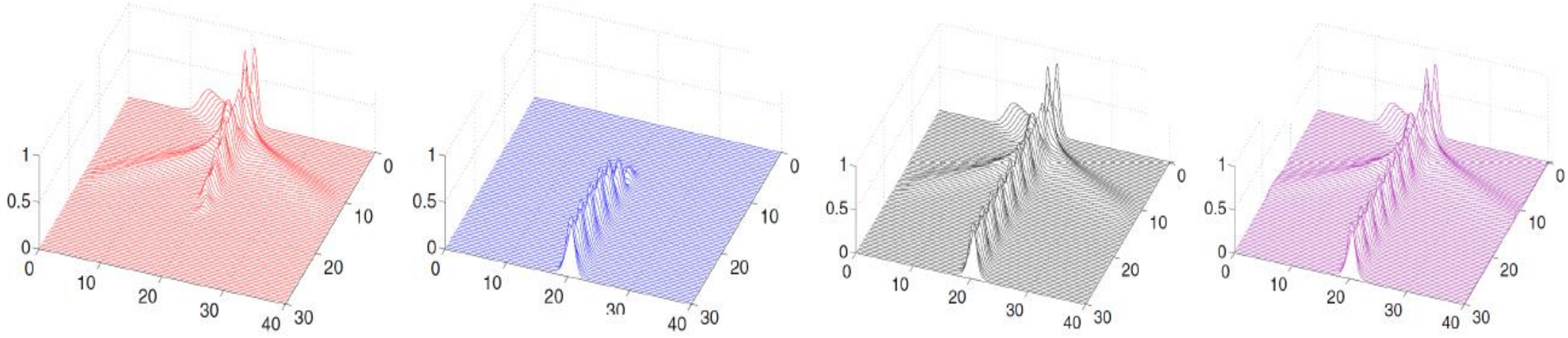

Absorbers as numerical tools – and measuring devices

OSLO METROPOLITAN UNIVERSITY
STORBYUNIVERSITETET

Sølve Selstø
Bad Honnef
December 19th

Background:

Atomic physics, light-matter interaction

Numerical simulations of dynamical unbound quantum systems

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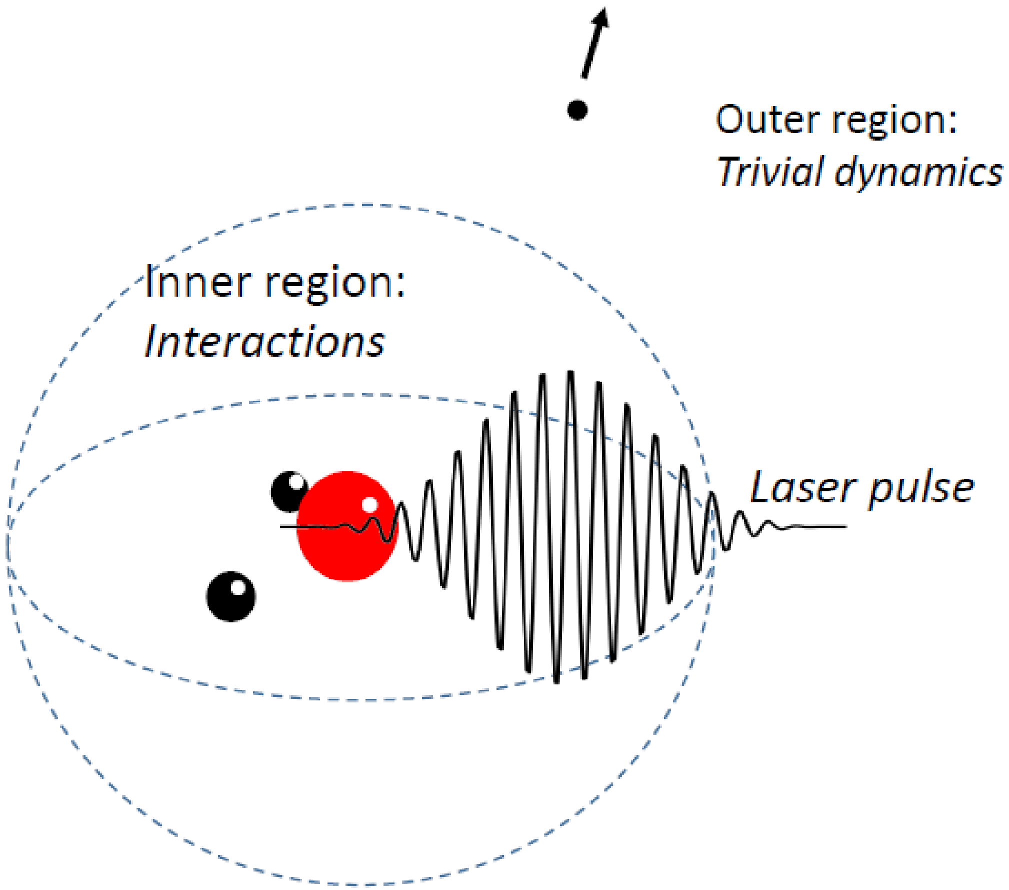

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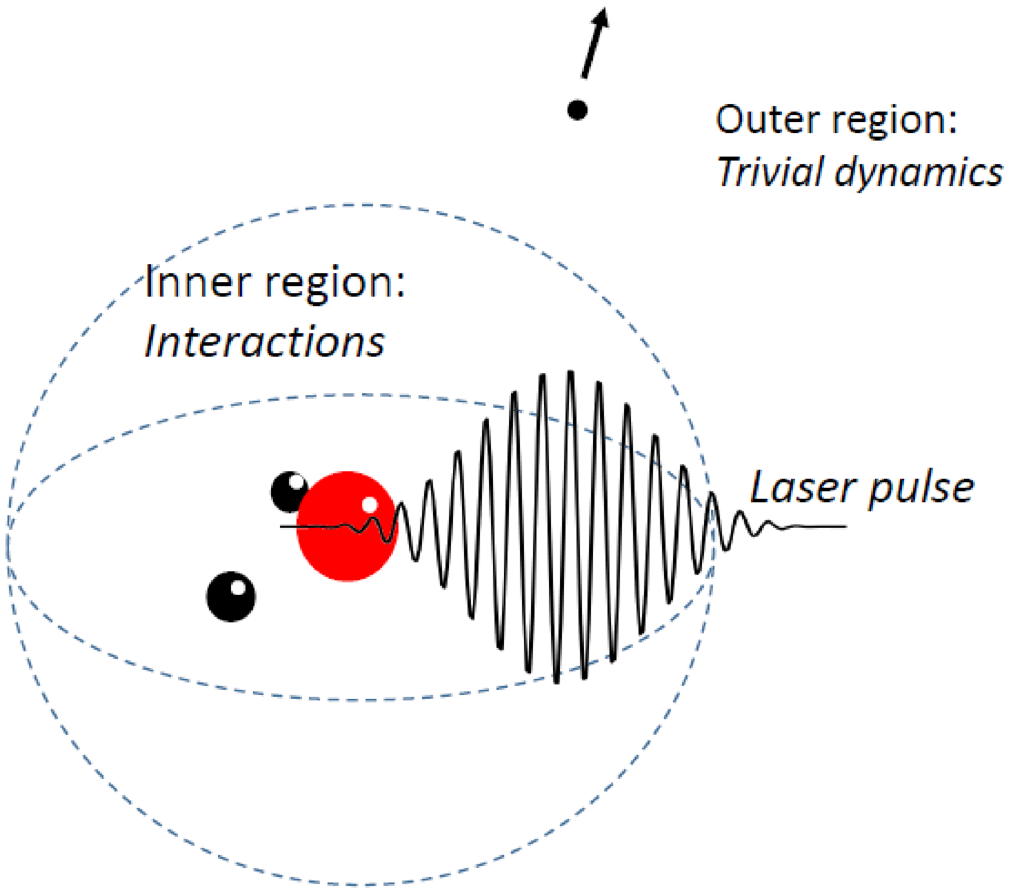

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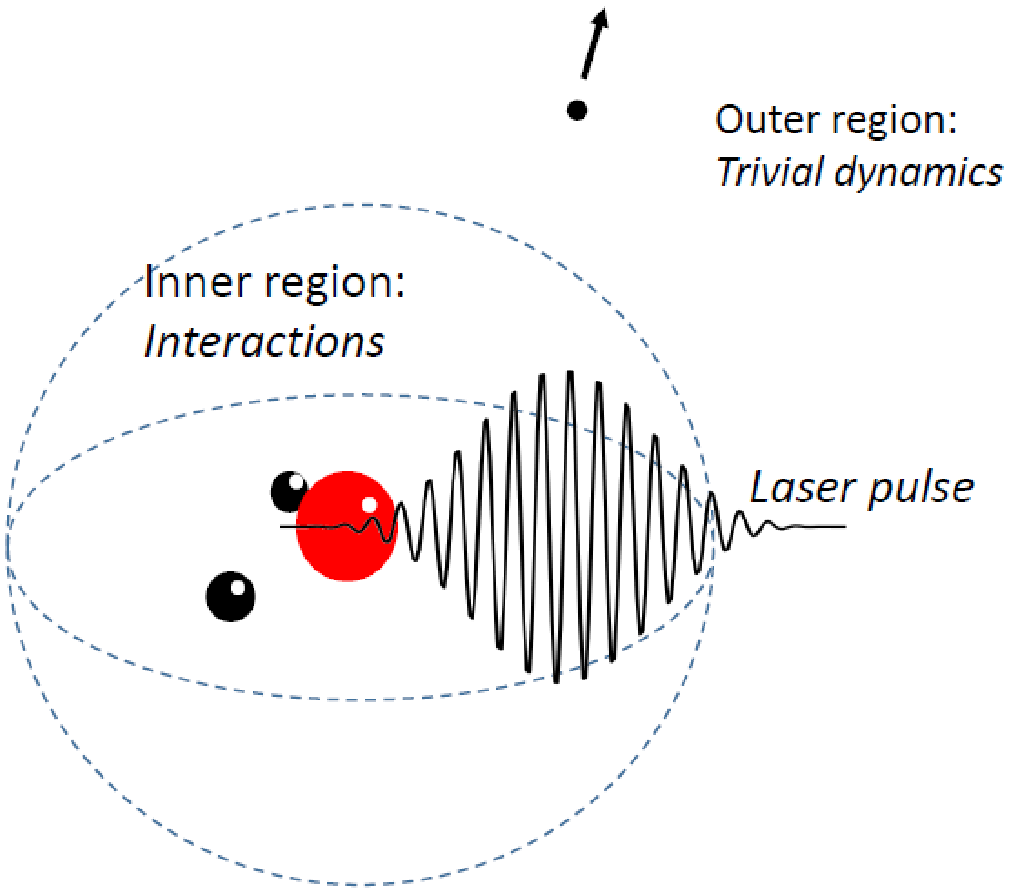
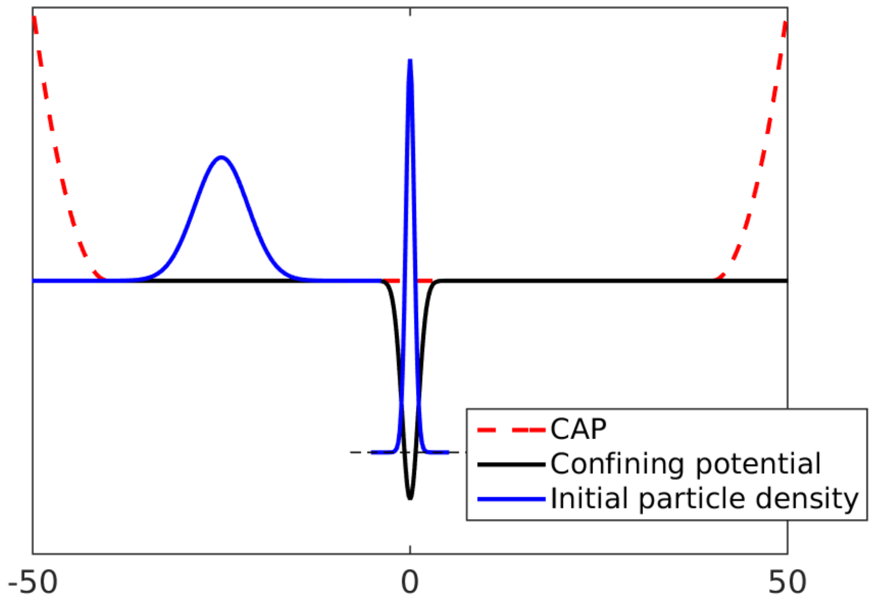
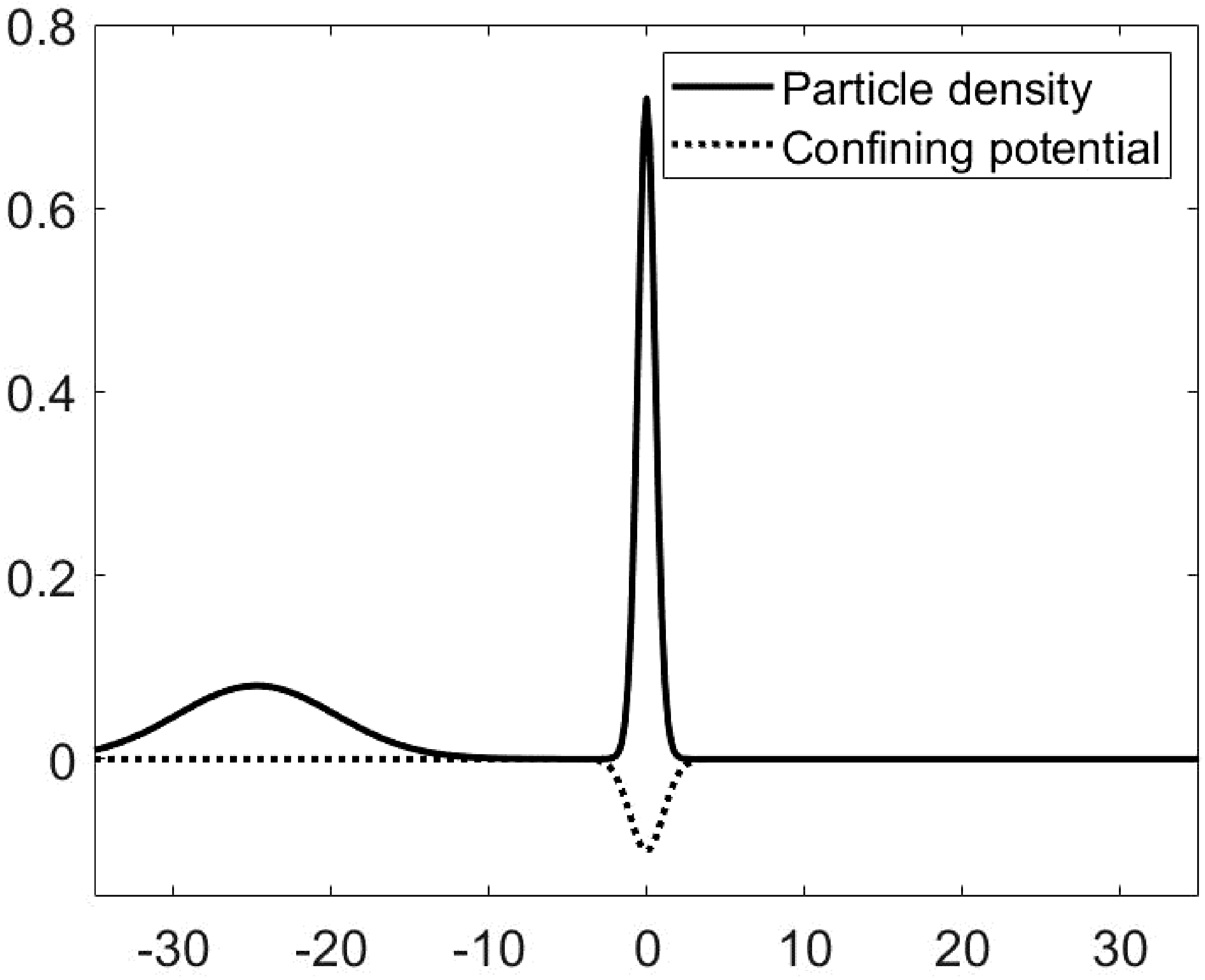
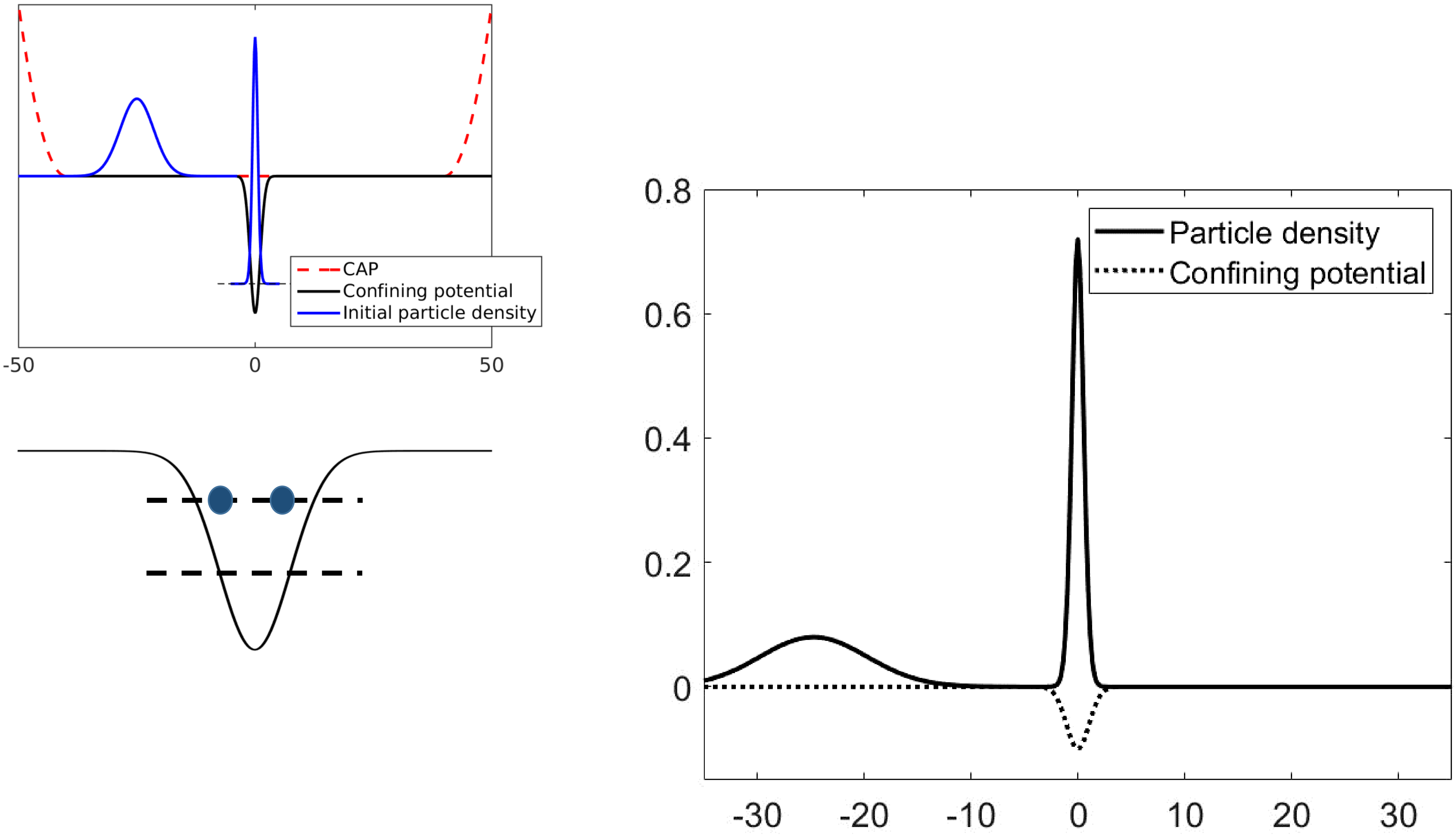


Another problem:

The curse of dimensionality


CAP
Confining potential
Initial particle density
-50
0
50


Particle density
Confining potential
0.8
0.6
0.4
0.2
0
-30
-20
-10
0
10
20
30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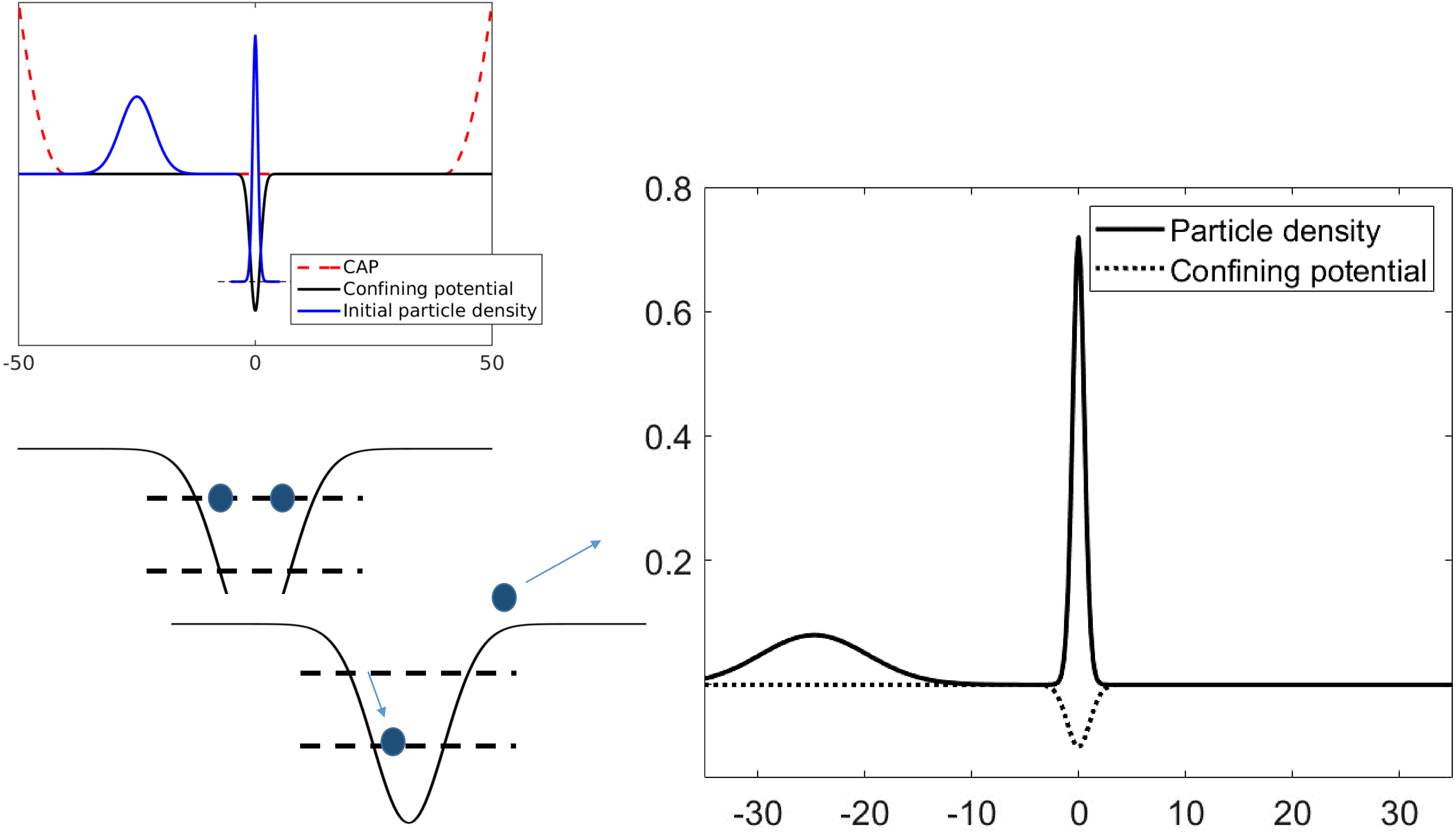

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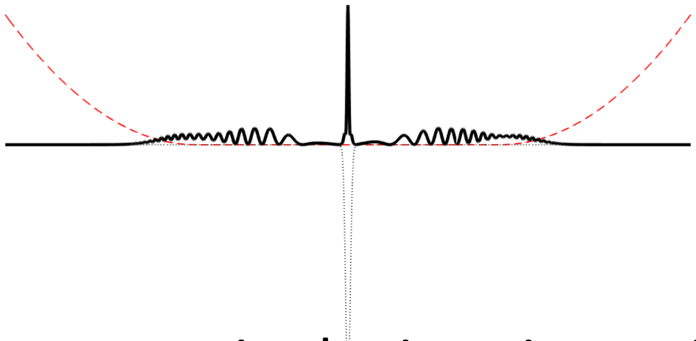
Absorber:

Augment the Hamiltonian with some (artificial) non-Hermitian term

$$H \rightarrow H_{eff} = H - i\,\hat{\Gamma}$$

Γ:



- Local potential larger than zero close to the boundary, zero in the interior region
- Exterior complex scaling/Perfectly matched layers
- Etc.

$$r \rightarrow \begin{cases} r, & r < r_0 \\ e^{i\theta}(r - r_o), & r \geq r_0 \end{cases}$$

Works fine for one-particle systems, not for any other system

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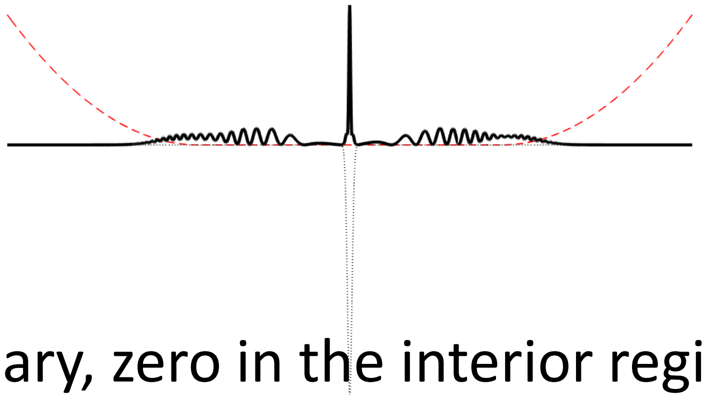

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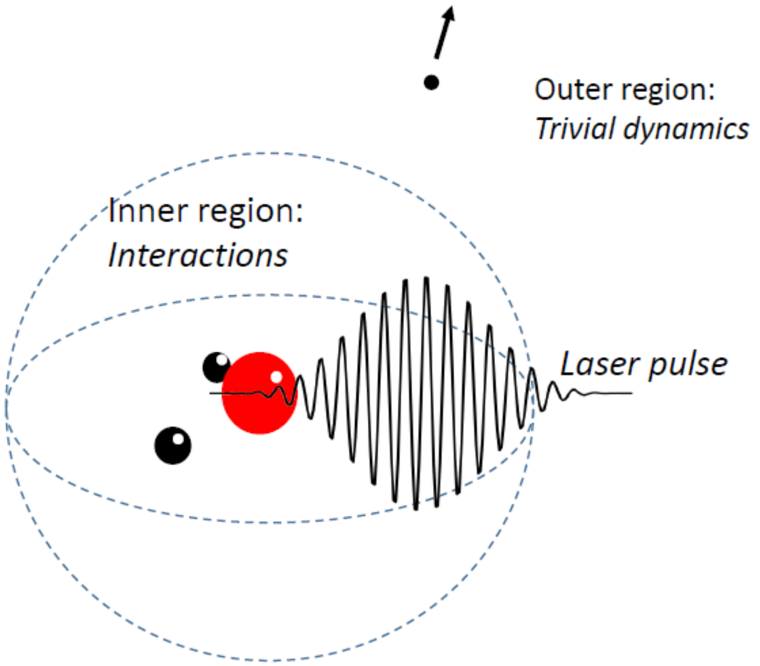
N-particle wave function Ψ:
Normalized to the probability of having *N* particles on the grid
If one or more particles are absorbed, this probability is zero – and so is Ψ

Is there no way we can retain the remainder?



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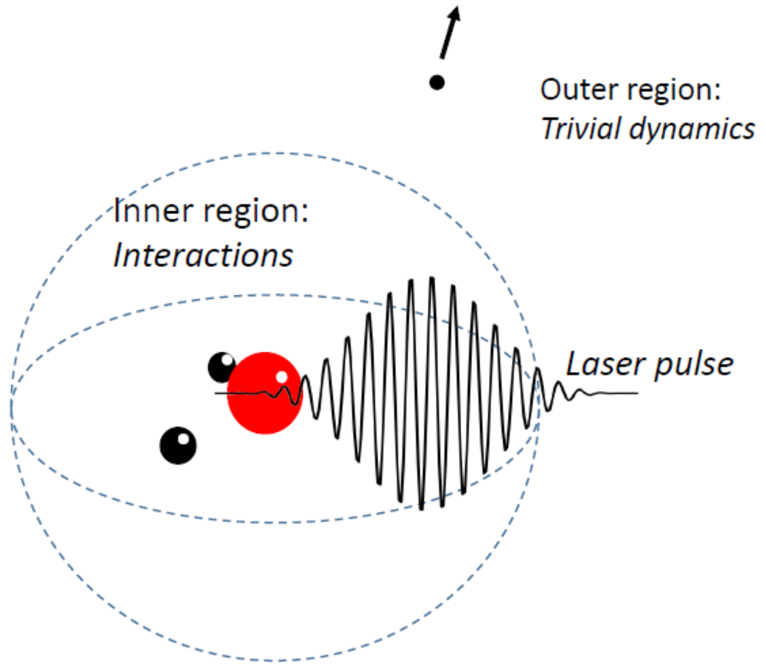
Using the Schrödinger equation:

NO



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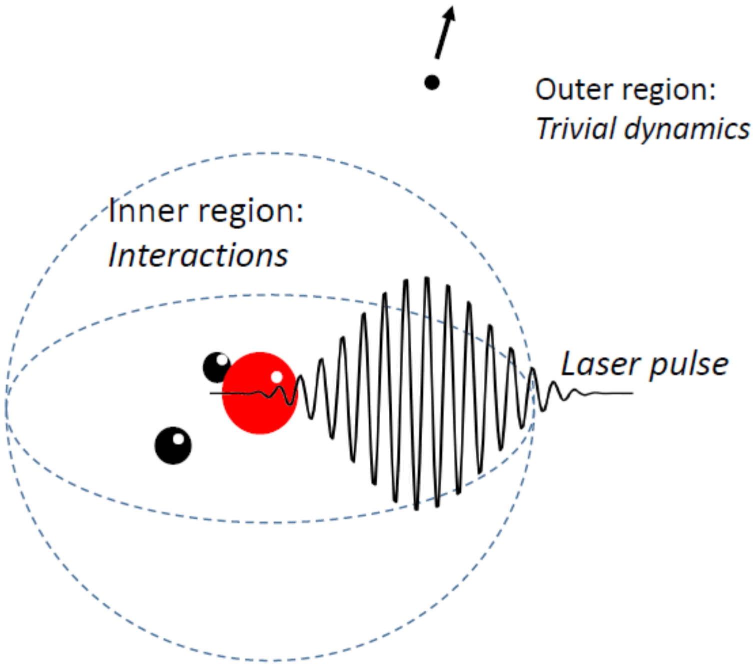
Lindblad

Using the ~~Schrödinger~~ equation:

YES



The **Lindblad equation:**

$$i\hbar \frac{d}{dt}\rho = [H, \rho] \; - i \, \Sigma_{k,l} \, \gamma_{k,l} \, (\{ a_k^\dagger a_l, \rho\} - 2 \, a_l \rho a_k^\dagger)$$

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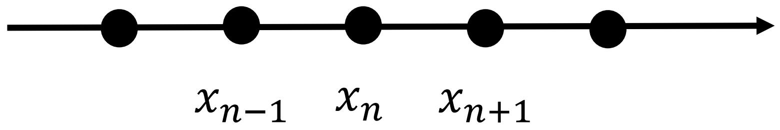
Absorber expressed using second quantization on a grid:

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



Zero for $|x\,| \leq x_0$, positive for $|x\,| > x_0$

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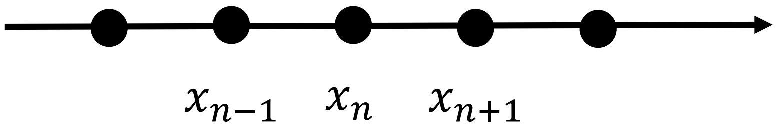

The non-Hermitian von Neumann equation (QLE), $H \rightarrow H_{eff} = H - i\,\hat{\Gamma}$

$$i\hbar \frac{d}{dt}\rho = H_{eff}\,\rho \; - \rho H_{eff}^\dagger = [H,\rho] \; - i\left\{\hat{\Gamma},\rho\right\} =$$

$$[H,\rho] \; - i\,\Sigma_k\, \Gamma(x_k) \left\{ c_k^\dagger c_k, \rho \right\}$$

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Feeds sub-system with less particles

The non-Hermitian von Neumann equation (QLE)

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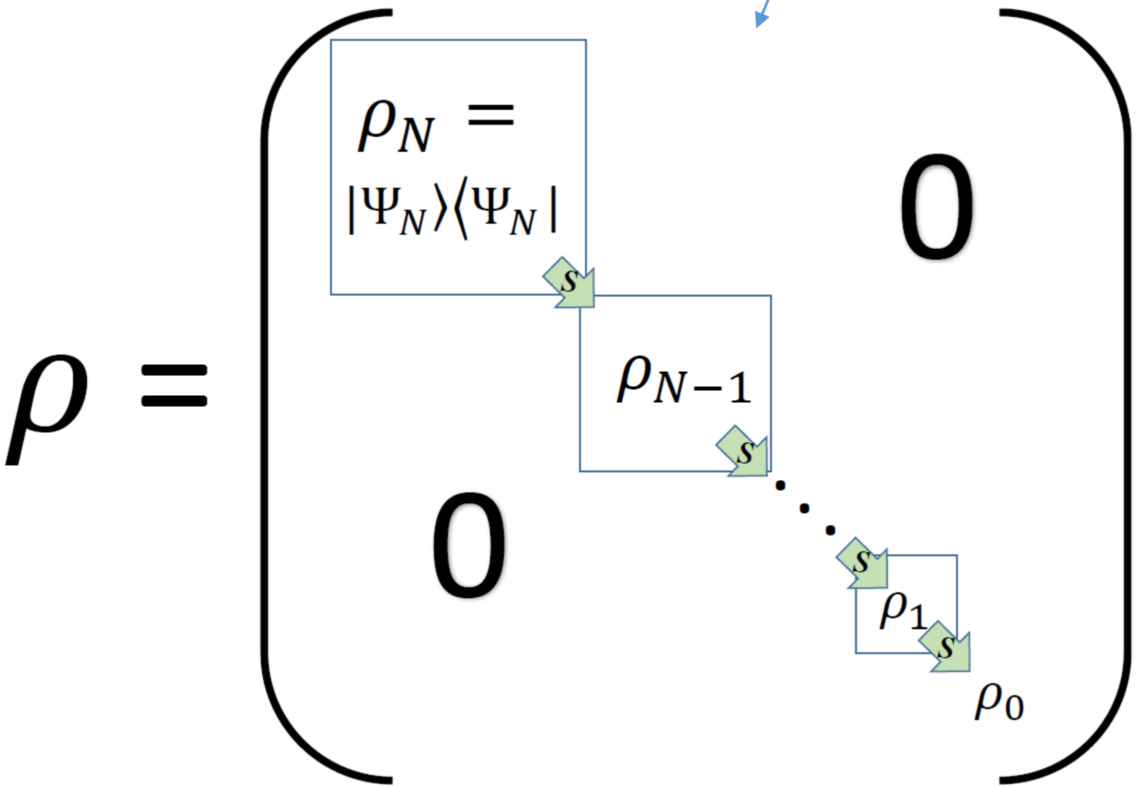
Hierarchy of equations

Source term

$$i\hbar \frac{d}{dt}\rho_n = H_{eff}\rho_n - \rho_n H_{eff}^{\dagger} + 2iS[\rho_{n+1}]$$

$$S[\rho] \equiv \Sigma_k \Gamma(x_k) c_k^{\dagger}\, \rho\, c_k$$

Diagonal flow



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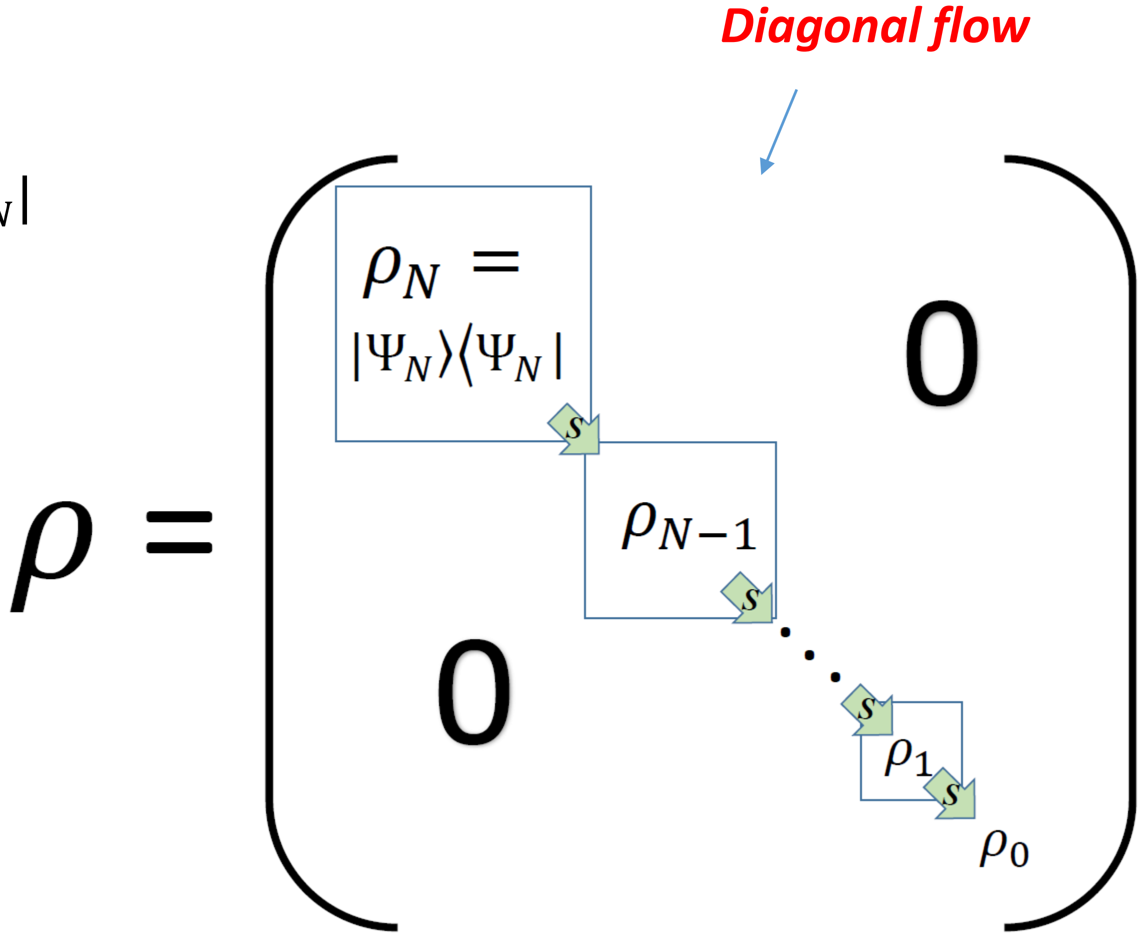
With initial *N*-particle pure state, $\rho_N = |\Psi_N >< \Psi_N|$

$$i\hbar \frac{d}{dt}\Psi_N = H_{eff}\Psi_N$$

Vacuum state

$$\hbar \frac{d}{dt}\rho_0 = 2S[\rho_1]$$

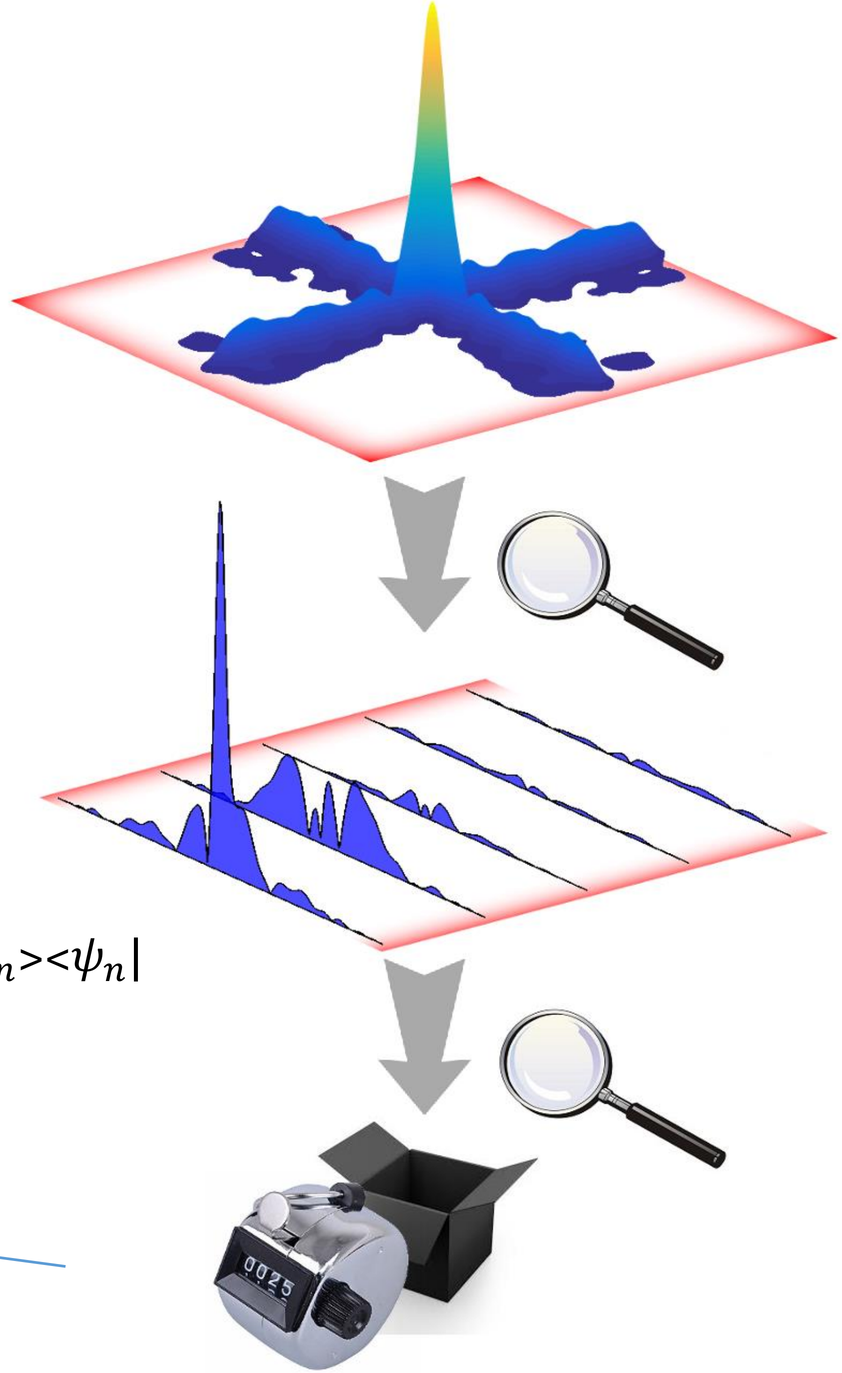


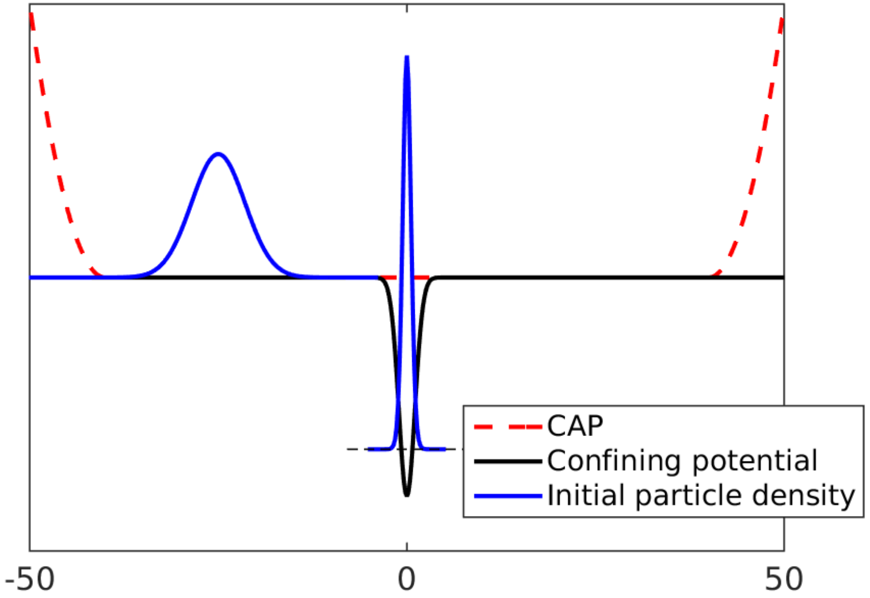
$$i\,\hbar\,\frac{d}{dt}\Psi_2 = \left(h_1 + h_2 + W_{1,2} - i\Gamma_1 - i\Gamma_2\right)\Psi_2$$

$$i\,\hbar\frac{d}{dt}\rho_1 = (h\; - i\,\Gamma)\rho_1 - \rho_1(h + i\Gamma) + 2i\,S[\Psi_2]$$

$$\frac{d}{dt}p_0 = 2\langle -|S[\rho_1]|-\rangle$$

$$\rho = \sum_n p_n|\psi_n><\psi_n|$$





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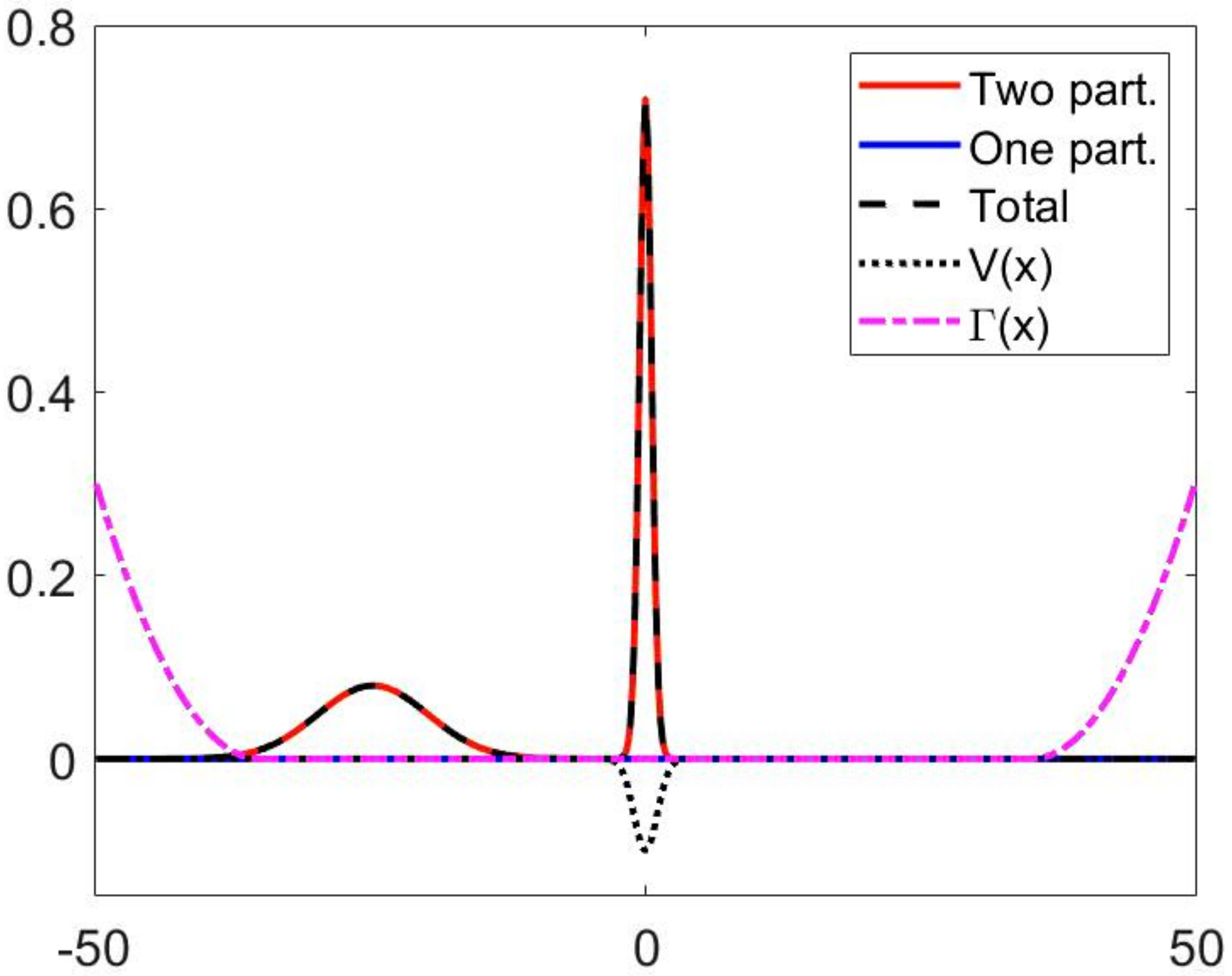

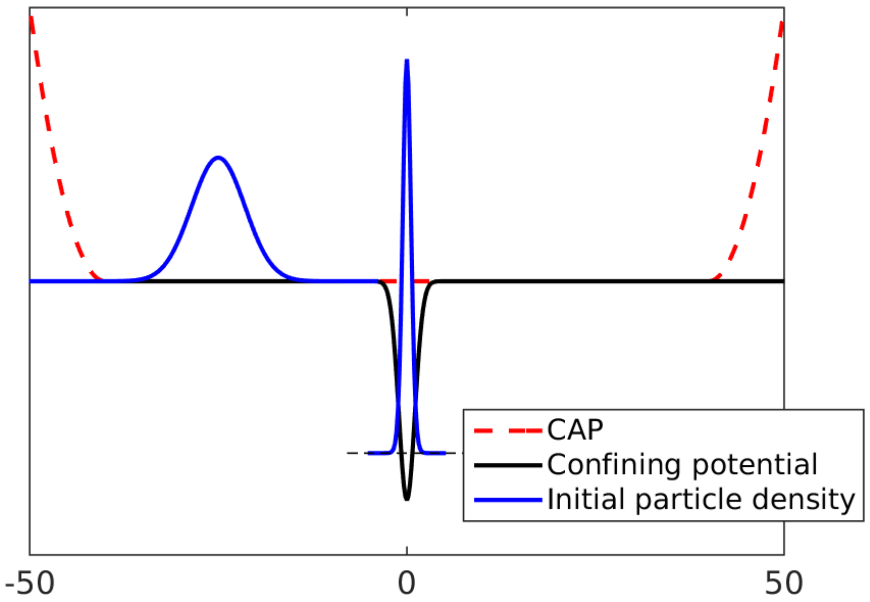

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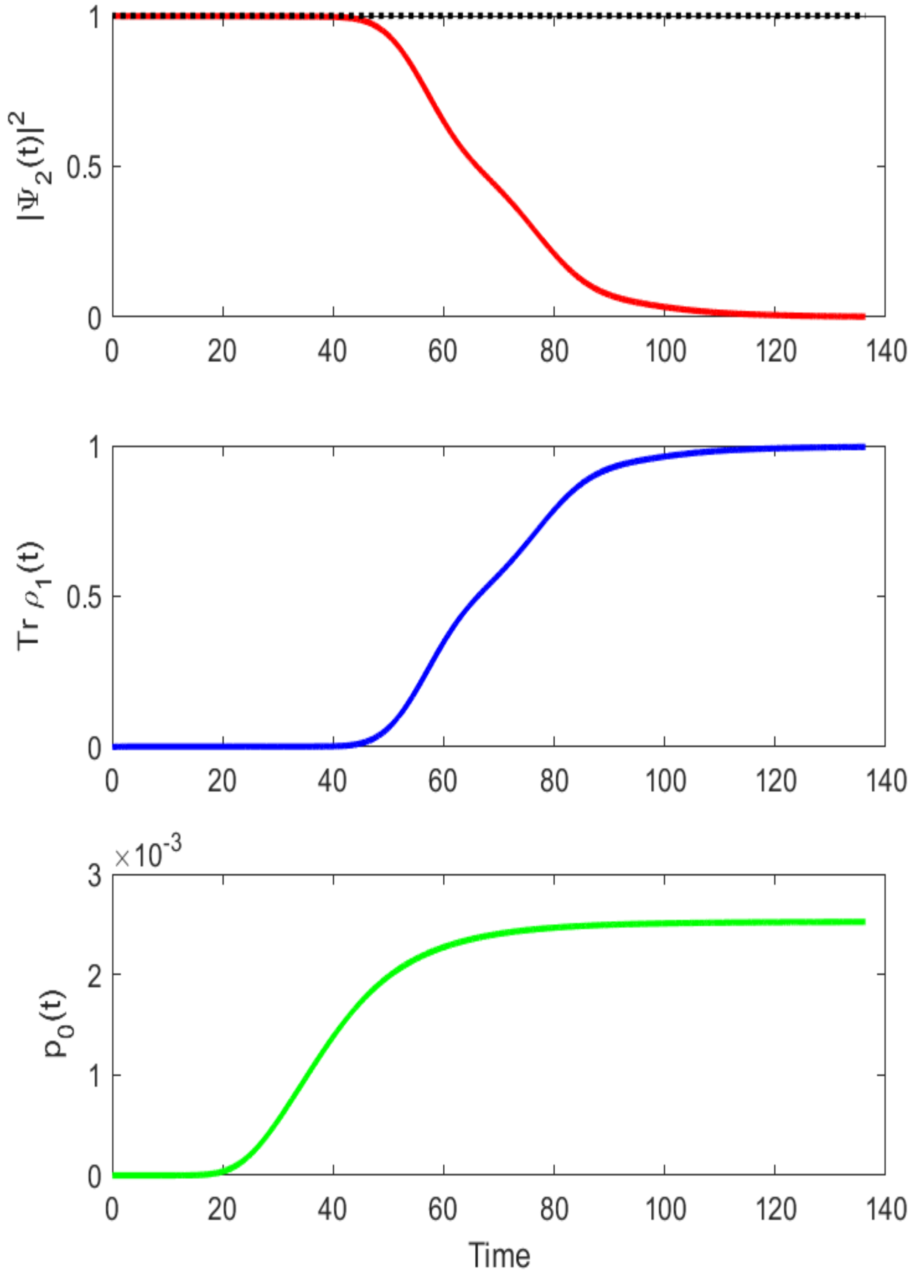

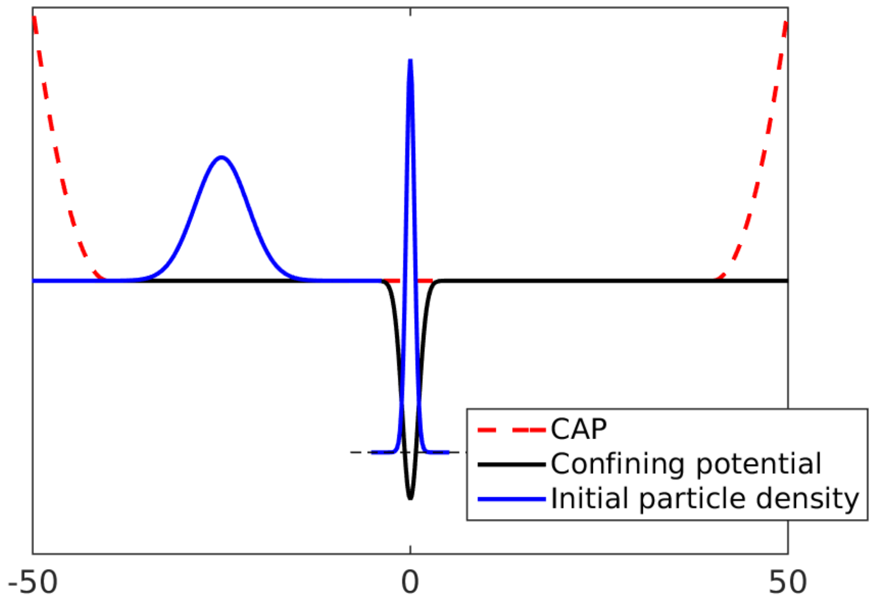

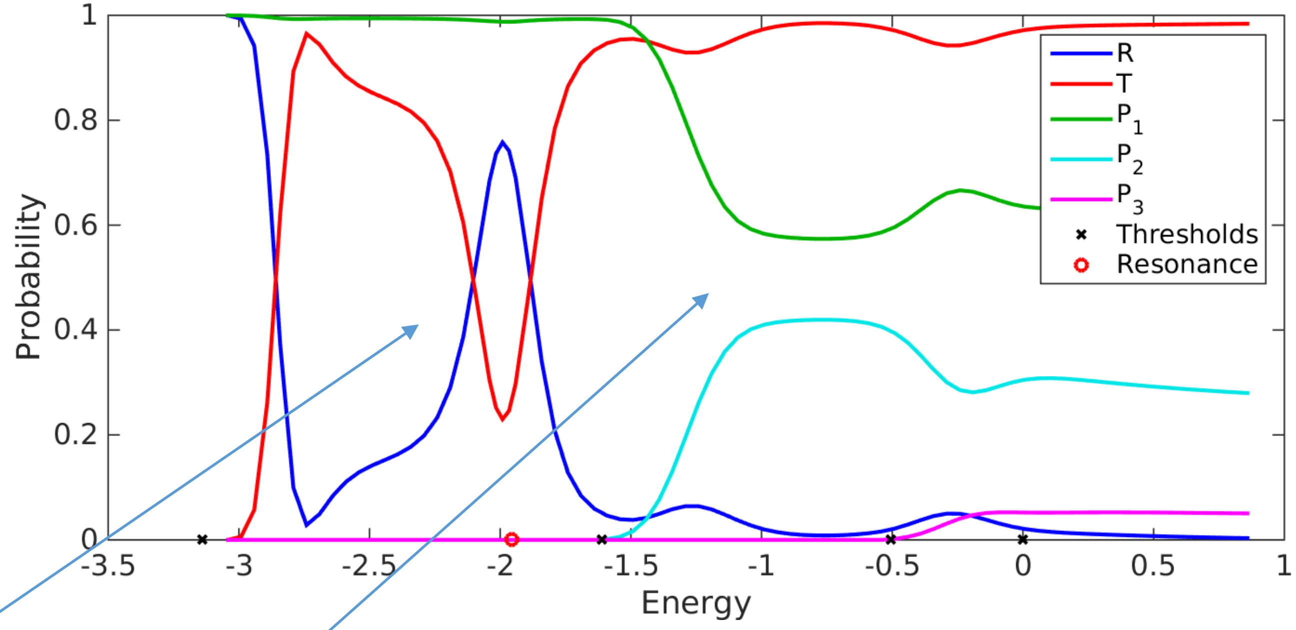

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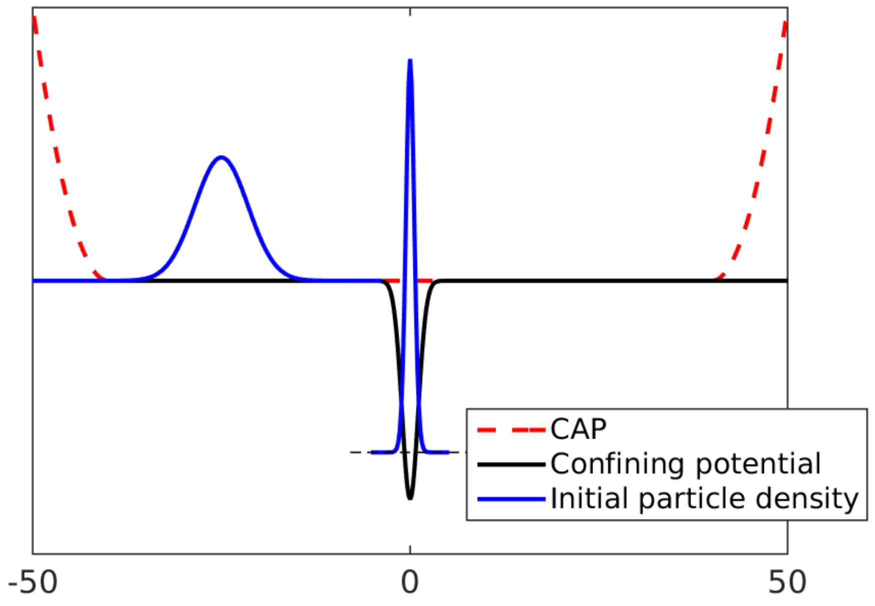

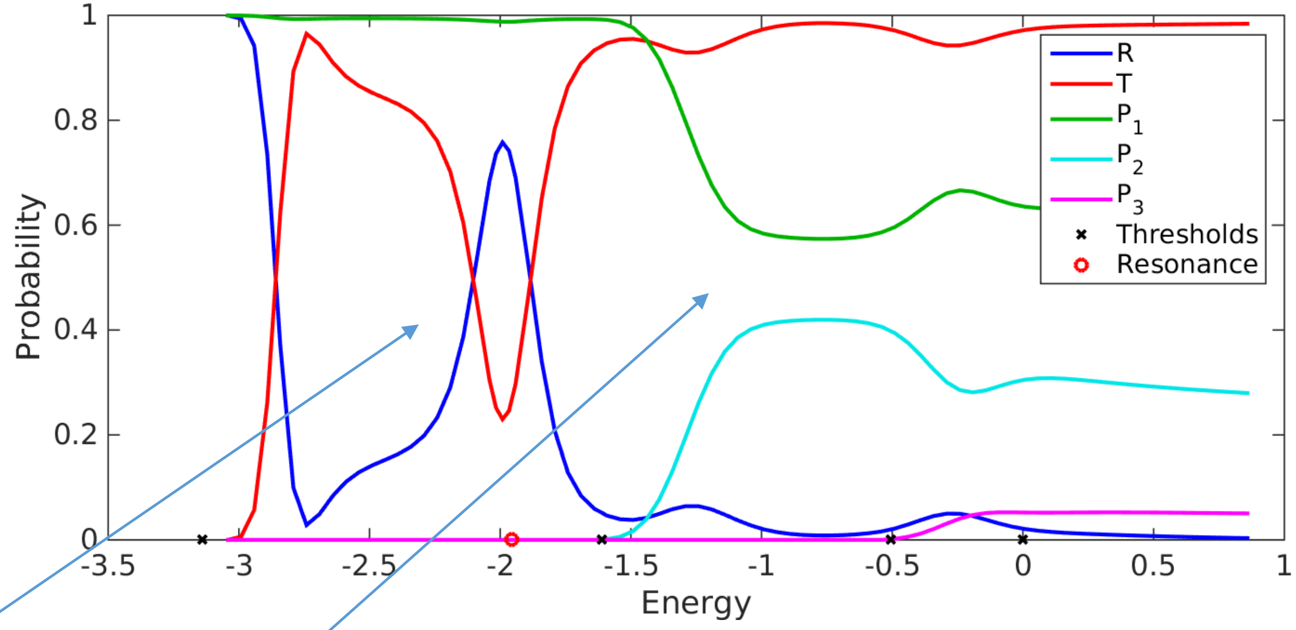

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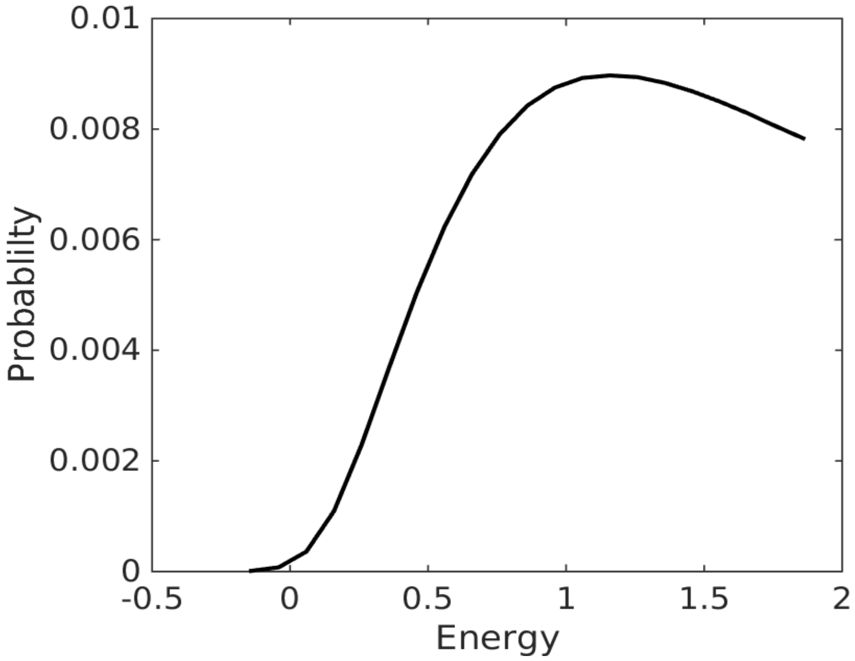
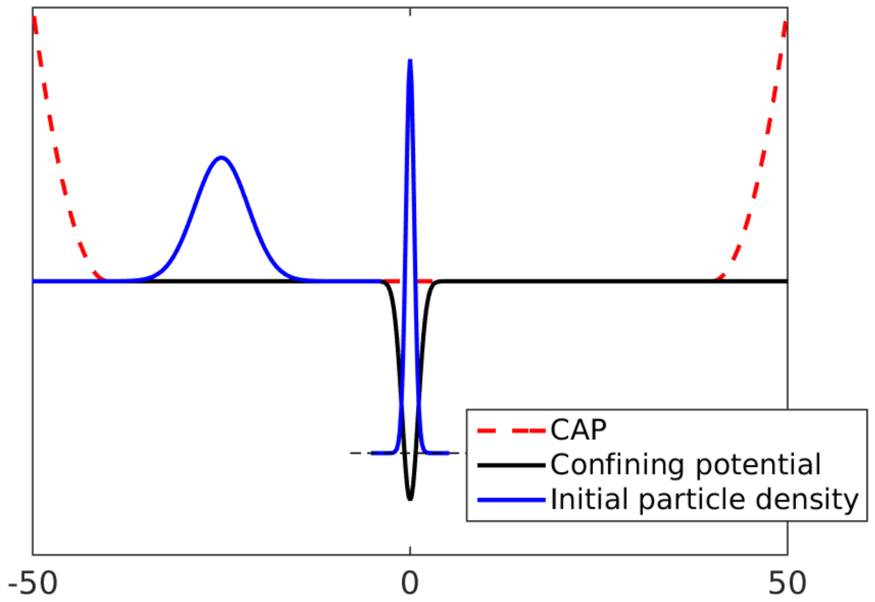
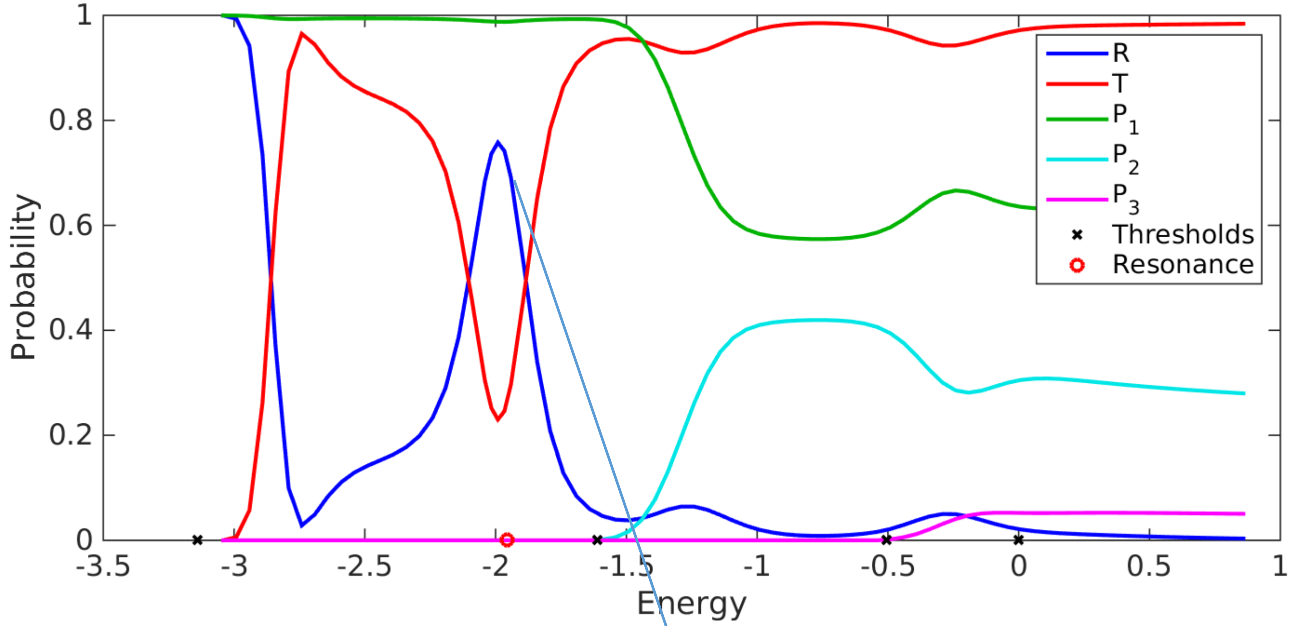
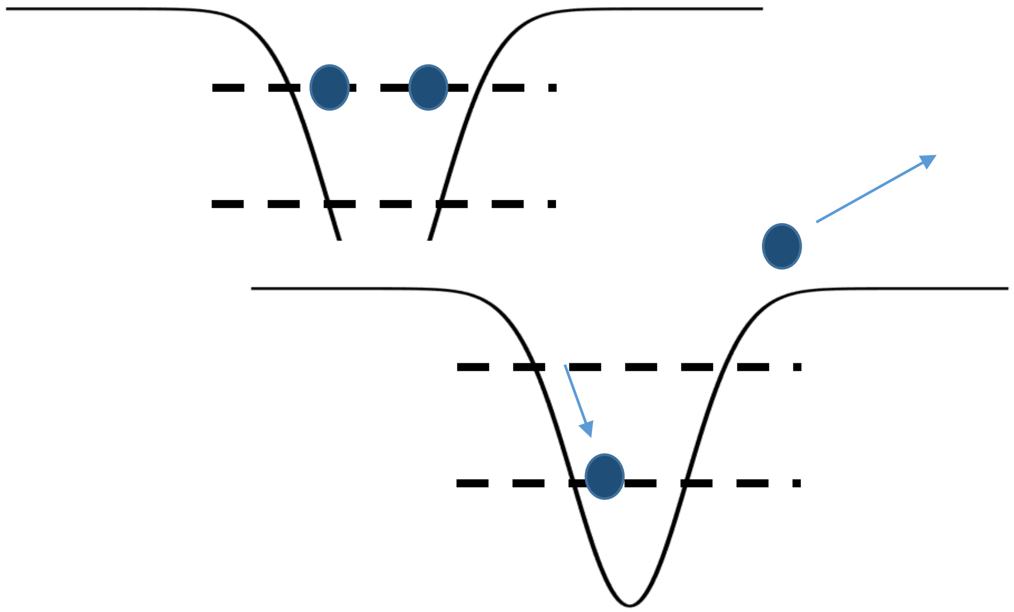
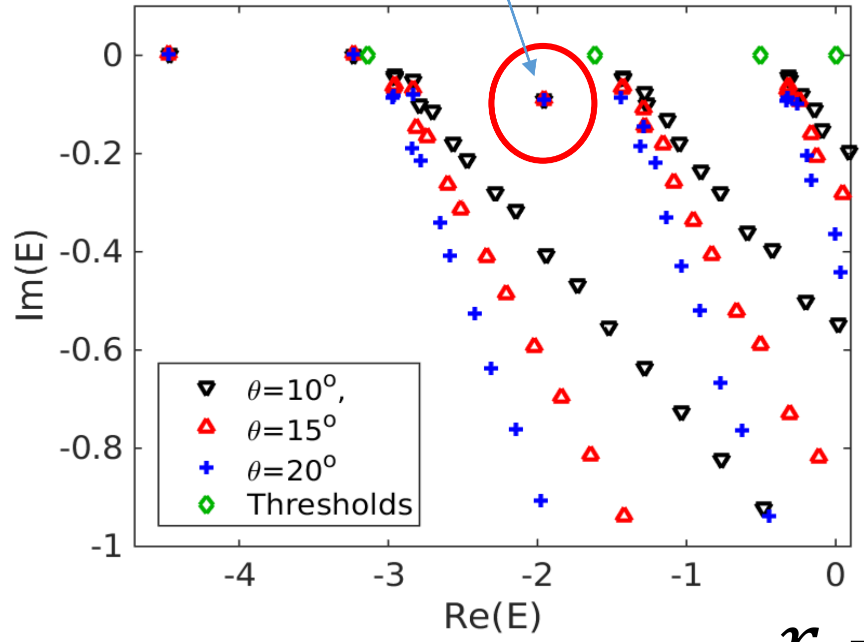






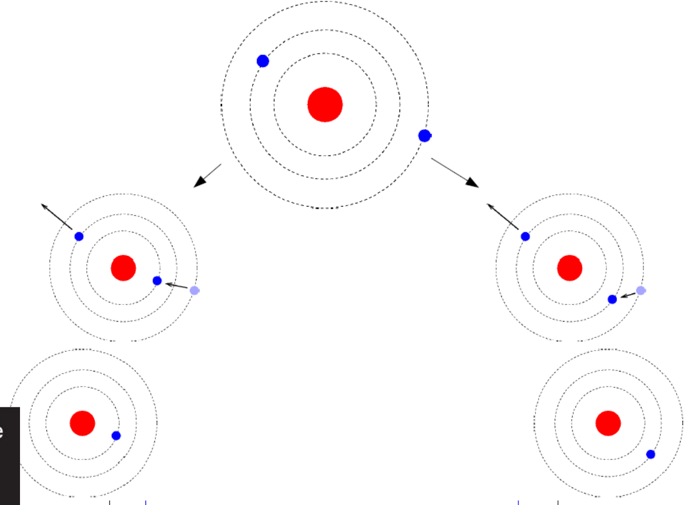


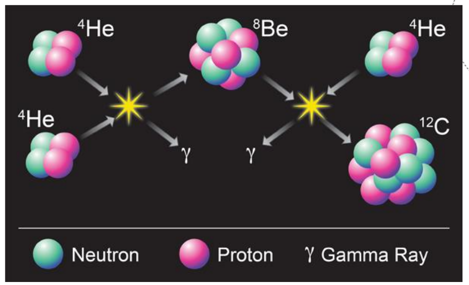


$$r \to e^{i\theta} r$$

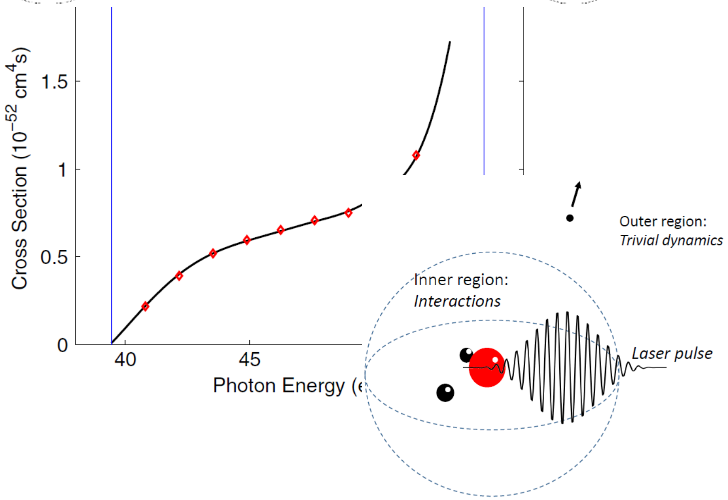
Applications – past, present and future(?):

- **Resonances**
  -Partial widths
  -Decay chains





- **Simulating dynamical few-particle quantum systems**
  -Small atoms and molecules in laser fields
  -Quantum dots exposed to perturbations



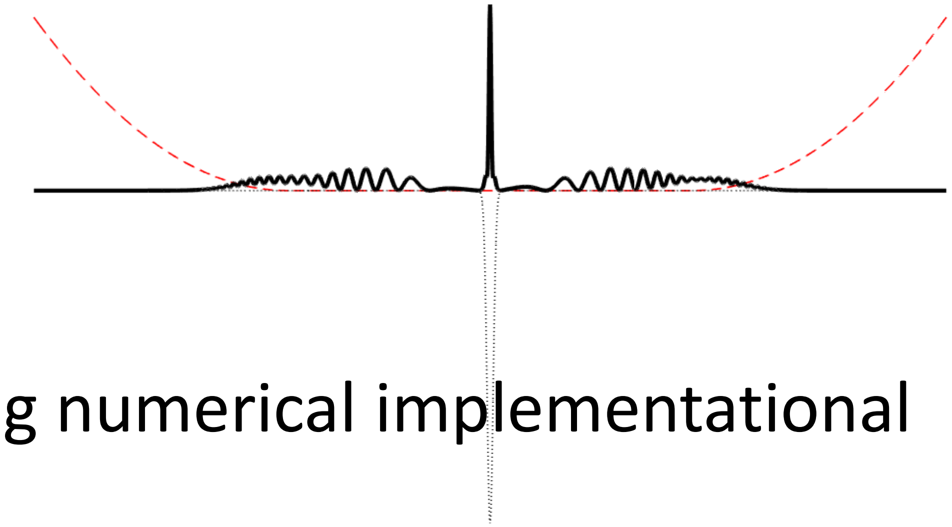
Simen Kvaal, Phys. Rev. A **84**, 022512 (2011)

- **Calls for new ways of approximating the density matrix**
  -Multi-configurational time-dependent Hartree-Fock method
  -Lower rank approximations
  -Correspondance with quantum jump/Monte Carlo wave packet-approach

$$\rho = \sum_n p_n |\psi_n><\psi_n|$$

Ihor Vakulchyc's talk later today

Main purpose of the absorber:



Remove unbound, outgoing part – facilitating numerical implementational

However, **we know what we remove**.
We may perserver that *information* although we do not perserve the particle

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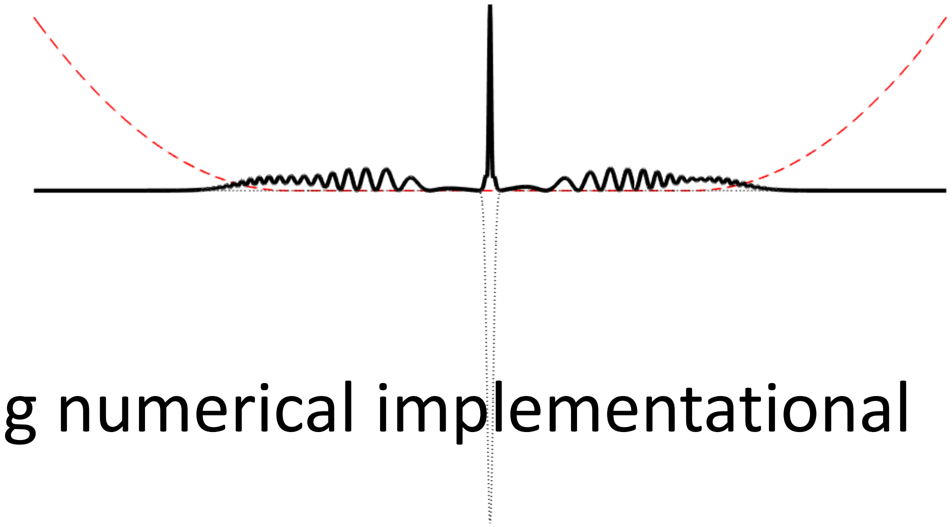

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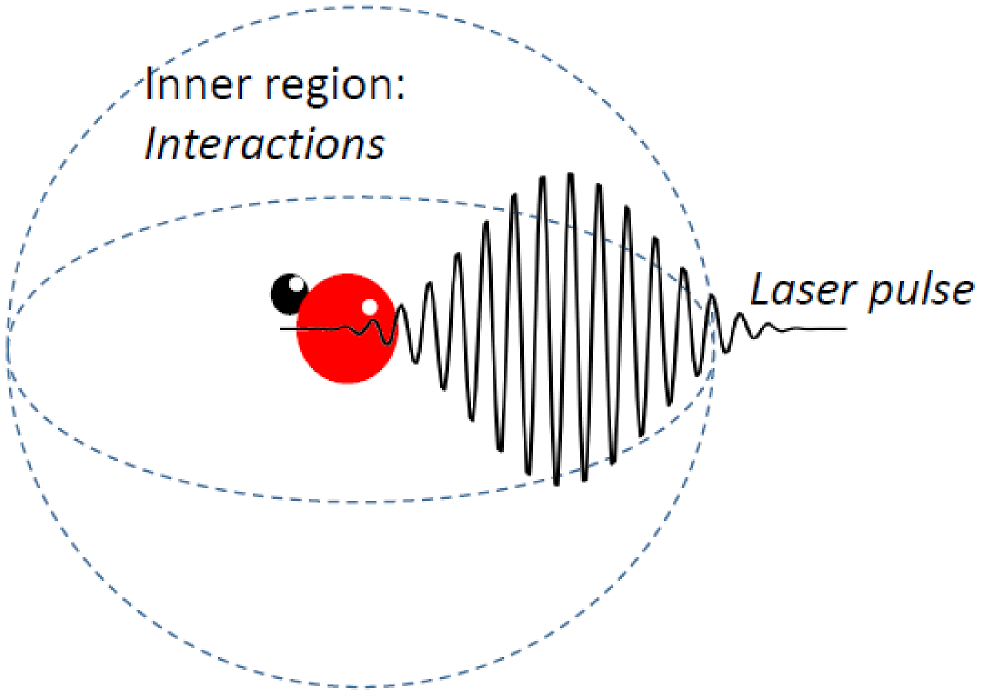
$$i\hbar \frac{d}{dt}\rho_n = [H, \rho_n] - i\{\hat{\Gamma}, \rho_n\} + 2iS[\rho_{n+1}]$$

One-particle examples

Angular distribution of the photo electron from a hydrogen atom exposed to a laser pulse

$$\Gamma(r) = \theta(r - r_0)\Gamma_0(r - x_0)^2$$
$$\Gamma_0 = 10^{-2}$$



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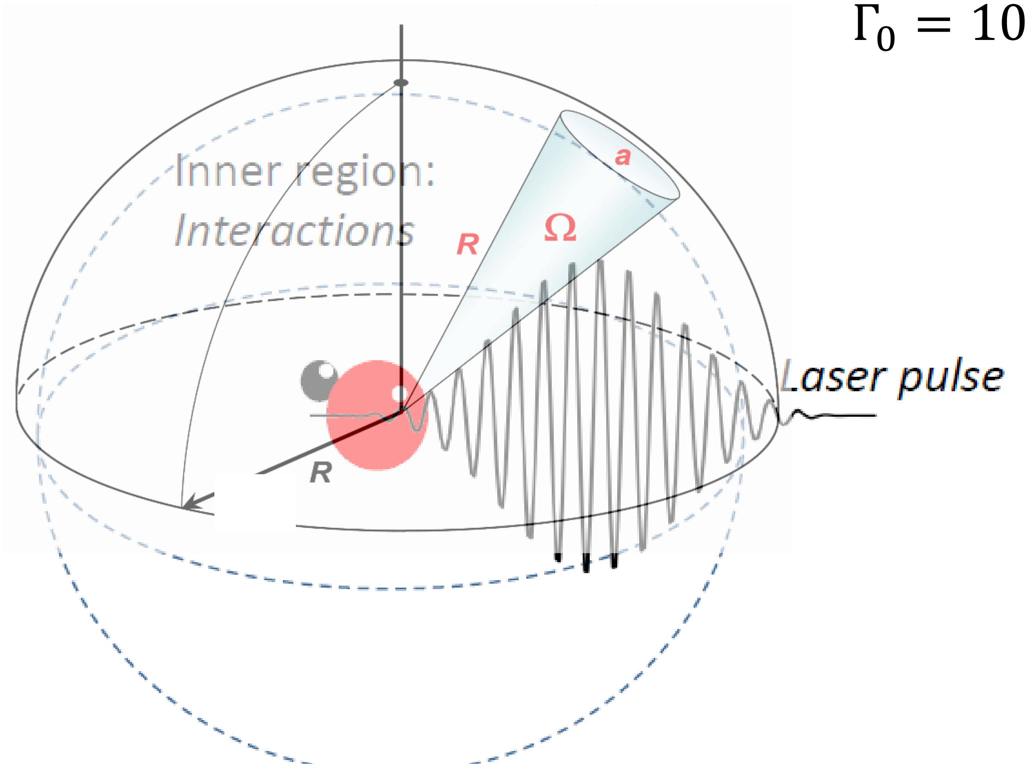

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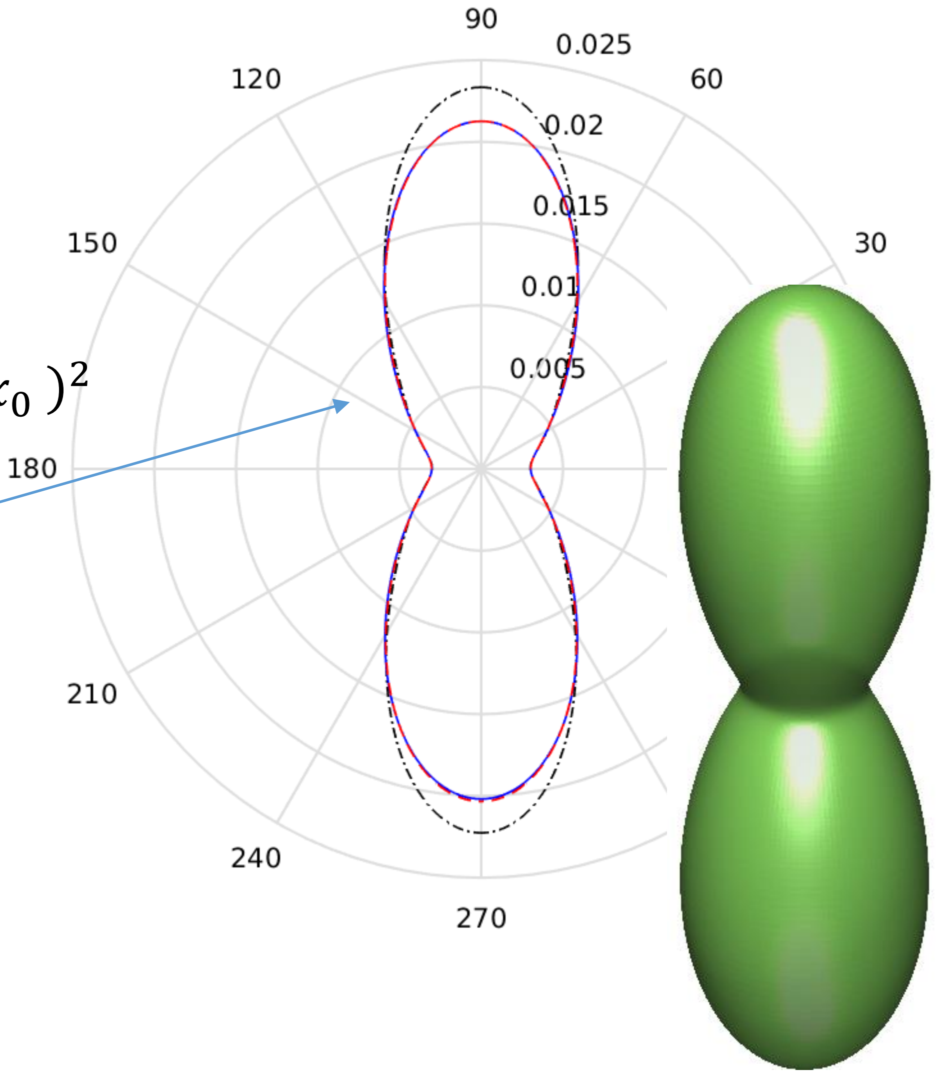
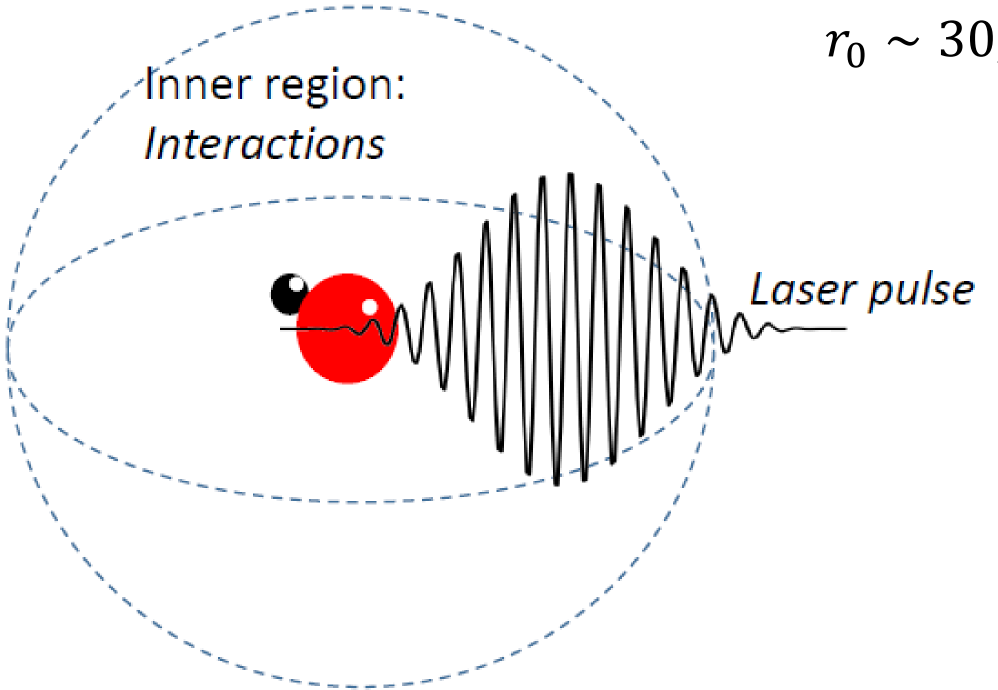
$$\Gamma_0 = 10^{-2}$$

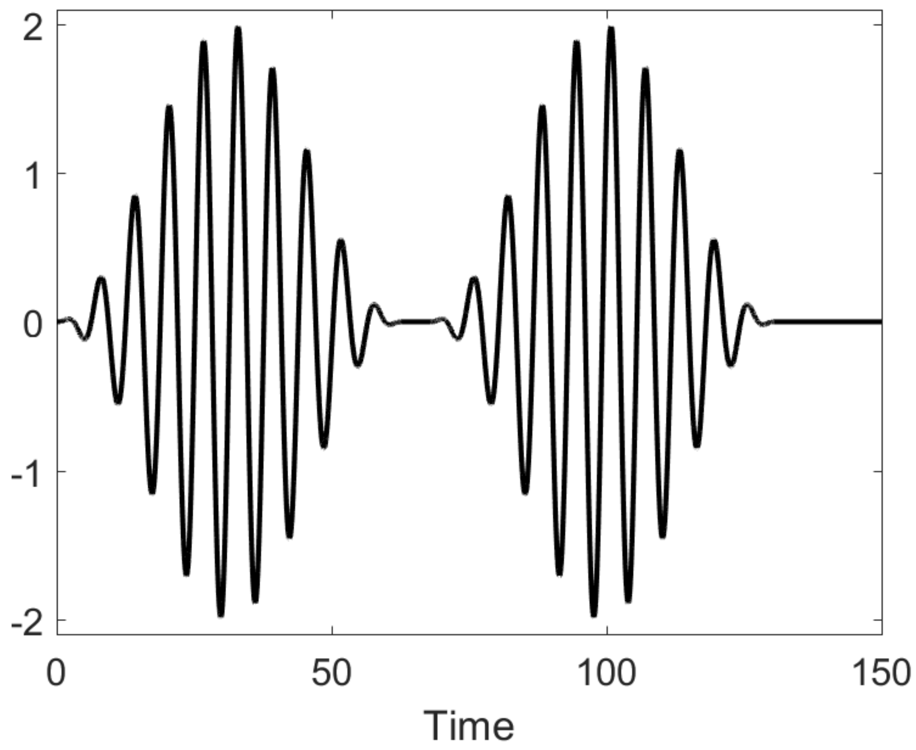
$$r_0 \sim 30, 40, 50$$

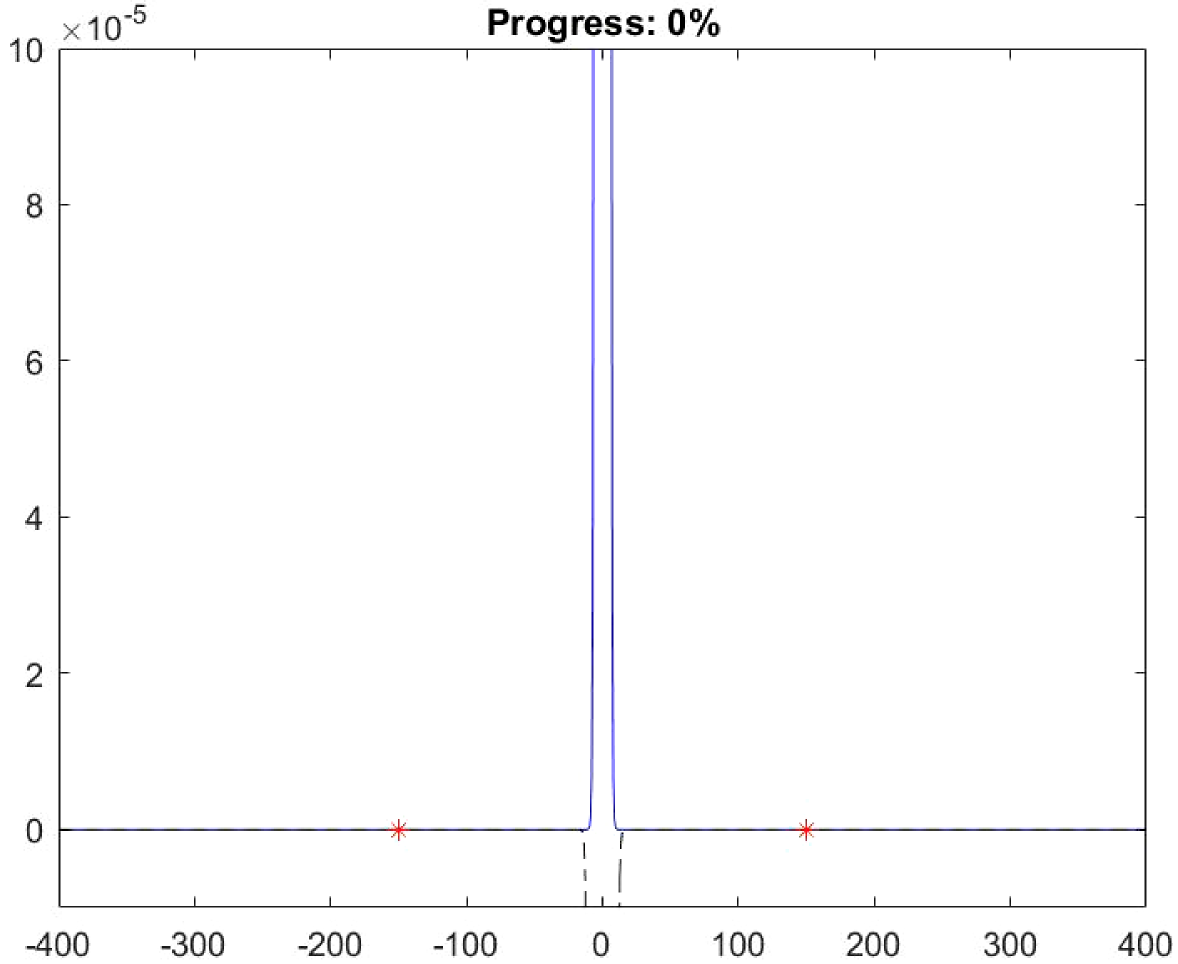




One-particle examples

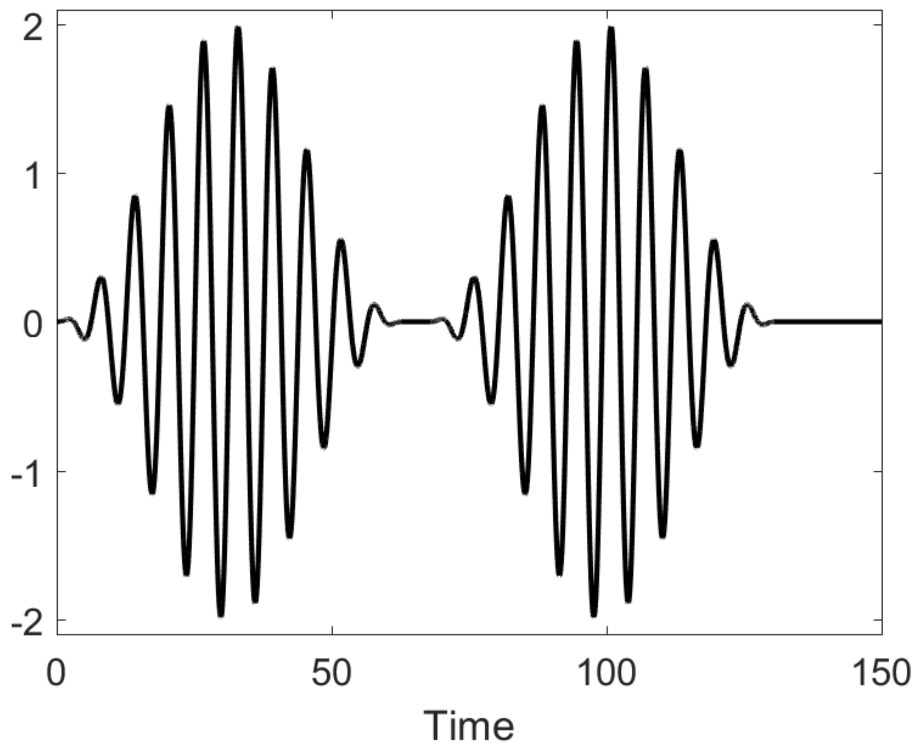
Momentum distribution for 1D “atom” exposed to two pulses of radiation

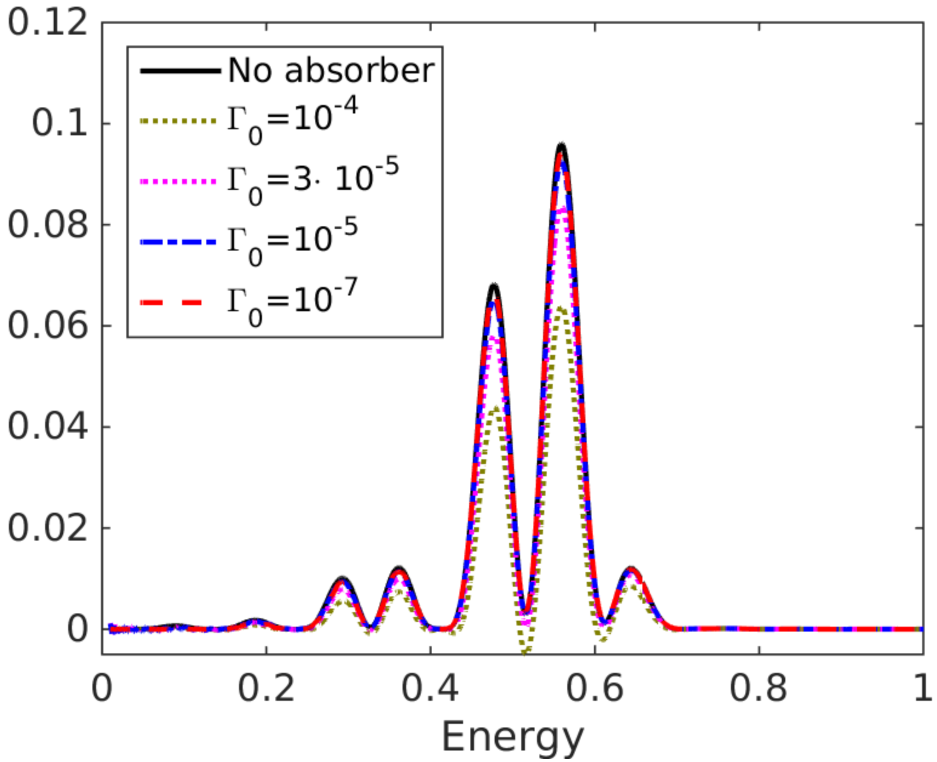




One-particle examples

$$\Gamma(x) = \begin{cases} 0, & |x| \le x_0 \\ \Gamma_0(|x| - x_0)^2, & |x| > x_0 \end{cases}$$

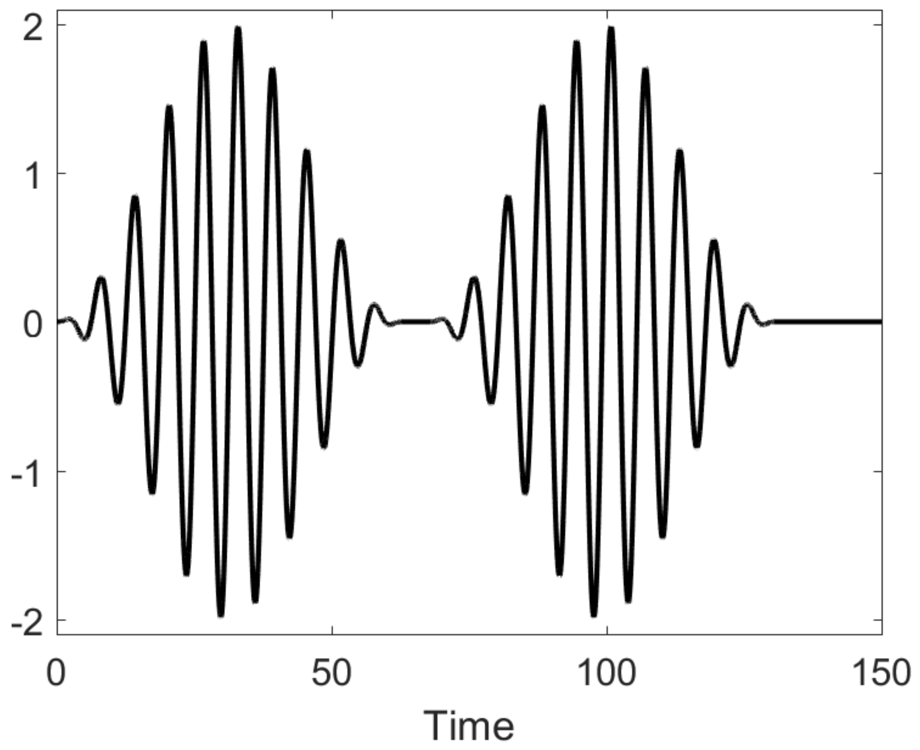


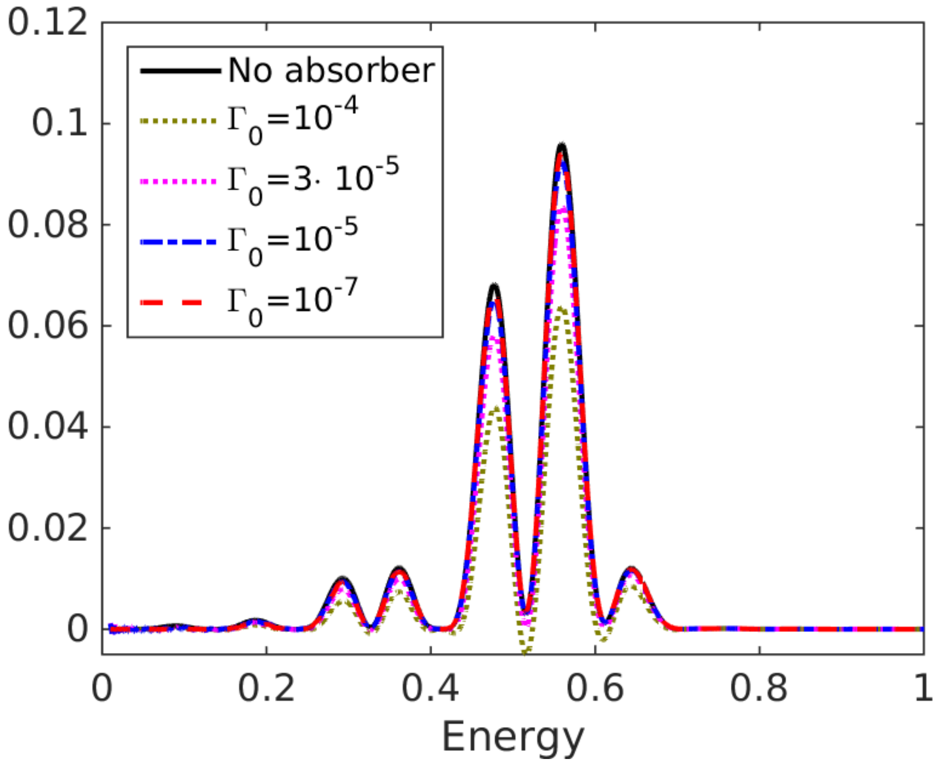


One-particle examples

But the absorber need not be diagonal in position representation.

$$\Gamma(x) = \begin{cases} 0, & |x| \leq x_0 \\ \Gamma_0(|x| - x_0)^2, & |x| > x_0 \end{cases}$$





One-particle examples

$$\Gamma(x,p) = \begin{cases} 0, & |x| \le x_0 \\ f_0 p^{2/3}, & |x| > x_0 \end{cases}$$

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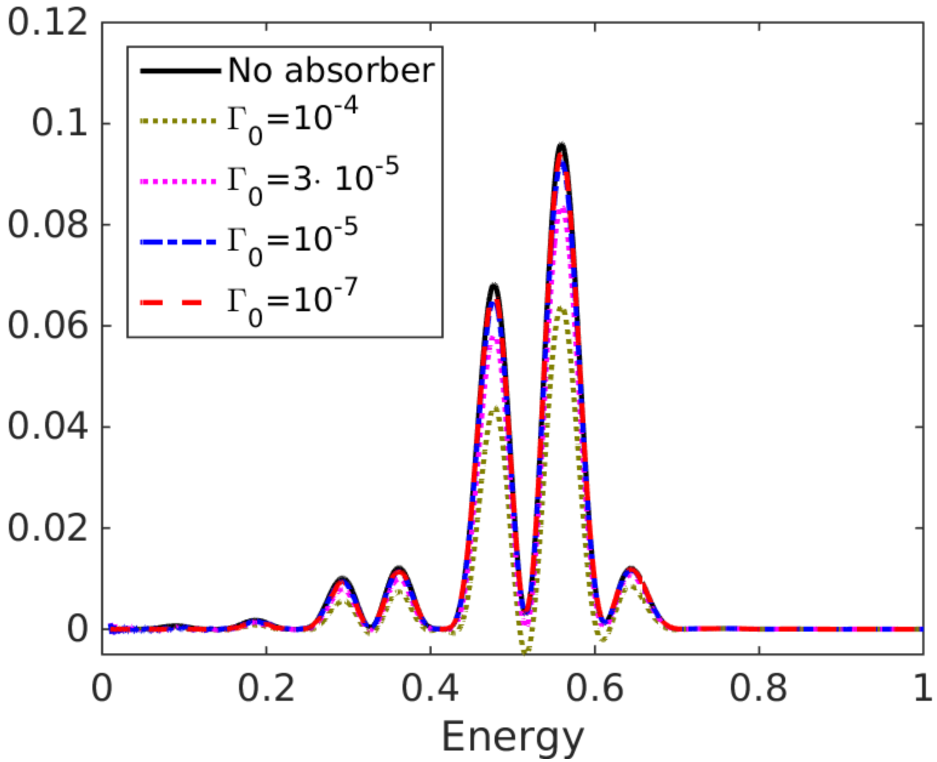

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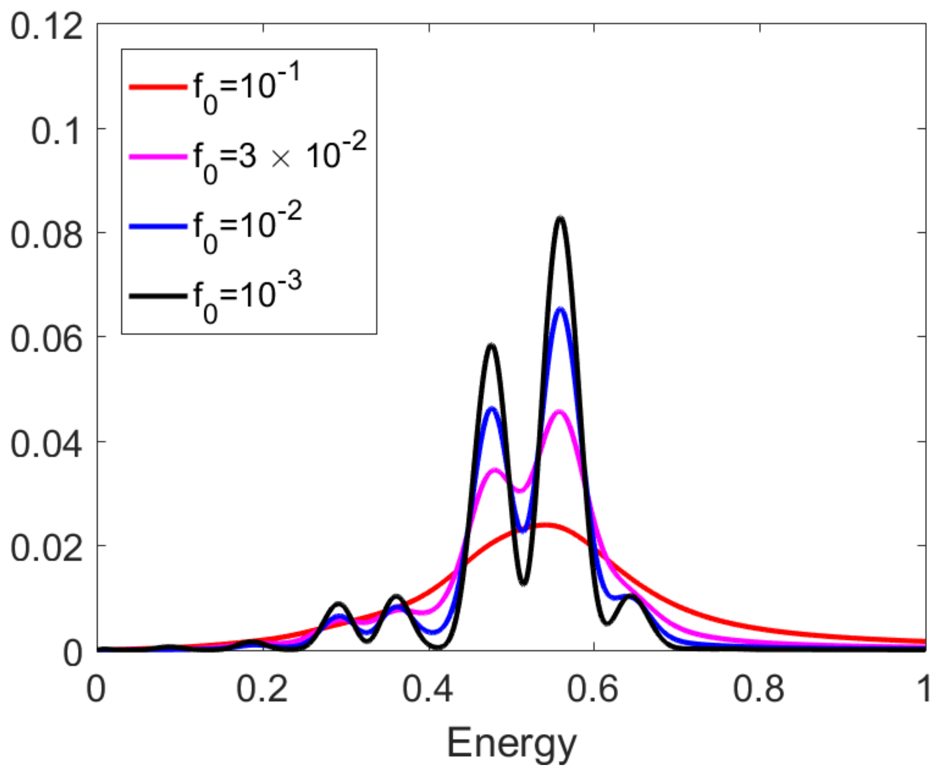

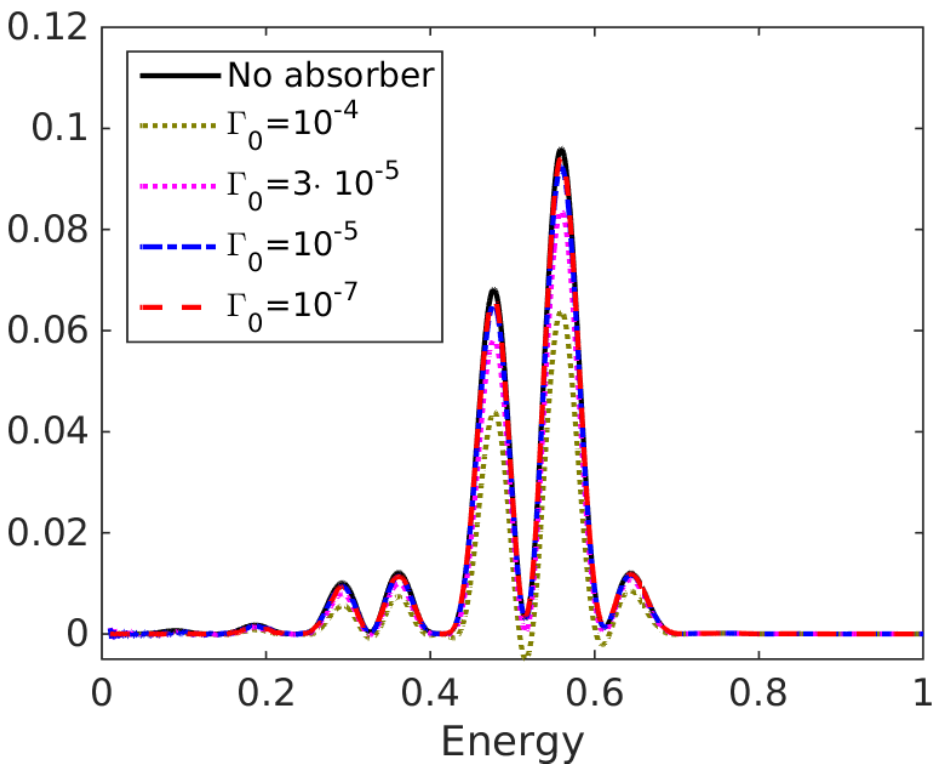

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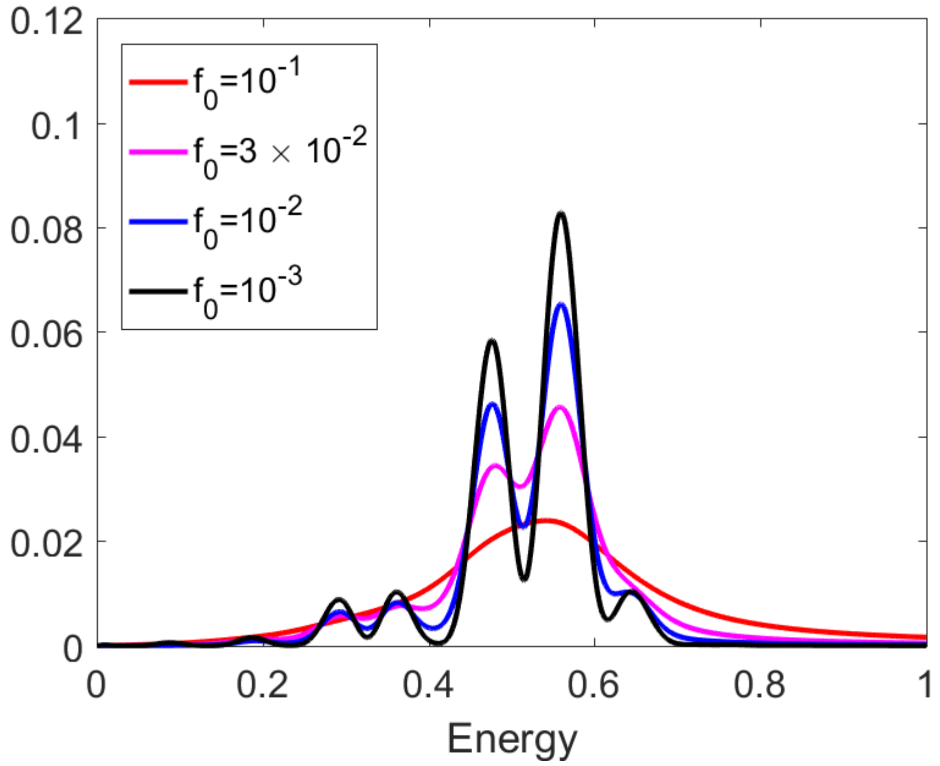
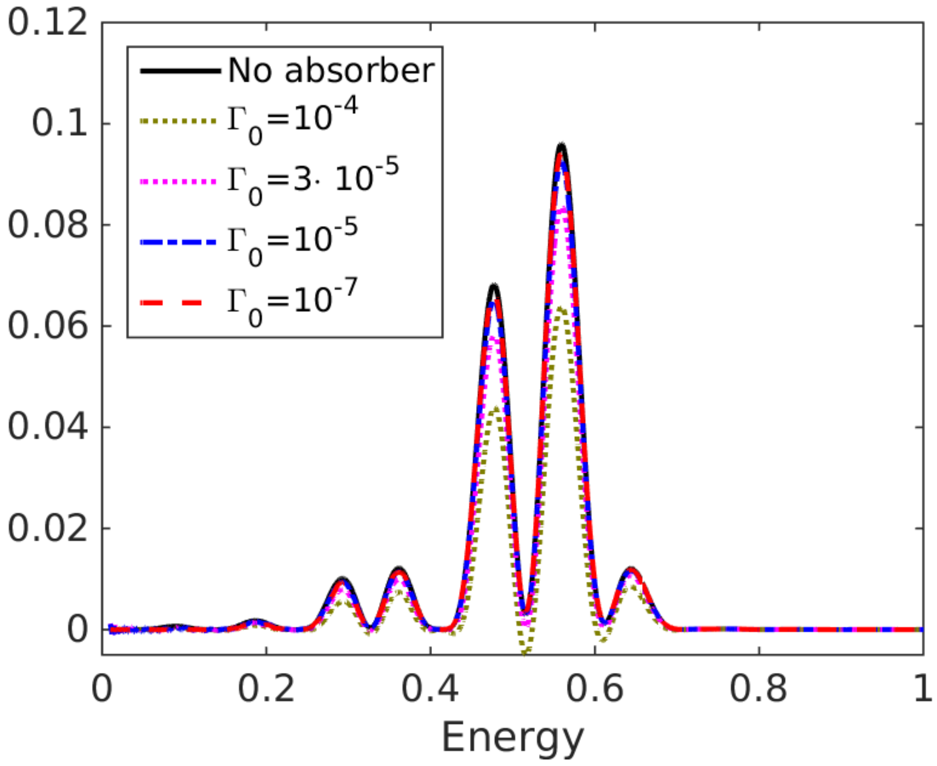
Momentum distribution from a momentum absorber: **Incoherent** sum.





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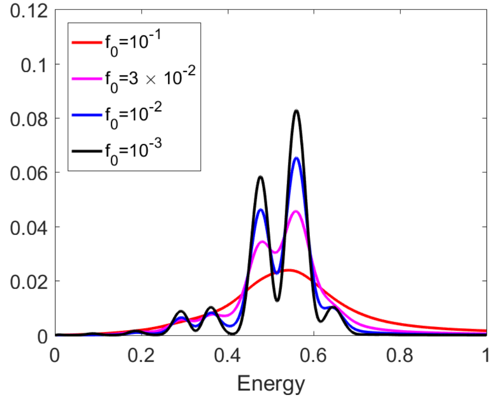

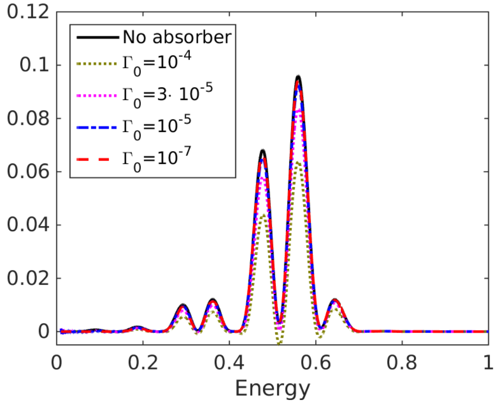

$$\hbar \frac{d}{dt}\frac{dP}{dp} = \int dp\, \Gamma(p) \left|\langle p | \Psi_{|x|>x_0}\rangle\right|^2$$
$$= \int dp\, \Gamma(p) |\mathcal{F}[\Psi(|x| > x_0)](p)|^2$$

$$\hbar \frac{d}{dt}\frac{dP}{dp} = \int dx\, \Gamma(x)\, \langle p|x\rangle\langle x|\Psi\rangle\langle\Psi|p\rangle$$
$$= \int dx\, \mathcal{F}[\Gamma(x)\Psi(x)](p)\, \left(\mathcal{F}[\Psi(x)](p)\right)^*$$

One-particle examples

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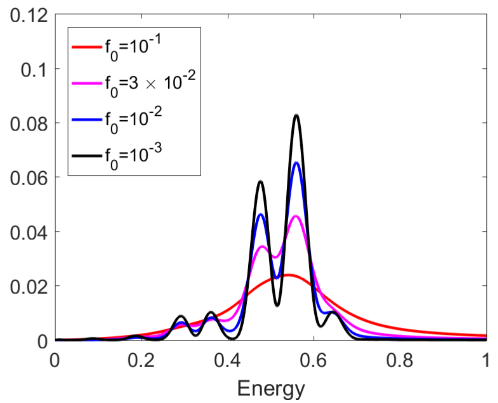
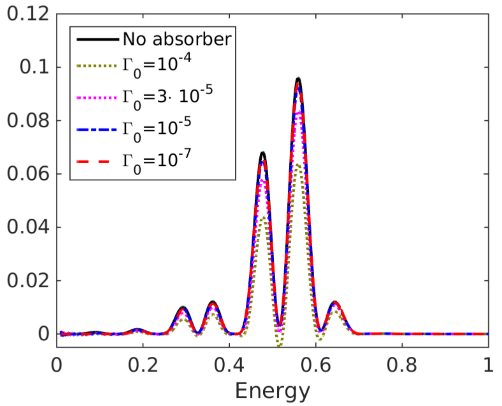
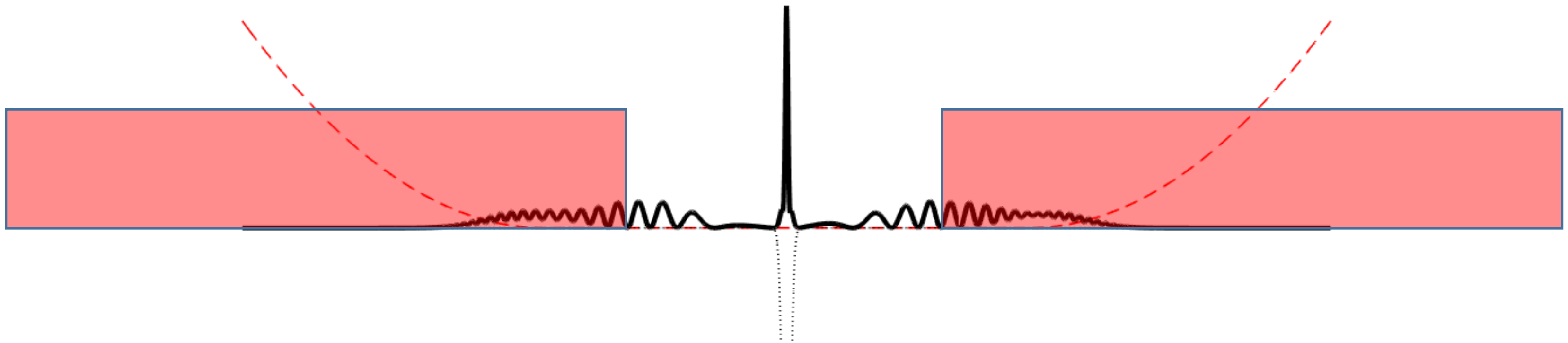






Why use the Lindblad equation for describing unbound many-particle systems?

- **The** proper way to impose absorbing boundaries, thus allowing us to use truncated domains.

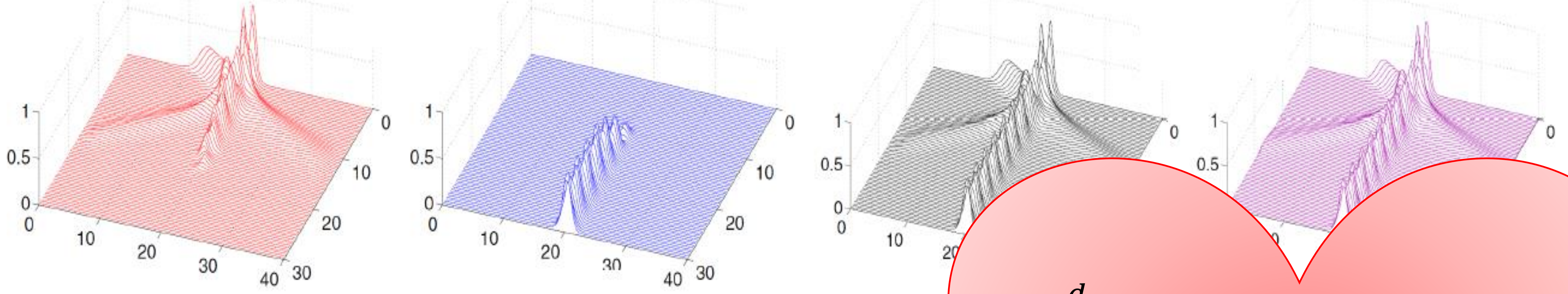
- When particles are removed, physical information about the removed particles (direction, energy, etc.) may still be perserved (*and not just for for one-particle systems*).

- *Analyse decay producs of resonances.*

- Allows us to model how coherence properties are lost by the act of measurement.

- Challenge: Finding efficient ways of propagating the density matrices for systems of many degrees of freedom.

$$i\hbar \frac{d}{dt}\rho = [H,\rho] - i\,\Sigma_n \Gamma_n \left(\{ a_n^\dagger a_n, \rho \} - 2\, a_n \rho a_n^\dagger \right)$$



$$i\hbar \frac{d}{dt}\rho = [H,\rho] \; - \; i\,\Sigma_n \Gamma_n \left(\{ a_n^\dagger a_n, \rho \} - 2\, a_n \rho a_n^\dagger \right)$$

Thank you for your attention!

References

- *"Absorbing boundary conditions for dynamical many-body quantum systems",* Journal of Physics B **43**, 065004 (2010)
- *"A master equation approach to double ionization of helium",* Journal of Physics B **44**, 215003 (2011)
- *"Formulae for partial widths derived from the Lindblad equation"*, Physical Review A **85**, 062518 (2012)
- "*Scattering in a quantum dot: the role of resonances*", Journal of Physics: Condensed Matter **25**, 315802 (2013)