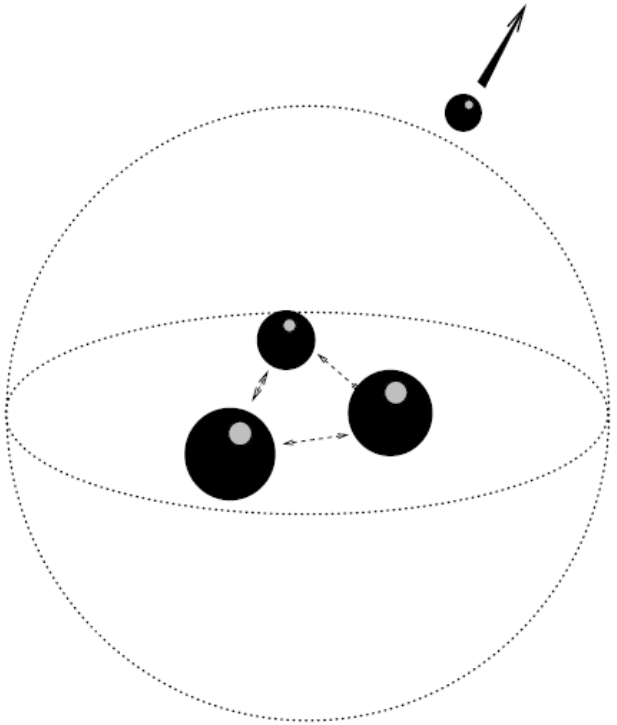
Absorbing boundaries for more than one particle

Technion, Haifa, Tuesday June 1st



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Collaborators

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Raymond Nepstad, UiB

Non-Hermitian Hamiltonians and absorbing boundaries

Complex scaling

Uniform: $r \longrightarrow r \cdot e^{i\theta}$

Exterior: $r \rightarrow \begin{cases} r, & r \leq R \\ R + (r - R)e^{i\theta}, & r > R \end{cases}$

Anti-Hermitian «potentials»

Phenomenological spontaneous decay: $H \longrightarrow H - i|\psi_n\rangle\langle\psi_n|$

Complex absorbing (local) potential: $V(r) \rightarrow V(r) - i\Gamma(r), \Gamma(r) \leq 0$

Masking function: $\Psi(t + \Delta t) = U\Psi(t) \rightarrow U\Psi(t) \cdot M(r), \quad M \in (0, 1]$

Non-unitary evolution

Typically: $H = X - iY, \quad X = X^\dagger, \quad Y = Y^\dagger, \quad Y \geq 0$

Evolution:

$$\Psi(t + \Delta t) \approx \exp(-iH\Delta t)\Psi(t)$$

Norm:

$$N^2(t + \Delta t) = \langle \Psi(t + \Delta t) | \Psi(t + \Delta t) \rangle = \langle \Psi(t) | e^{+iH^\dagger \Delta t}\, e^{-iH\Delta t} | \Psi(t) \rangle$$

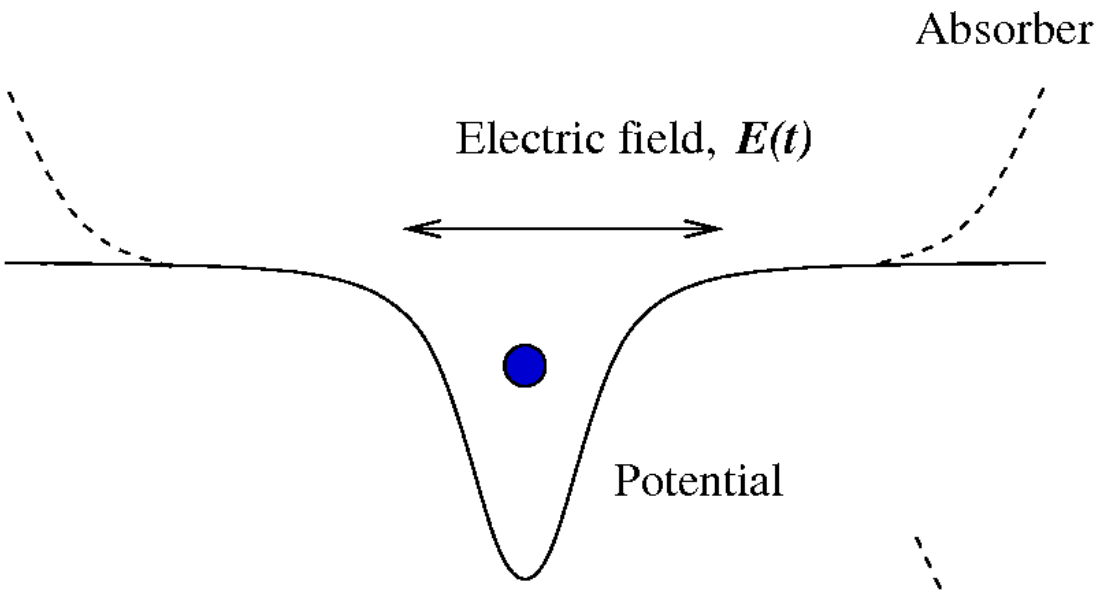
$$\langle \Psi(t) | e^{-2Y\Delta t} | \Psi(t) \rangle \leq N^2(t)$$

Thus, N^2 *decreases in time*

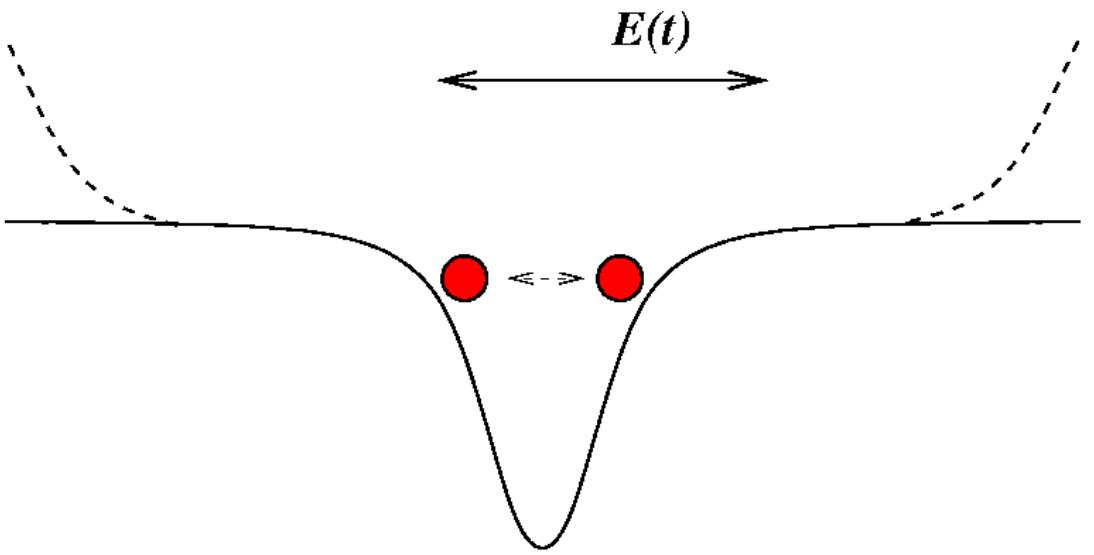
May be useful – but also problematic...

The problem...

One particle



Two particles



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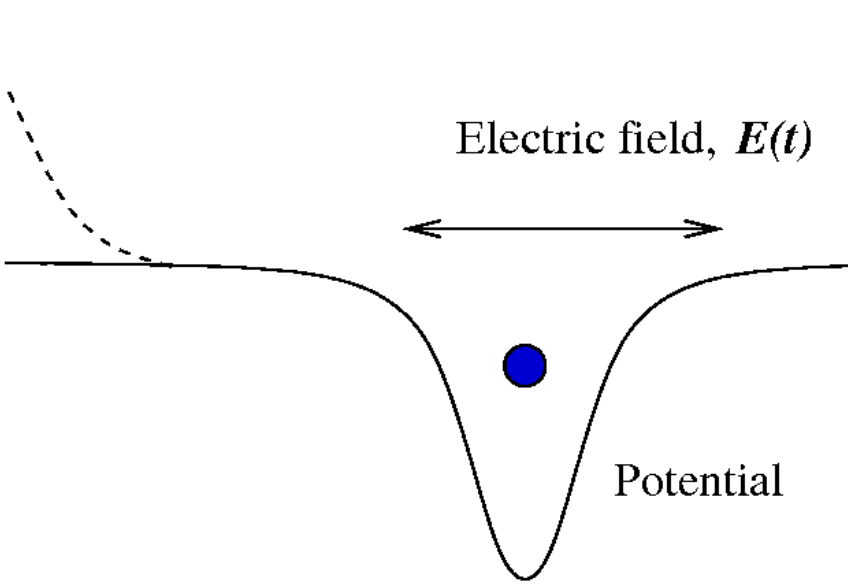
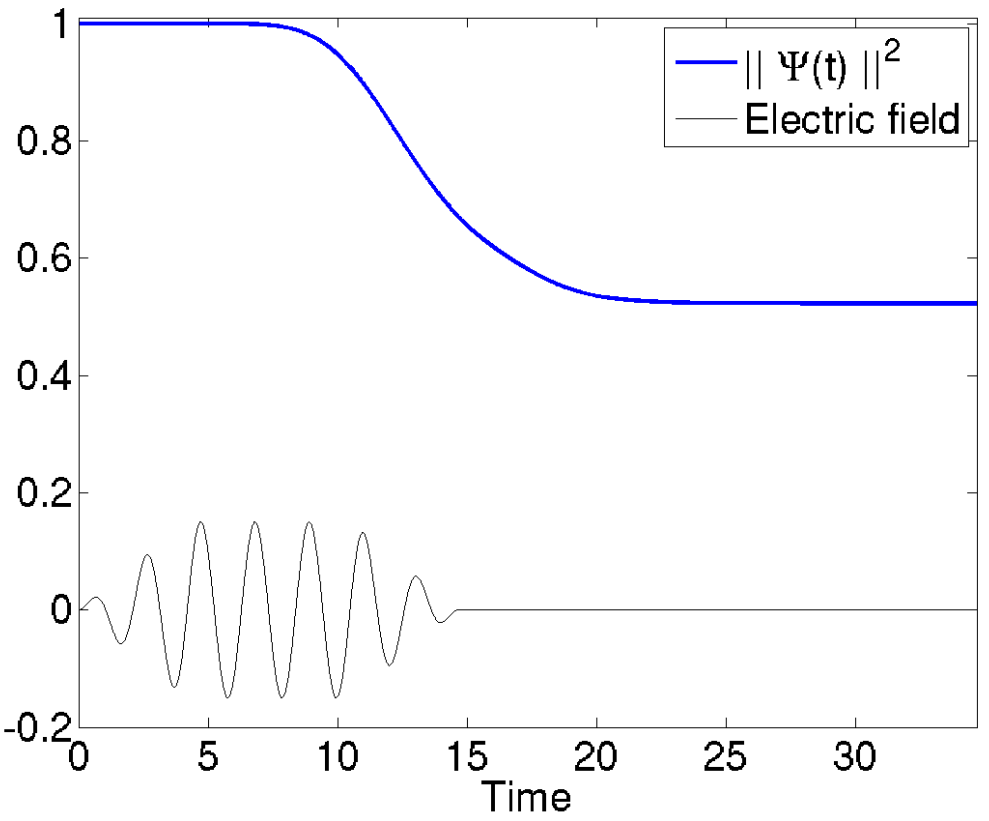
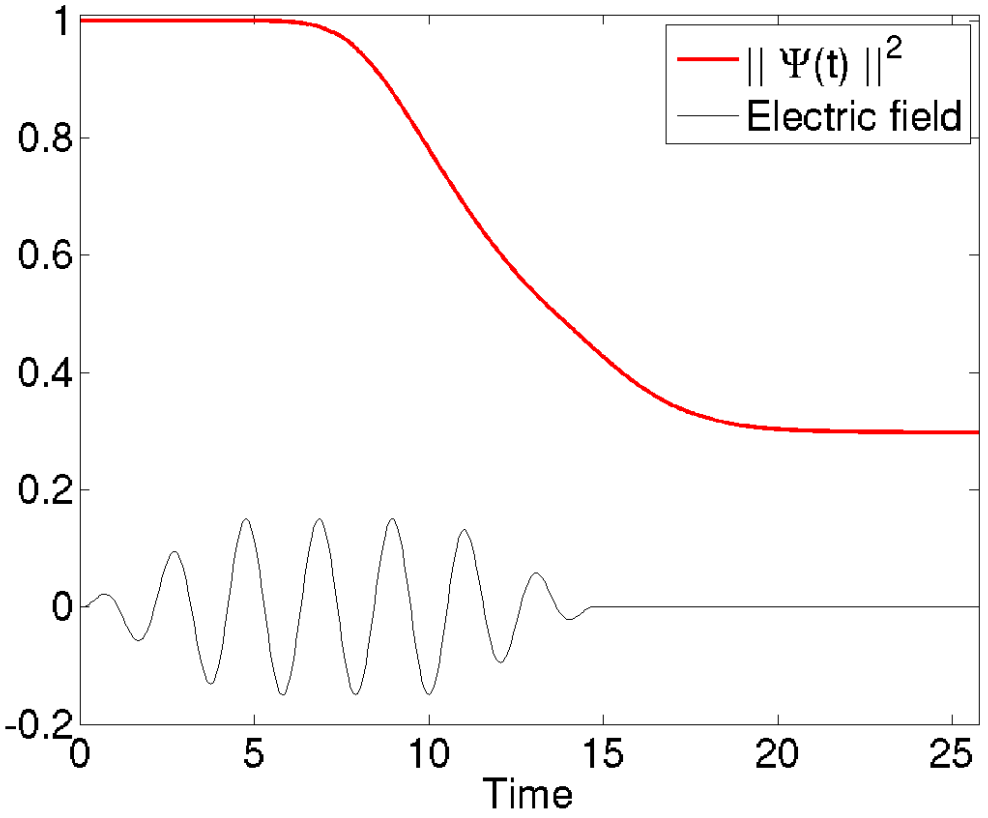
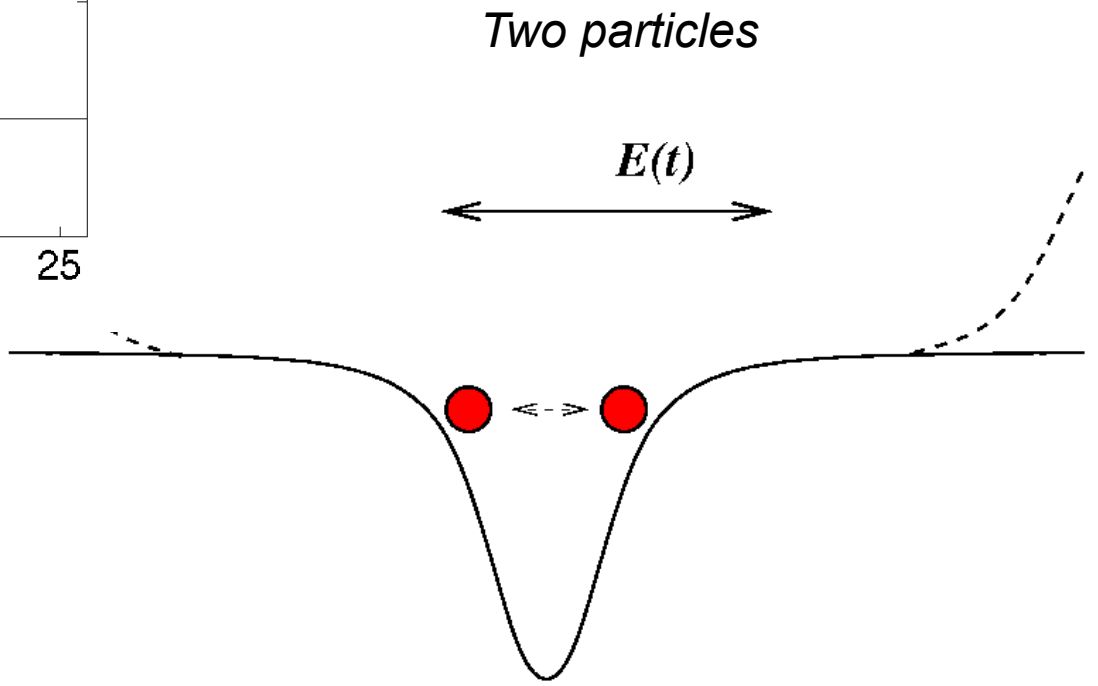
One particle



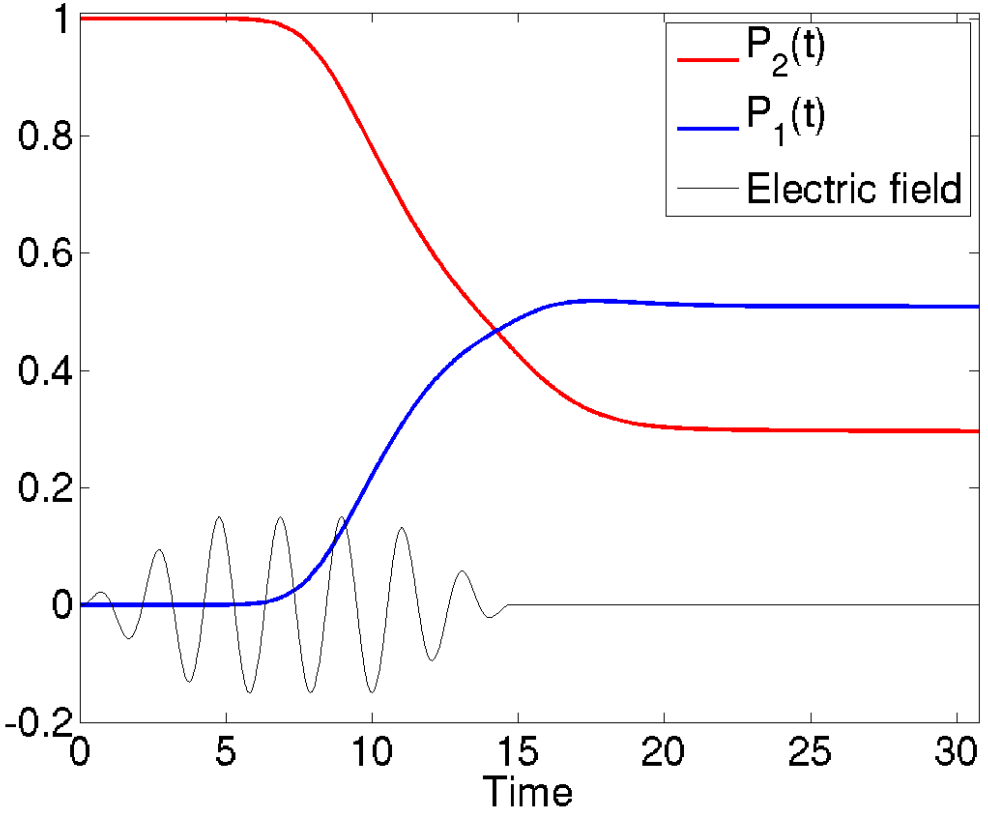


The problem...


|| Ψ(t) ||2
Electric field
1
0.8
0.6
0.4
0.2
0
-0.2
0
5
10
15
20
25
Time


Two particles
E(t)

The problem...


1
0.8
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Time
P2(t)
P1(t)
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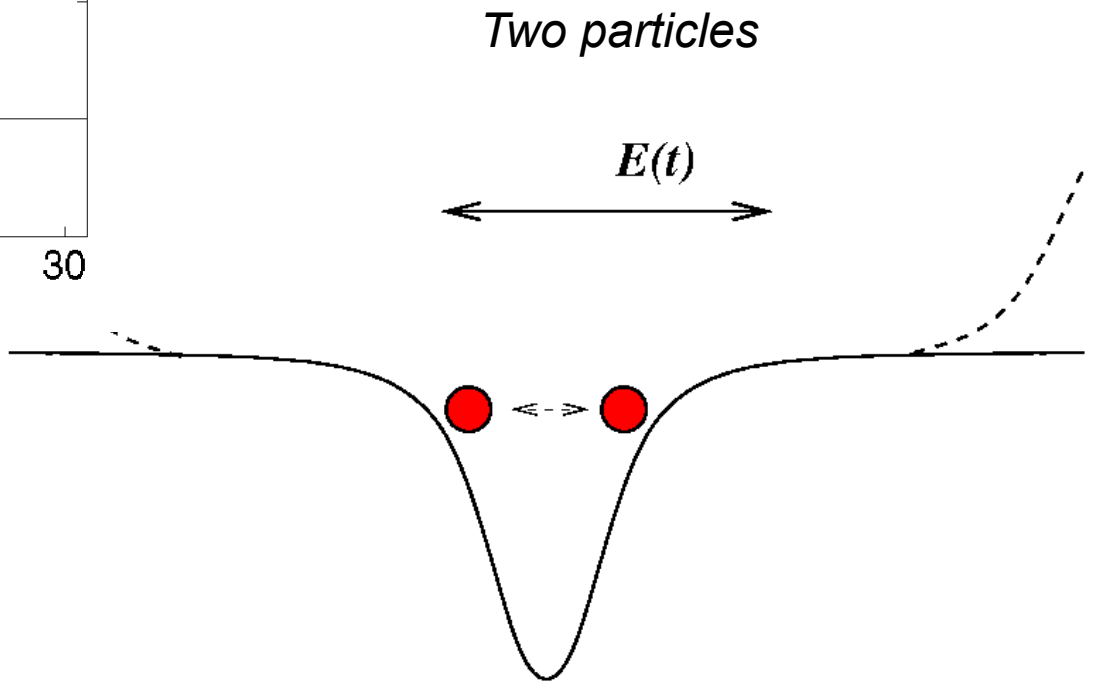
Two particles
E(t)

Formulation with variable number of particles

Fock space:

$$\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \mathcal{H}_3 \oplus \ldots$$

Field operators for identical fermions:

$$\{\psi(x), \psi^\dagger(x')\} = \delta(x - x')$$

$\psi^\dagger(x)$ *creates a particle in position* x

$\psi(x)$ *removes a particle in position* x

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One-particle operators:

$$\hat{h} = \int dx\, \psi^\dagger(x) h(x) \psi(x)$$

Two-particle operators:

$$\hat{V} = \frac{1}{2} \int dx\, \psi^\dagger(x) \psi^\dagger(x') V(x, x') \psi(x') \psi(x)$$

$$H = \hat{h} + \hat{V}$$

Formulation with variable number of particles

Foch space:

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Point:
H independent of the number of particles

One-particle operators:

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Two-particle operators:

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$$H = \hat{h} + \hat{V}$$

The absorber

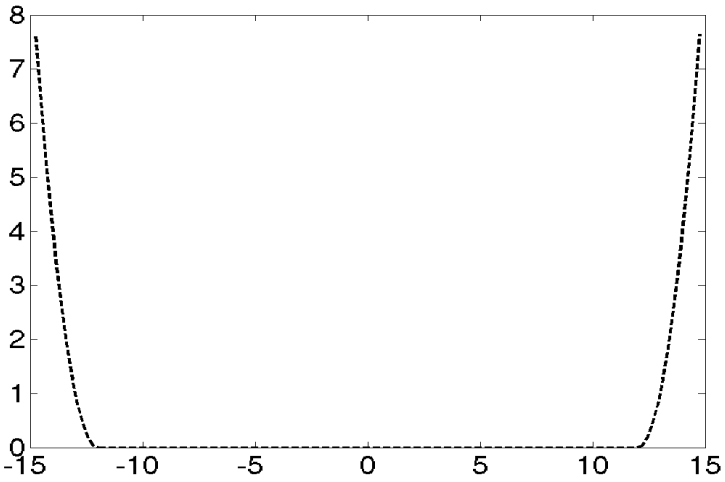
$$-i\hat{\Gamma} = -i \int dx\, \Gamma(x) \boldsymbol{\psi}^{\dagger}(x) \boldsymbol{\psi}(x)$$

$\Gamma(x)$ is zero for x in a certain (interaction) region, and positive outside of this region

Typcal choices:

Power form, $\Gamma(x) = C\xi^n, \quad \xi \equiv \max(0, x - x_T, -x_T - x)$

Manolopoulos from, *J. Chem. Phys.* **117**, 9952 (2002)



Why the Lindblad equation?

Markovian:
There is no memory of any absorbed particle

Positive:
Probabilites should remain positive at all times

Trace conserving:
The probability of having N, N-1, ..., 1 or zeros particles should always be unity

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The evolution of any such quantum mechanical process is goverened by an equation of form

$$
\begin{aligned}
i\hbar\frac{d}{dt}\rho &= [H,\rho] - i\mathcal{D}(\rho) \\
\mathcal{D} &= \sum_{m,n} \gamma_{m,n}\left(A_m^\dagger A_n\rho + \rho A_m^\dagger A_n - 2A_n\rho A_m^\dagger\right)
\end{aligned}
$$

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

Von Neumann equation (equivalent to the Schrödinger equation):

$$i\hbar\frac{d}{dt}\rho = [H, \rho]$$

Von Neumann equation with absorbing potential:

$$i\hbar\frac{d}{dt}\rho = [H, \rho] - i(\hat{\Gamma}\rho + \rho\hat{\Gamma})$$

Lindblad equation with Lindbladian on diagonal form:

$$i\hbar\frac{d}{dt}\rho = [H, \rho] - i\sum_n \left(A_n^\dagger A_n \rho + \rho A_n^\dagger A_n - 2A_n \rho A_n^\dagger\right)$$

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Identification:

$$\sum_n A_n^\dagger A_n \to \int dx A^\dagger(x)A(x) \longrightarrow \int dx\, \Gamma(x)\boldsymbol{\psi}^\dagger(x)\boldsymbol{\psi}(x) = \int dx\, A^\dagger(x)A(x)$$

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Identification:

$$A(x) \equiv \sqrt{\Gamma(x)}\boldsymbol{\psi}(x)$$

$$i\hbar\frac{d}{dt}\rho = [H,\rho] - i\{\hat{\Gamma},\rho\} + 2i\int dx\,\Gamma(x)\boldsymbol{\psi}(x)\rho\boldsymbol{\psi}^{\dagger}(x)$$

«Normal» dynamics

Absorption

Transition to system with fewer particles

$$\boldsymbol{\psi}(x) : \mathcal{H}_N \rightarrow \mathcal{H}_{N-1}$$

$$\rho = |\Psi_N\rangle\langle\Psi_N| \Rightarrow \boldsymbol{\psi}\rho\boldsymbol{\psi}^{\dagger} \sim |\Psi_{N-1}\rangle\langle\Psi_{N-1}|$$

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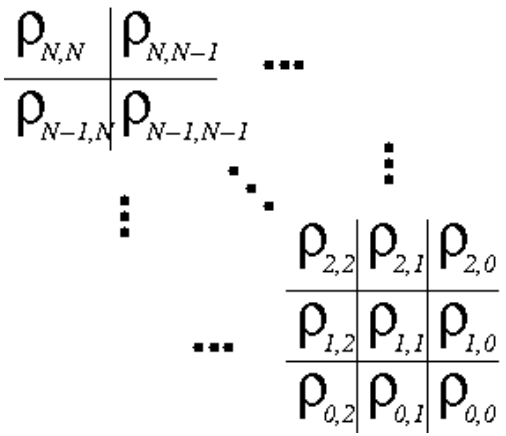
Structure of the denstity matrix:



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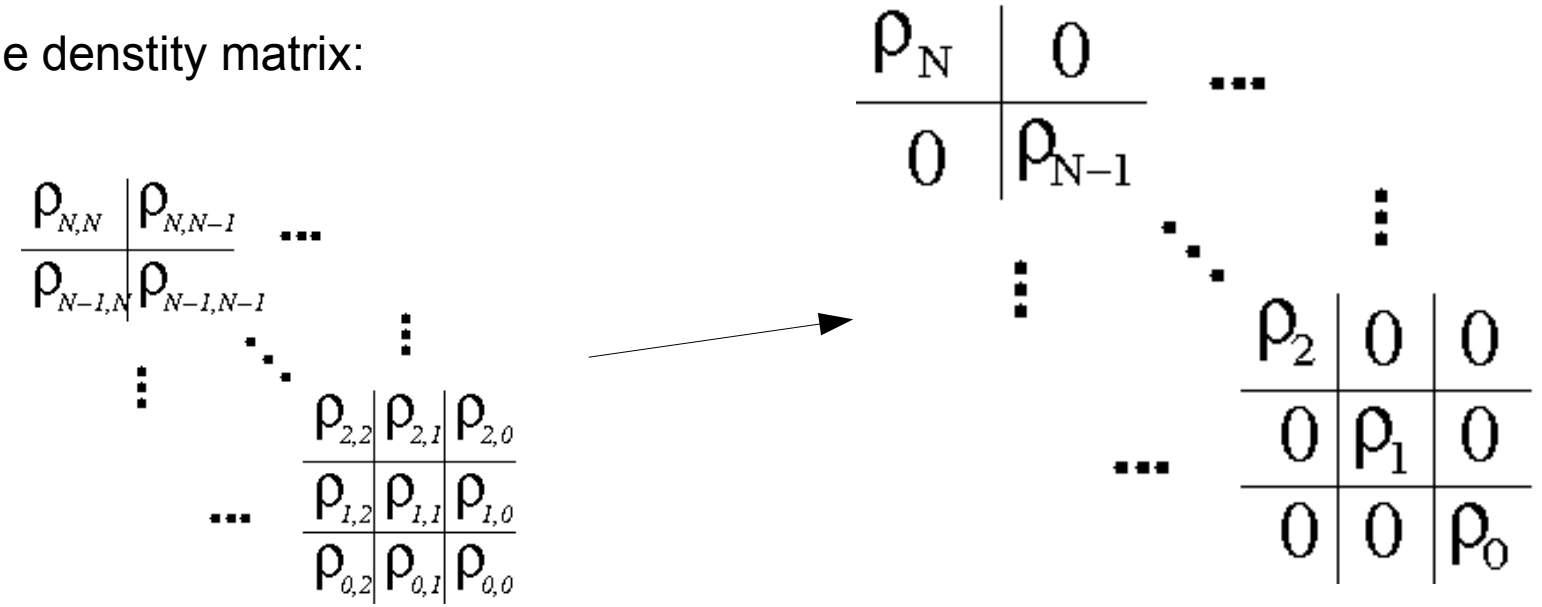


Finally:

$$i\hbar\frac{d}{dt}\rho_n = [H,\rho_n] - i\{\hat{\Gamma},\rho_n\} + 2i\int dx\,\Gamma(x)\boldsymbol{\psi}(x)\rho_{n+1}\boldsymbol{\psi}(x)$$

Special cases:

Pure initial state

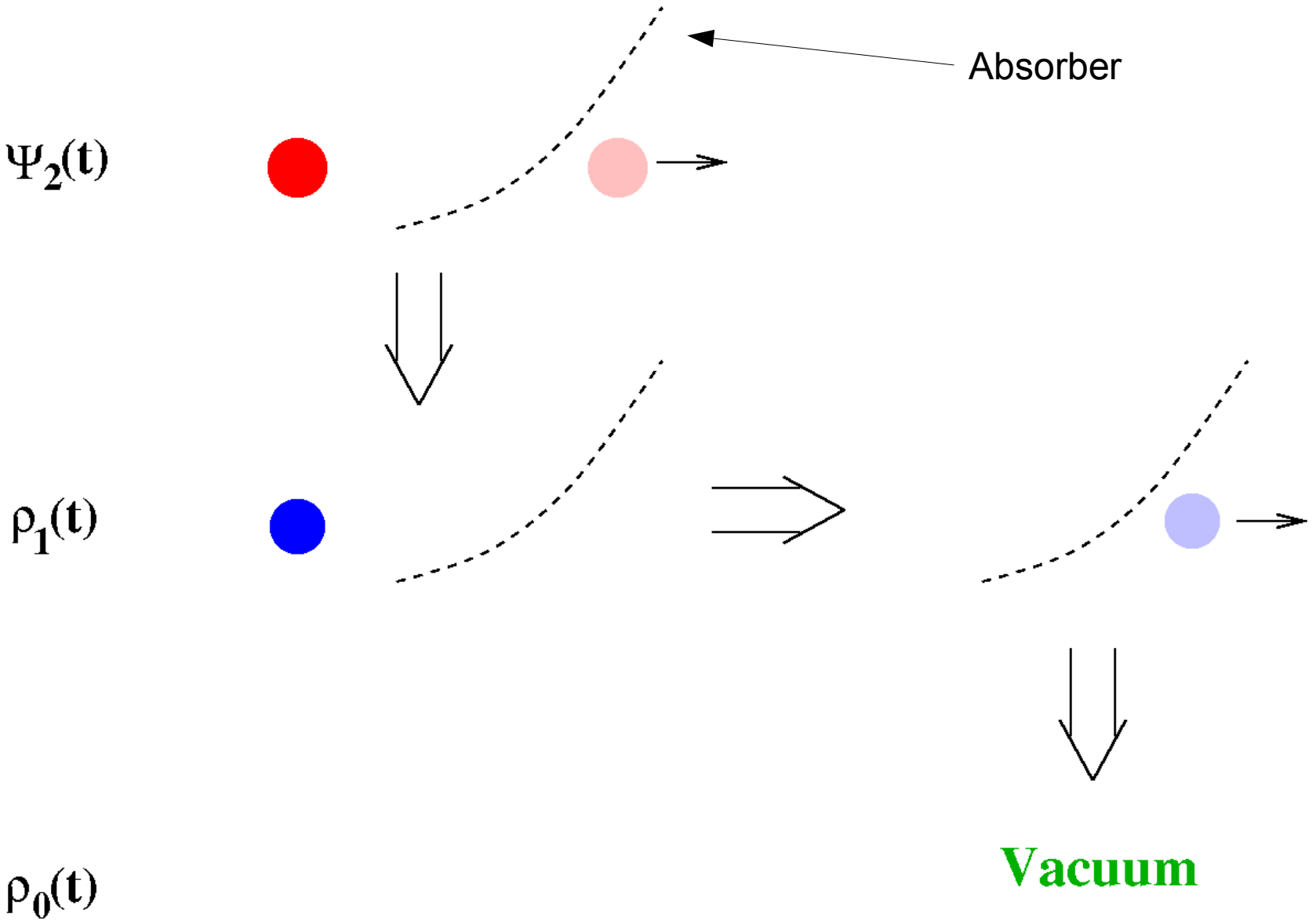
$$\rho(t=0) = |\Psi_N\rangle\langle\Psi_N| \Rightarrow i\hbar\frac{d}{dt}|\Psi_N\rangle = (H - i\hat{\Gamma})|\Psi_N\rangle$$

Vacuum (no particles)

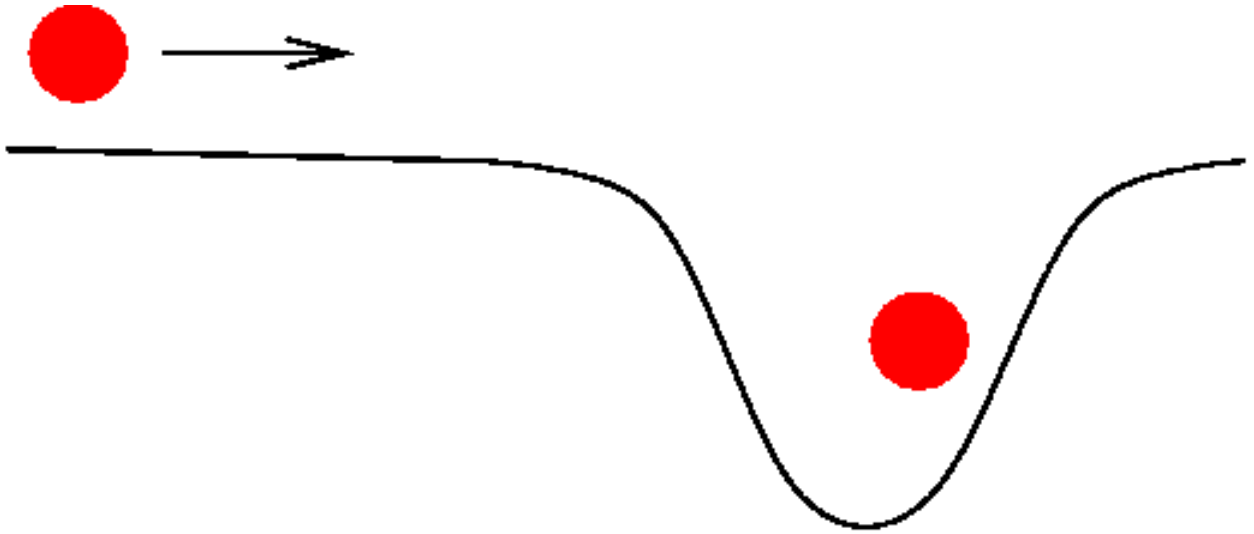
$$\rho_0 = p_0(t)|-\rangle\langle -|, \quad \hbar\frac{dp_0}{dt}|-\rangle\langle -| = 2\int dx\,\Gamma(x)\boldsymbol{\psi}(x)\,\rho_1\,\boldsymbol{\psi}^\dagger(x)$$

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

Schematically (two particles):



Example: Collision in a Gaussian well



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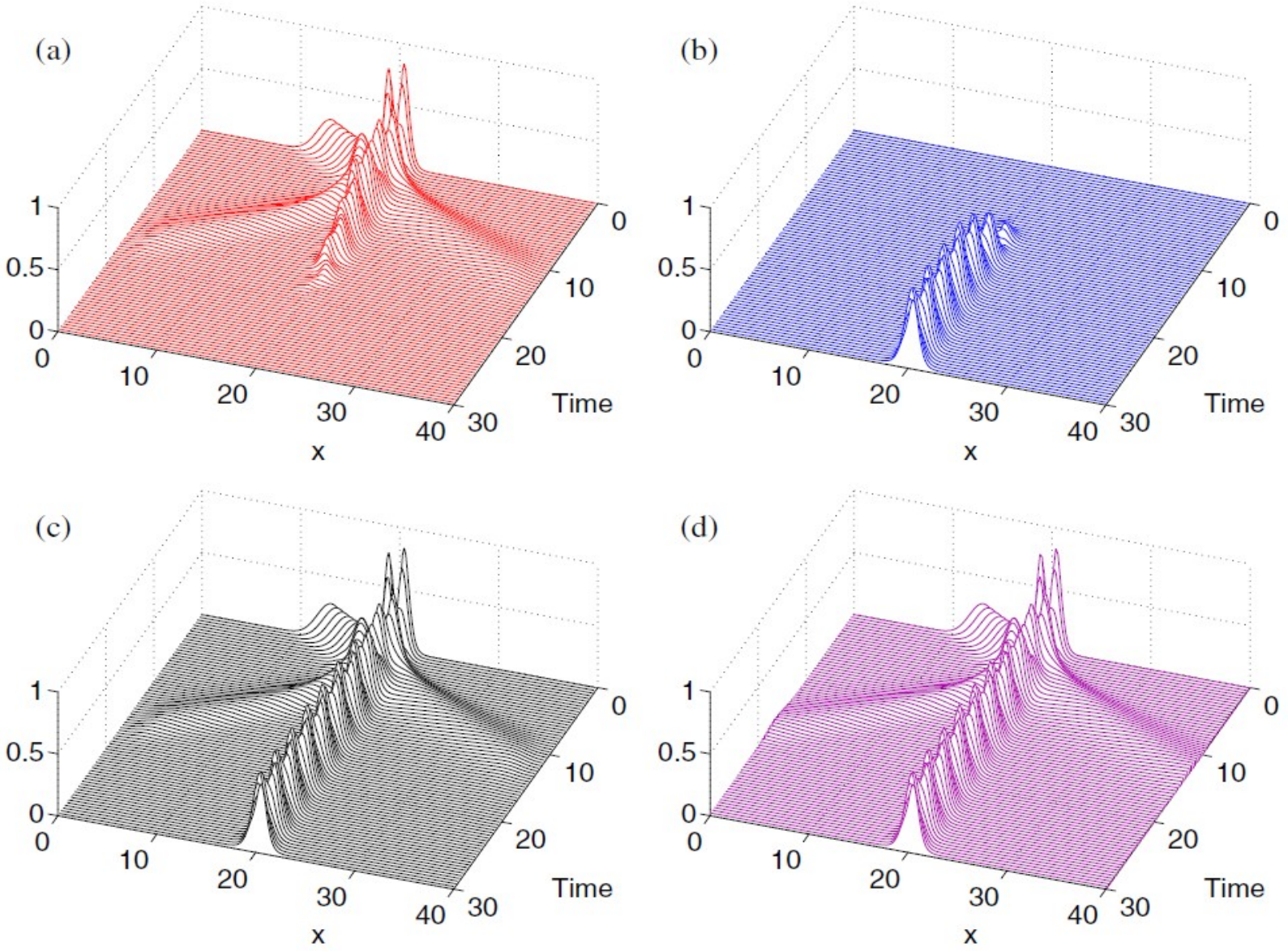

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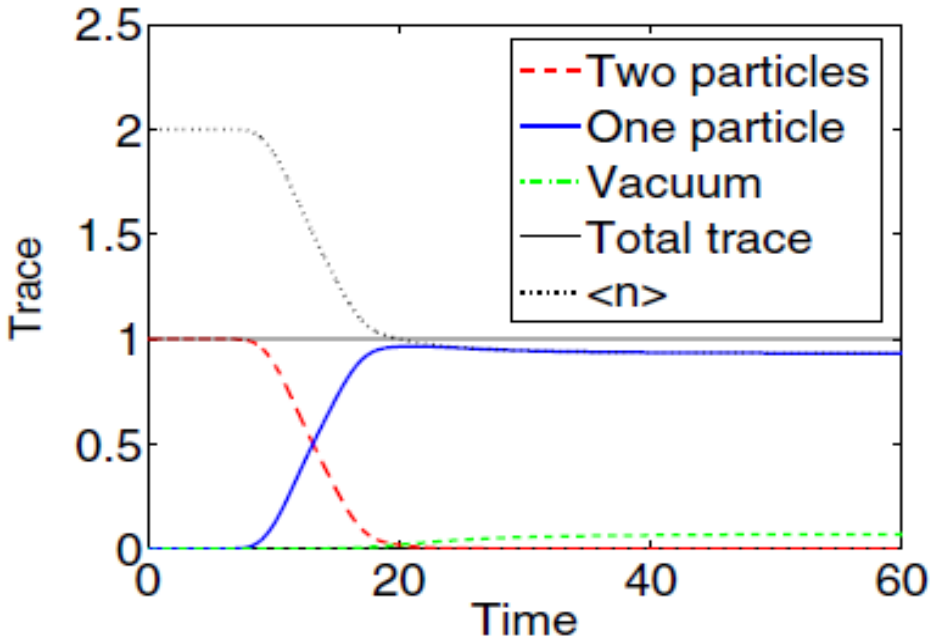
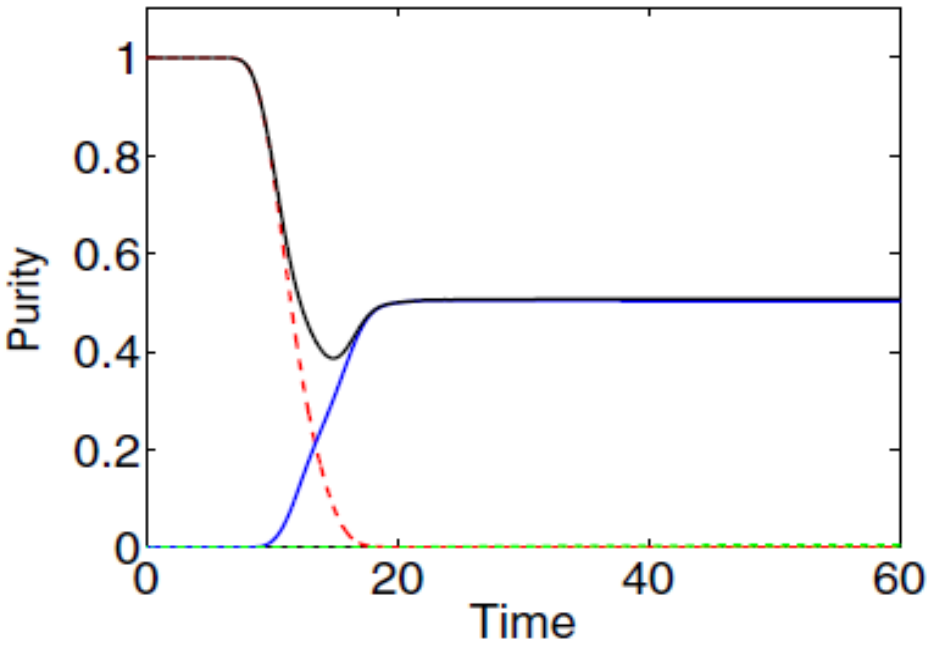
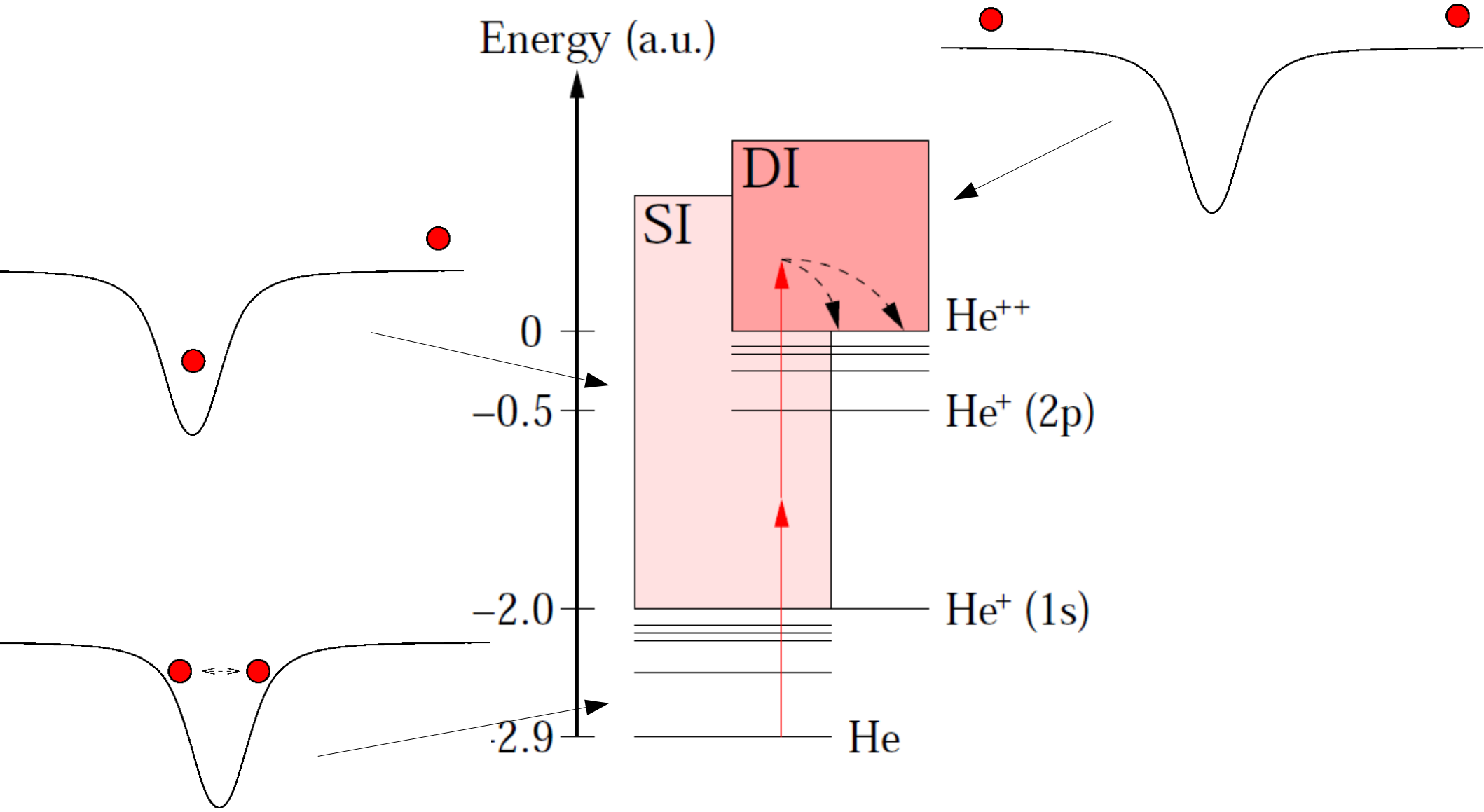


$$\rho \sim \begin{pmatrix} |\Psi_2(x_1,x_2,t)\rangle\langle\Psi_2(x_1',x_2',t)| & 0 & 0 \\ 0 & \rho_1(x,x',t) & 0 \\ 0 & 0 & p_0(t) \end{pmatrix}$$

Purity: $\zeta \equiv \mathrm{Tr}(\rho^2)$



Application: *Non-sequential two-photon double ionization of helium*



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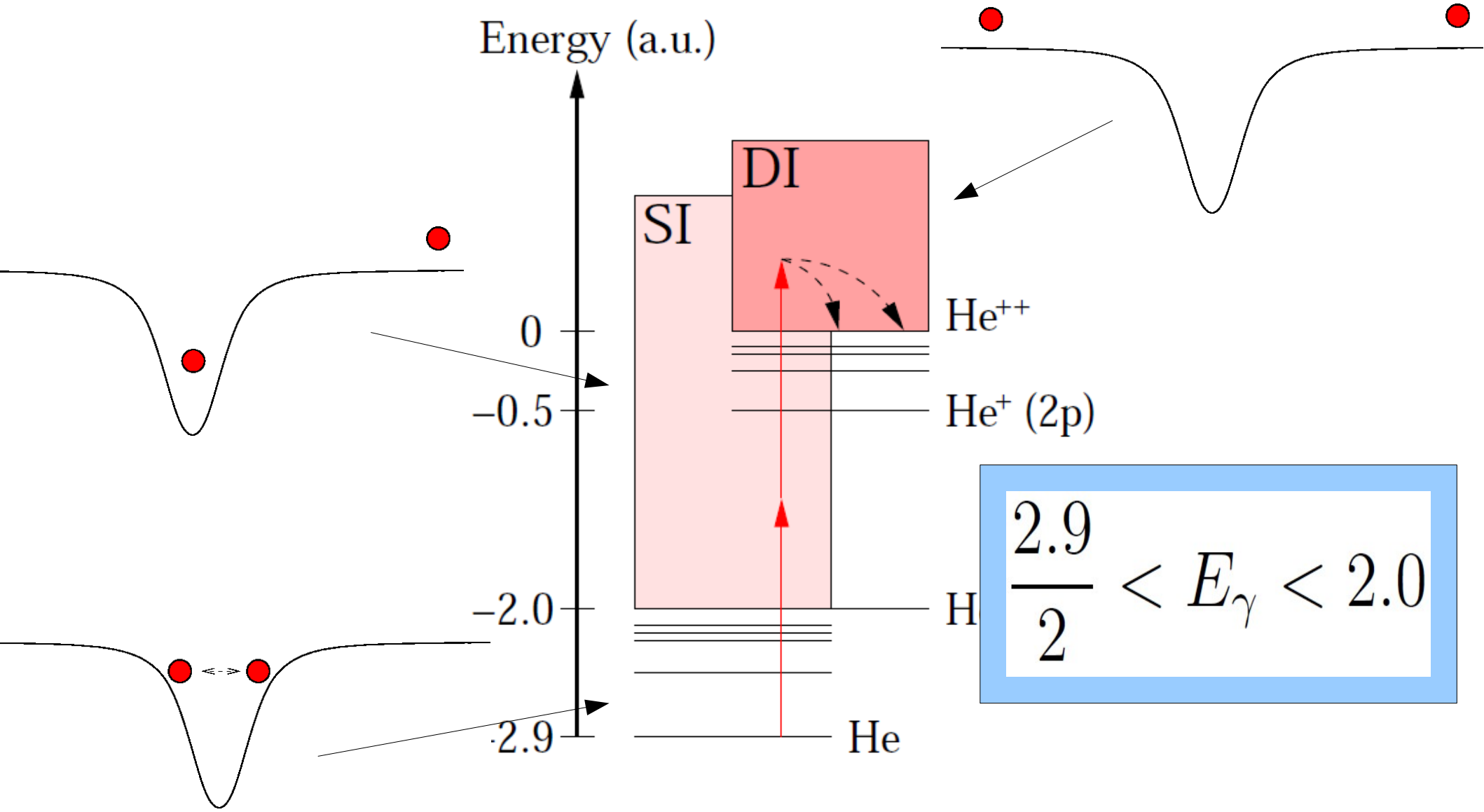


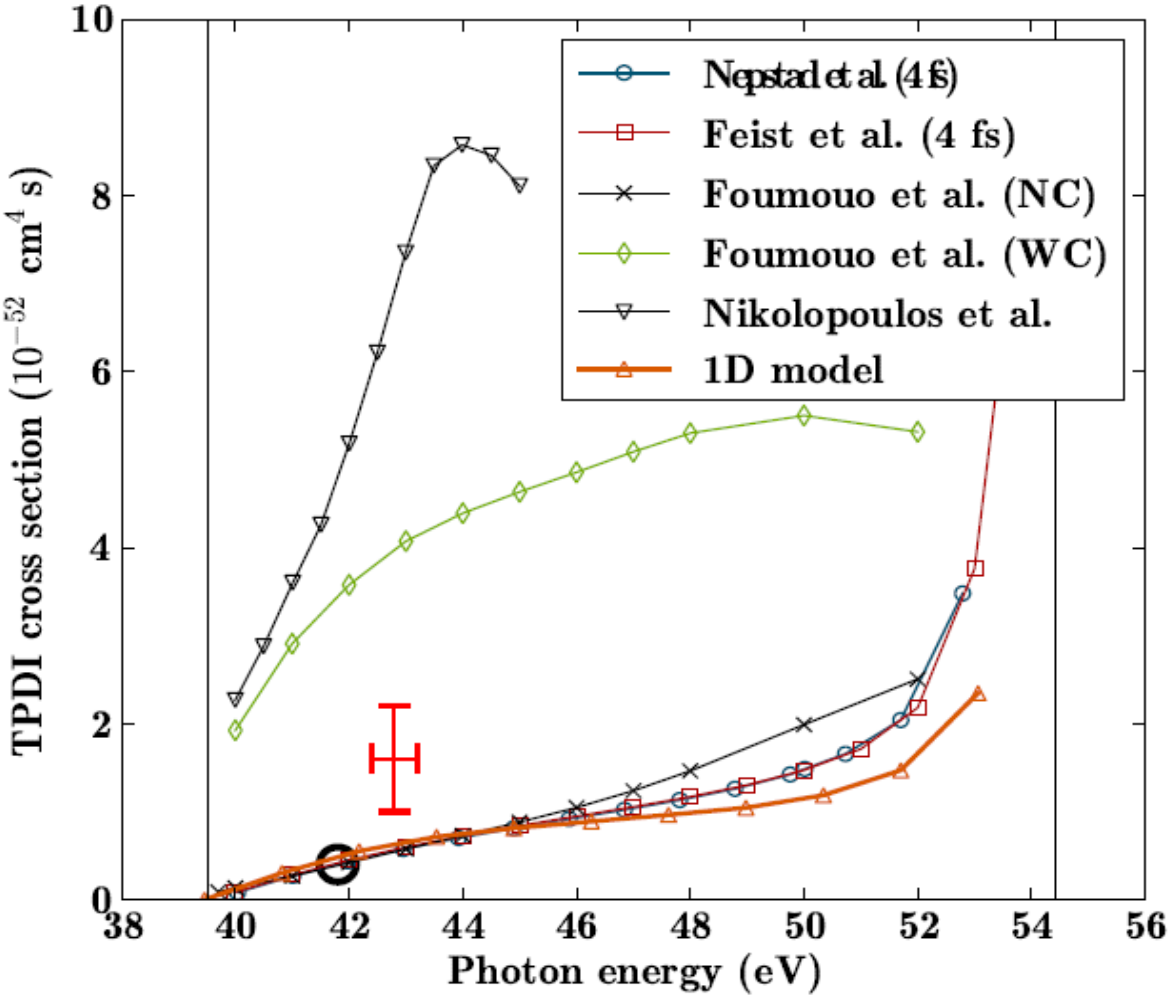
$$\frac{2.9}{2} < E_\gamma < 2.0$$

Results still debated

$$P_{\mathrm{DI}} = \sum_k |\langle \Phi_k^{\mathrm{DC}} | \Psi(t > T) \rangle|^2$$

$$\approx \sum_{n,m} |\langle \{\phi_n^{\mathrm{UC}} \phi_m^{\mathrm{UC}}\} | P_{\mathrm{UB}} | \Psi(t \to \infty) \rangle|^2$$

?

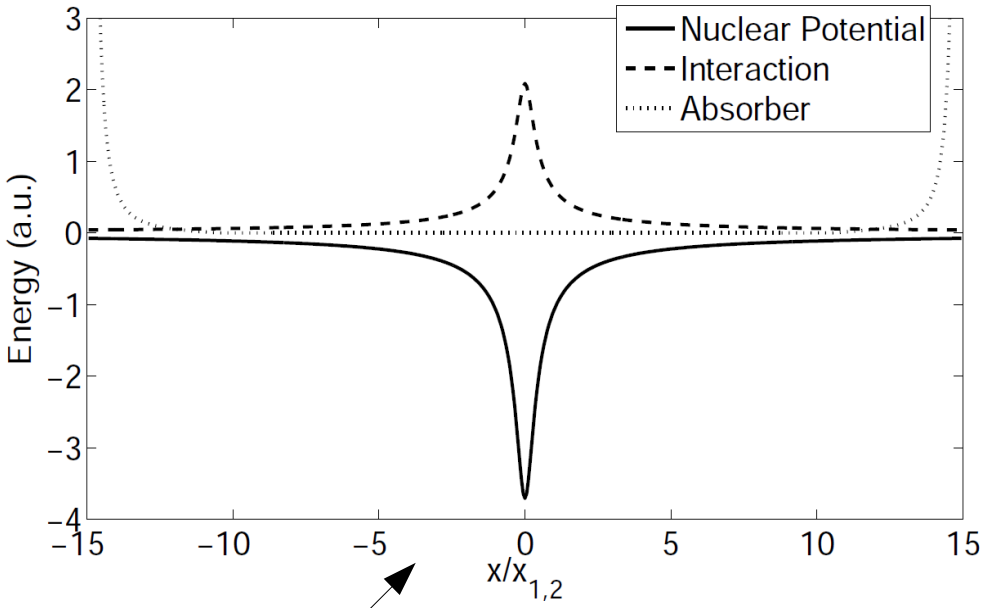


DI: *Direct ionization*
DC: *Double continuum*
UC: *Uncorrelated*
UB: *Unbound*

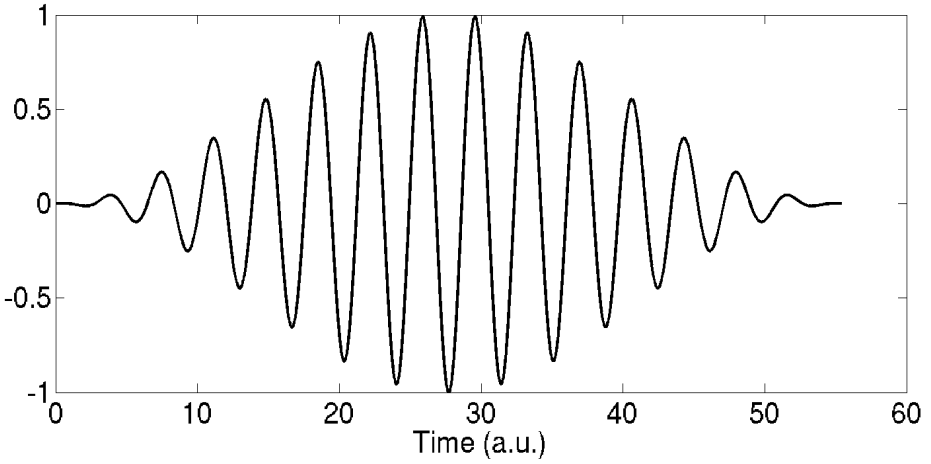
$$H = h(x_1) + h(x_2) + V(x_{1,2})$$

$$x_{1,2} \to \infty \Rightarrow V(x_{1,2}) \to 0$$

Ionization probabilities via the Lindblad equation

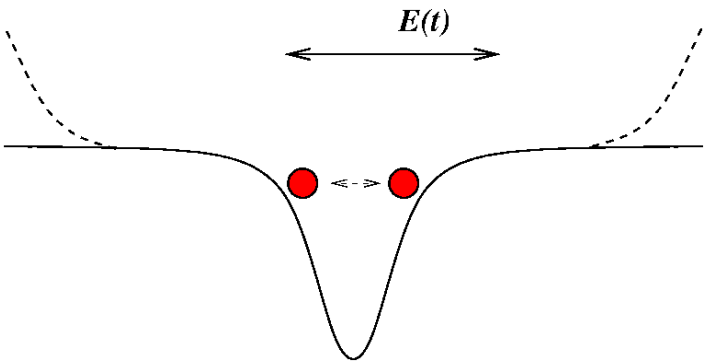


$$E(t) = E_0 \sin^2\left(\frac{\pi t}{T}\right) \sin(\omega t + \varphi)$$



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

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



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

Ionization probabilities via the Lindblad equation

Two particles

$$i\hbar\frac{d}{dt}|\Psi_2\rangle = (H - i\Gamma(x_1) - i\Gamma(x_2))\,|\Psi_2\rangle$$

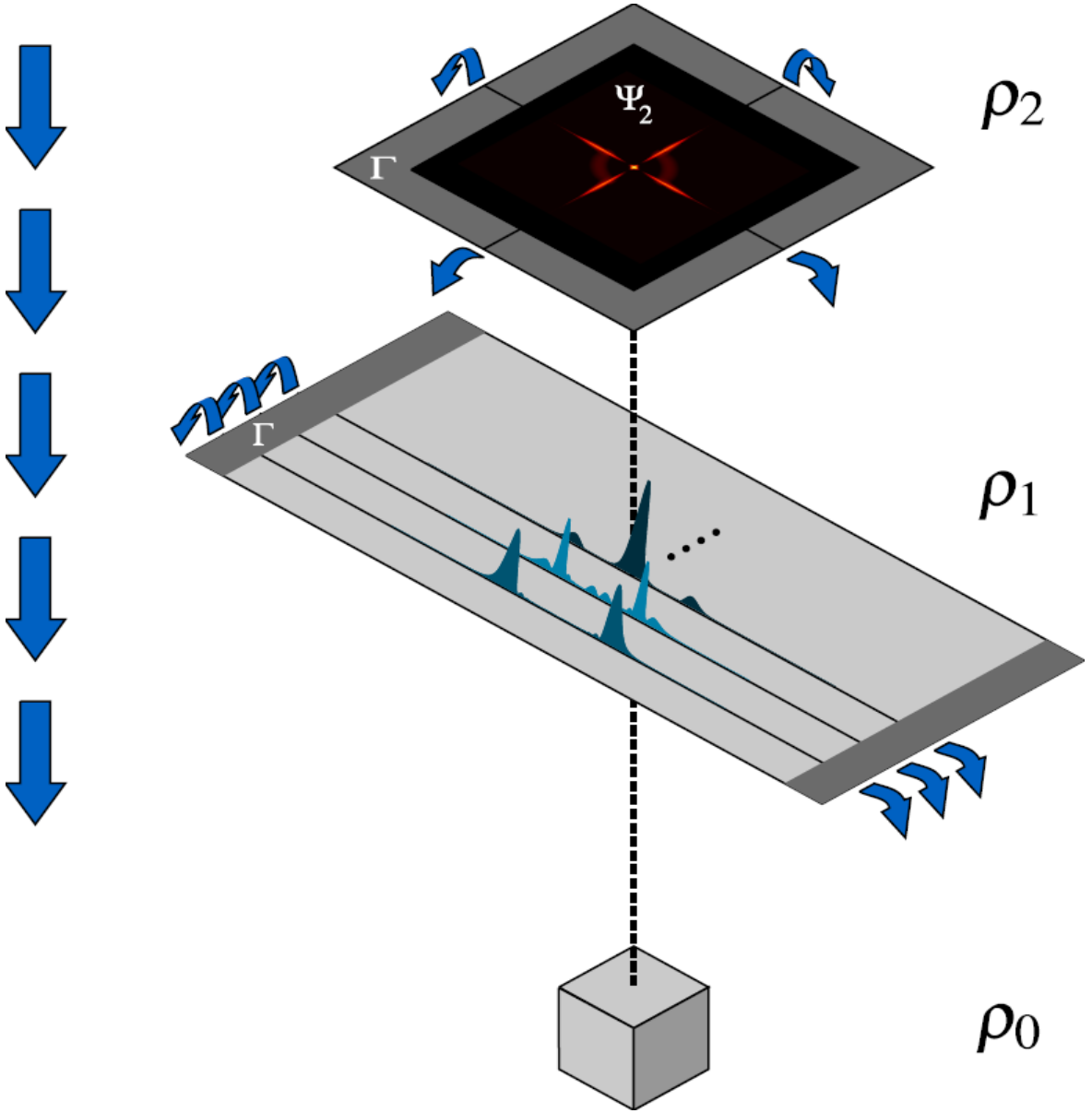
One particle

$$i\hbar\frac{d}{dt}\rho_1 = [h,\rho_1] - i\{\Gamma,\rho_1\} + 2i\int \Gamma(x)\boldsymbol{\psi}(x)|\Psi_2\rangle\langle\Psi_2|\boldsymbol{\psi}^\dagger(x)\,dx$$

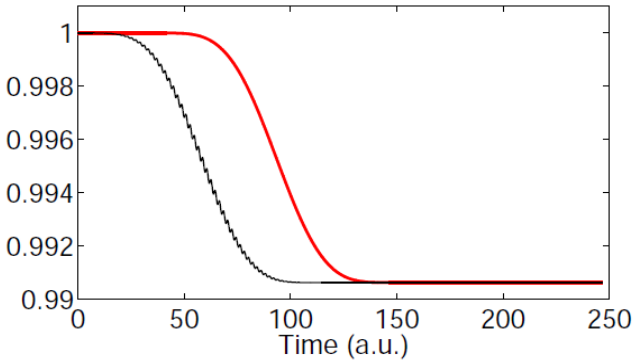
No particles

$$\hbar\frac{d}{dt}\rho_0 = 2\int \Gamma(x)\boldsymbol{\psi}(x)\rho_1\boldsymbol{\psi}^\dagger(x)\,dx,$$

Ionization probabilities via the Lindblad equation



Ionization probabilities via the Lindblad equation

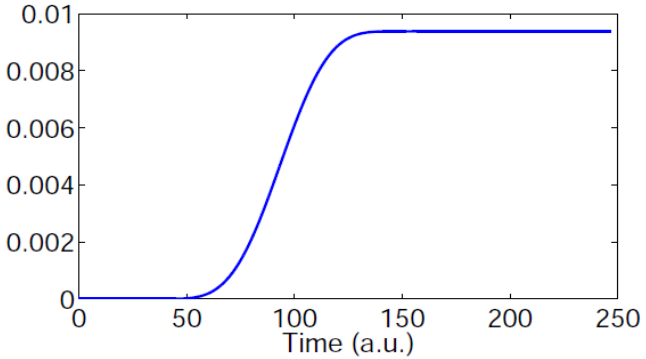


$$p_2(t) = \|\Psi_2(t)\|^2$$

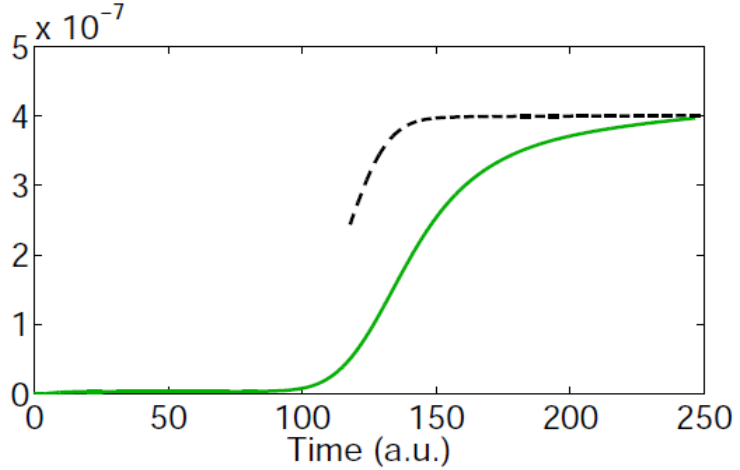
Pulse duration: 30 cycles (118 a.u.)

Intensity: 2.2×10^{13} W/cm^2

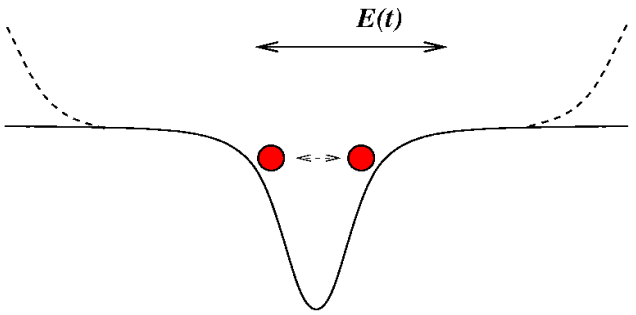
Photon energy: 43.5 eV



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



$$p_0(t) \xrightarrow{?} P_{\mathrm{DI}}$$

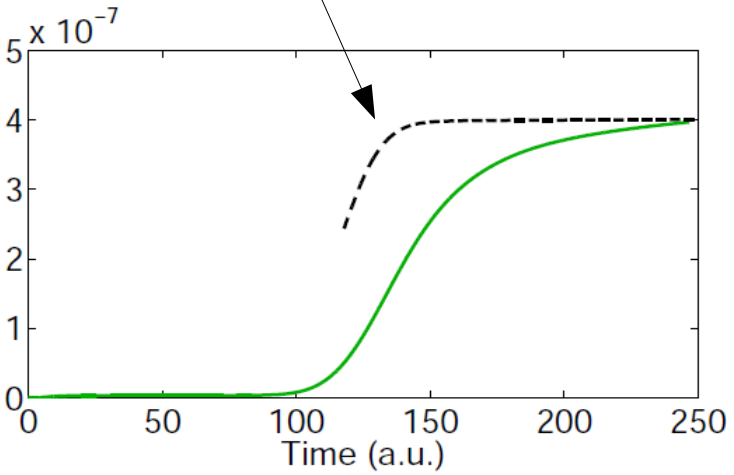


Ionization probabilities via the Lindblad equation

Analyze source-term on the fly

$$\Delta\rho_1^{\text{source}}(t) \approx \Delta t \times \frac{2}{\hbar}\int dx\,\Gamma(x)\boldsymbol{\psi}(x)|\Psi_2\rangle\langle\Psi_2|\boldsymbol{\psi}^\dagger(x)$$

$$P_{\text{DI}}(t+\Delta t) = P_{\text{DI}}(t) + \text{Tr}(\Delta\rho_1^{\text{source}}(t)\sum_n |\varphi_n^{\text{cont}}\rangle\langle\varphi_n^{\text{cont}}|)$$



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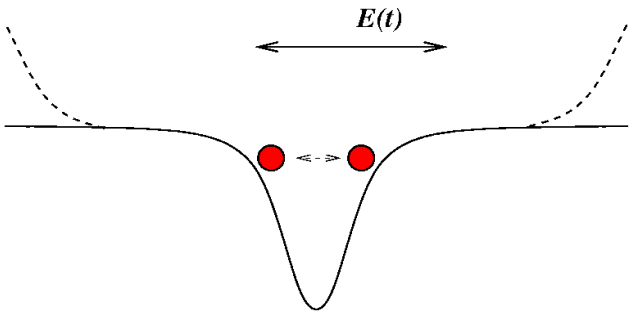
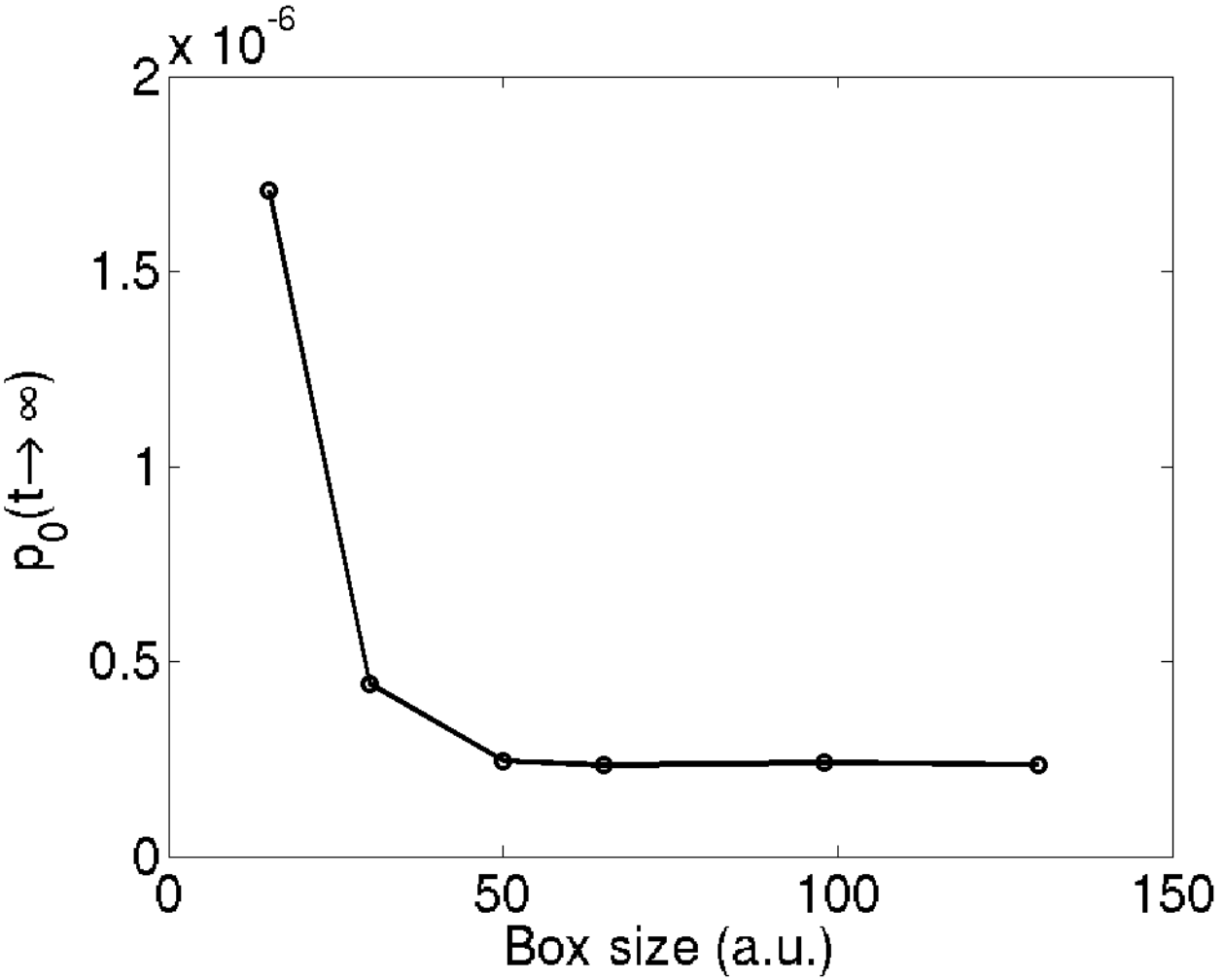


Convergence in «box size»



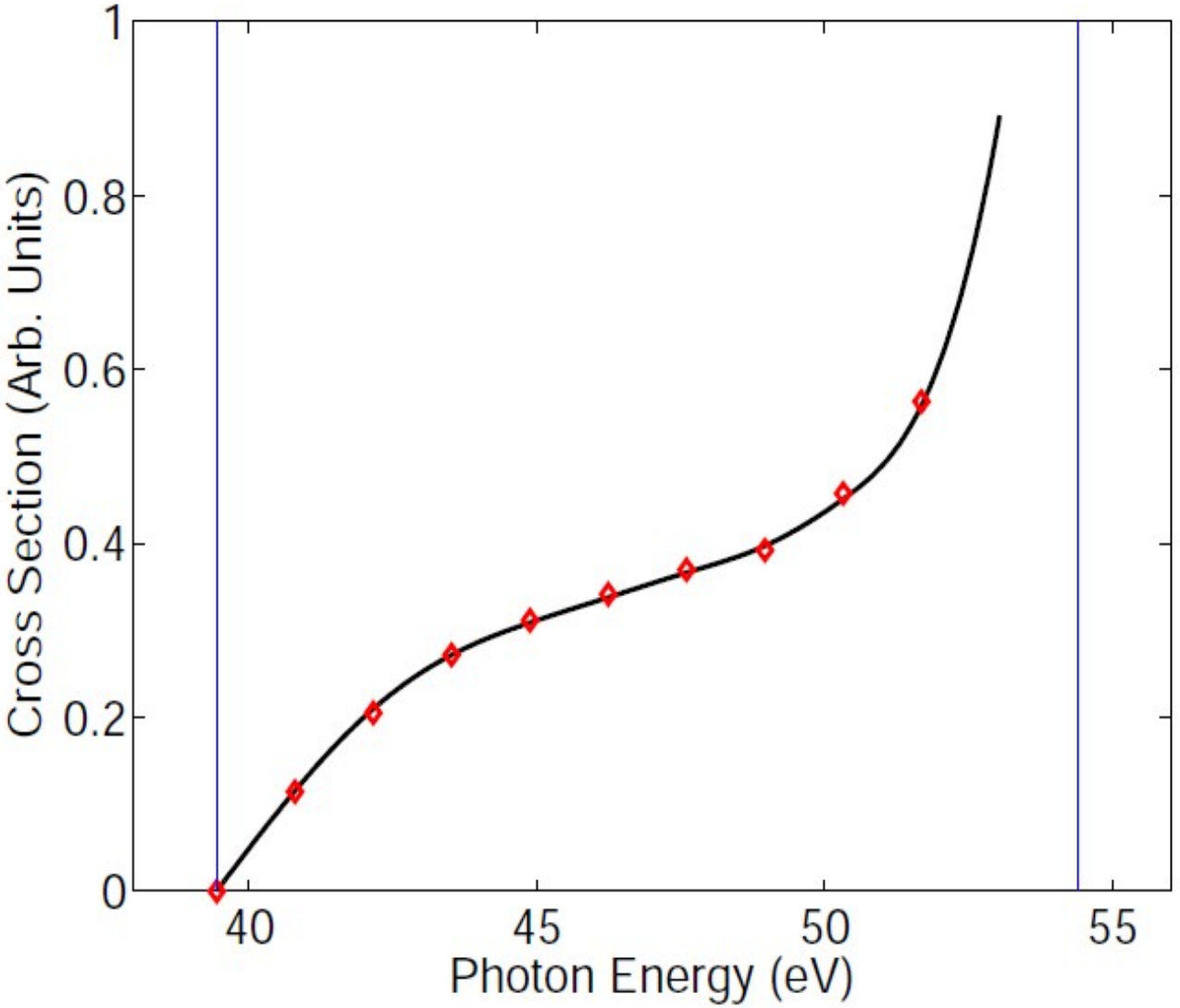
Pulse duration: 16 cycles

Intensity: 2.2×10^{13} W/cm^2

Photon energy: 46.2 eV

Absorber «turned on» at distances less than 20% of the box size from the edges

Does it work?


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

Partial widths?

Partial widths?

Maybe...

Resonance N-particle wave function(?):

$$\Psi_{\rm res}(t) = e^{-i(E_p - iE_w)t/\hbar}\,\psi_{\rm res}$$

Solves the N-particle equation,

$$\begin{aligned} \rho_N &\equiv |\Psi_{\rm res}\rangle\langle\Psi_{\rm res}| = e^{-2E_w t/\hbar}|\psi_{\rm res}\rangle\langle\psi_{\rm res}| \\ i\hbar\dot{\rho}_N &= [H,\rho_N] - i\{\Gamma,\rho_N\} \end{aligned}$$

Partial widths?

Bound (remaining) part

Electron travelling outwards

Assume asymptotic form:

$$\Psi_{\rm res} \sim \sum_c \{\Phi_c(\{x\})\chi_c(r)\}$$

Gives *N-1* system of form:

$$\rho_{(N-1)}(t) = \sum_c p_c(t)|\Phi_c(\{x\};t)\rangle\langle\Phi_c(\{x\};t)|$$

$p_c(t)$ may then provide the partial width corresponding to channel c

Partial widths?

$$\begin{aligned}
\mathcal{N} &= |\Psi_N(t)|^2 = e^{-\Gamma t} \Rightarrow \qquad (\hbar = 1) \\
\dot{\mathcal{N}} &= -\Gamma \mathcal{N} \\
\dot{p}_c(t) &= \Gamma_c \mathcal{N} \Rightarrow \\
p_c(t \to \infty) &= \frac{\Gamma_c}{\Gamma}, \quad \sum_c \Gamma_c = \Gamma
\end{aligned}$$

$p_c(t)$ found as eigenvalues to ρ_{N-1} or, if it the decay products are know, as:

$$p_c(t) = \langle \Phi_c(\{x\}) | \rho_{N-1} | \Phi_c(\{x\}) \rangle$$

Particularely:

Analyze what is left instead of what is leaving

Summary

-Applying absorbing boundry conditions to the time dependent Schrödinger equation may be problematic in an many-body context.

-The proper generalization of the concept of complex absorbing potentials is achieved through the Lindblad equation.

-The remaining system after absorbption is subject to loss of coherence (i.e. it is not a pure state),

-Within this formalism it is possible to describe the dynamics of remaining particles while others have been absorbed.

-The formalism facilitates the distinction between single, double etc. ionization.

-Suggest a method for distinguishing decay into varous channels?

What about complex rotation?

$$H(\{\mathbf{r}_i\},\{\mathbf{p}_i\}) \rightarrow H^{\theta} \equiv H(\{\mathbf{r}_i e^{i\theta}\},\{\mathbf{p}_i e^{-i\theta}\})$$

$$H = \sum_i^n \left(\cos(2\theta)\frac{p_i^2}{2m} + \mathrm{Re}(V^{\theta}(x_i)) \right) + \sum_{j<i}^n \mathrm{Re}\left(u^{\theta}(x_i,x_j)\right)$$

$$\begin{aligned} \Gamma^{(1)} &= \sum_i^n \left(\sin(2\theta)\frac{p_i^2}{2m} - \mathrm{Im}\left(V^{\theta}(x_i)\right) \right) \\ \Gamma^{(2)} &= -\sum_{j<i}^n \mathrm{Im}\left(u^{\theta}(x_i,x_j)\right), \end{aligned}$$

$$
\begin{aligned}
A^{(1)}_n &= c_n, \\
\gamma^{(1)}_{m,n} &= \langle \varphi_m | \Gamma^{(1)} | \varphi_n \rangle
\end{aligned}
$$

$$
\begin{aligned}
A^{(2)}_{(m,n)} &= c_n c_m \\
\gamma^{(2)}_{(k,l),(m,n)} &= \langle \varphi_k \varphi_l | \Gamma^{(2)} | \varphi_m \varphi_n \rangle
\end{aligned}
$$

$$
\begin{aligned}
& i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \rho_{m,n} = [H, \rho_{m,n}] - i\{\Gamma, \rho_{m,n}\} + \\
& 2i \sum_{i,j} \langle \varphi_i | \Gamma^{(1)} | \varphi_j \rangle c_j \rho_{m+1,n+1} c_i^\dagger + \\
& i \sum_{i,j,k,l} \langle \varphi_i \varphi_j | \Gamma^{(2)} | \varphi_k \varphi_l \rangle c_l c_k \rho_{m+2,n+2} c_i^\dagger c_j^\dagger
\end{aligned}
$$

Rquirement: Γ (γ-tensors) must be positive semi-definite

Interaction: $E(t) \cdot \boldsymbol{x}\, e^{i\theta}$ or $A(t) \cdot \boldsymbol{p}\, e^{-i\theta}$

Γ ***no longer positive semi-definite***

Consequently: The flow does no longer have a well-defined direction