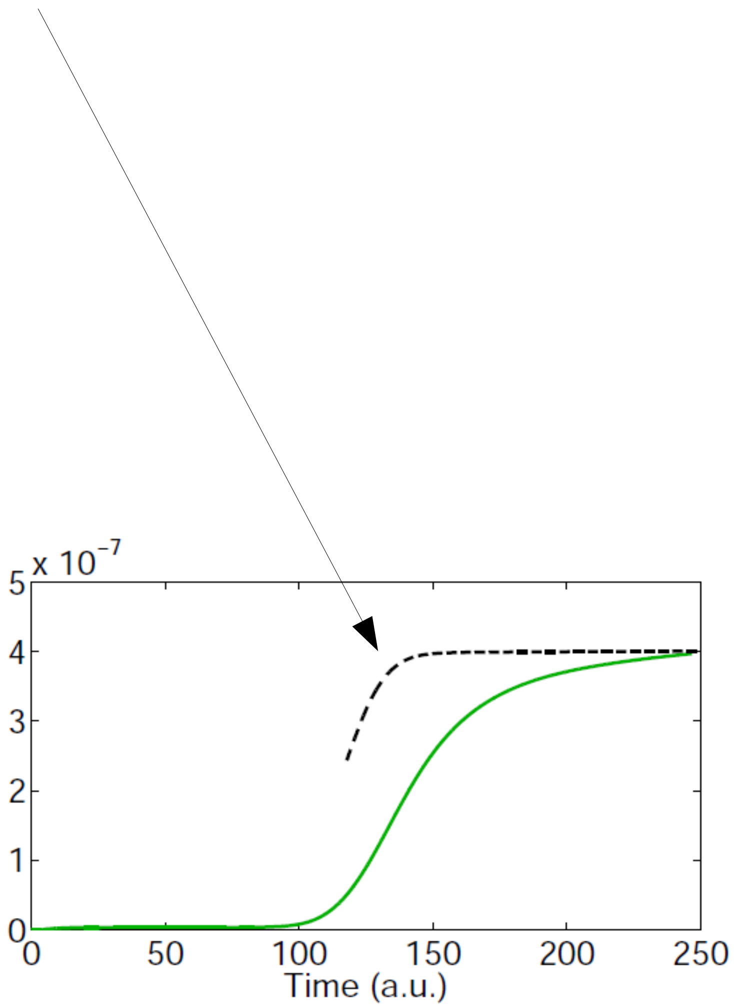
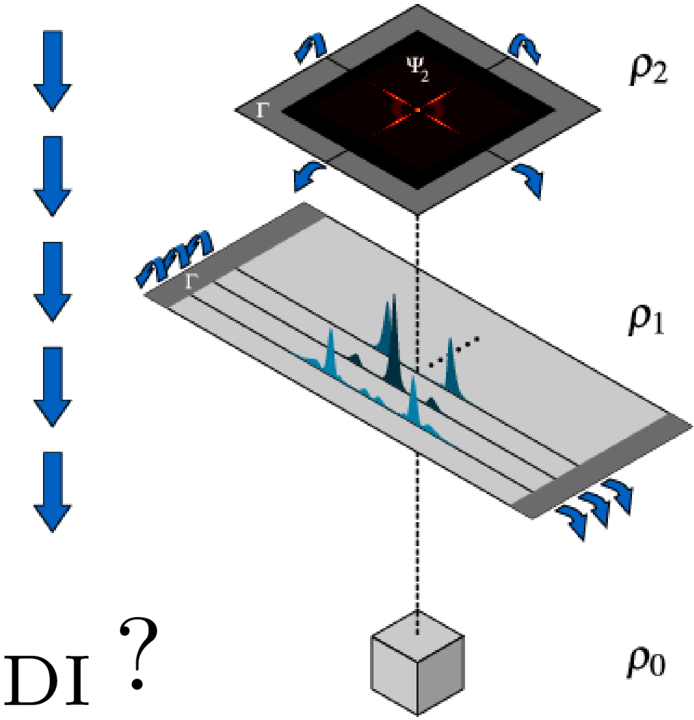
Does it work?


x 10^−6
2.5
2
1.5
1
0.5
0
$p_{DI}(t \to \infty)$
0
50
100
L (a.u.)


1
0.8
0.6
0.4
0.2
0
Cross Section (Arb. Units)
40
45
50
55
Photon Energy (eV)

Analyse source term «on the fly» for $t>T$





$$p_0(t) \rightarrow p_{\mathrm{DI}}\,?$$

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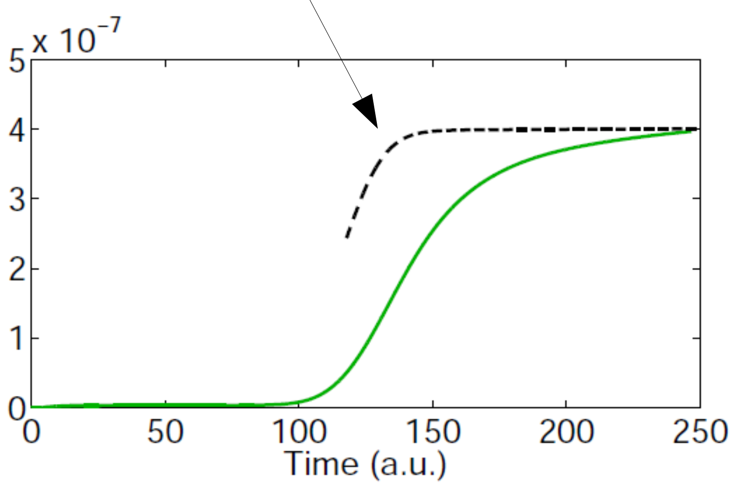
Analyse source term «on the fly» for $t > T$

$$p_{\mathrm{DI}}(t = T) = p_0(T) + \mathrm{Tr}(P_{\mathrm{unbound}} \rho_1)$$

$$\dot{p}_{\mathrm{DI}}(t > T) = \frac{2}{\hbar} \mathrm{Tr}(P_{\mathrm{unbound}} \mathcal{S}[\Psi_2])$$



$$p_0(t) \rightarrow p_{\mathrm{DI}} \, ?$$

Partial widths?

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