Solving the Dirac equation for hydrogenlike systems exposed to intense electromagnetic pulses

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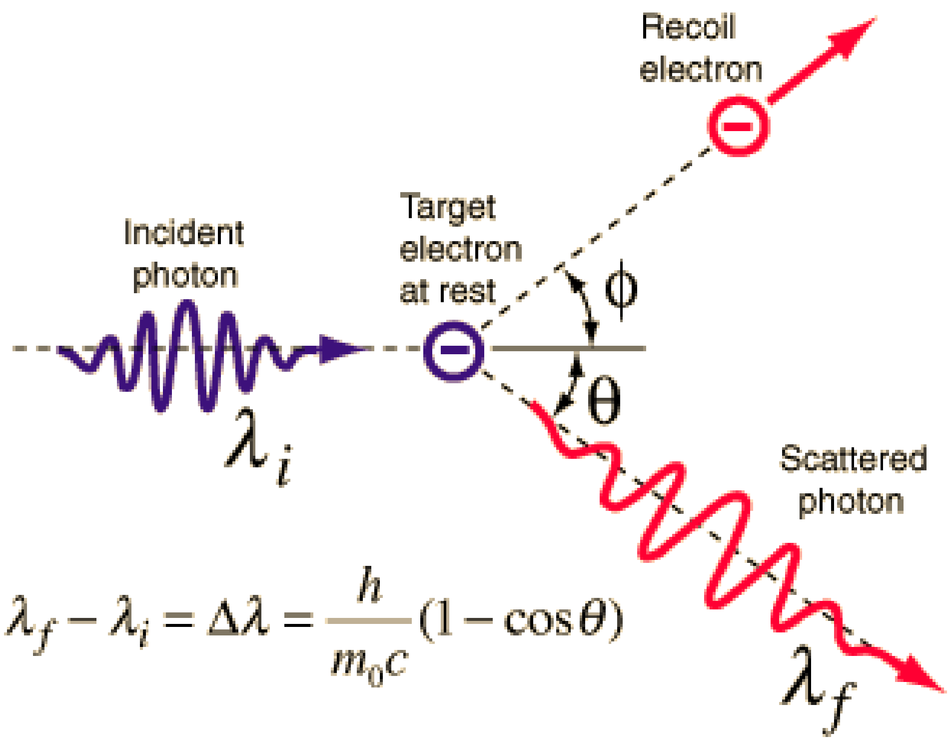
Thomson scattering
(low energy Compton scattering)



$$\lambda_f - \lambda_i = \Delta\lambda = \frac{h}{m_0 c}(1-\cos\theta)$$

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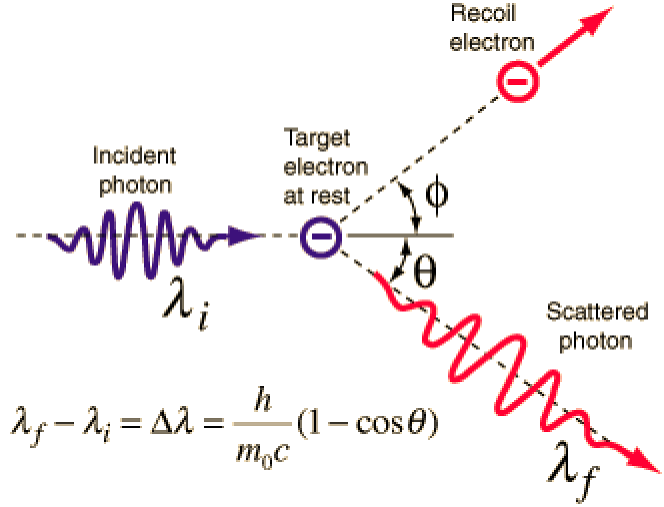
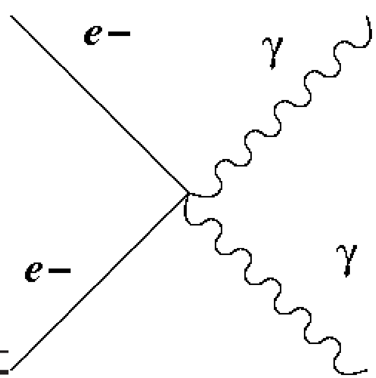
Thomson scattering



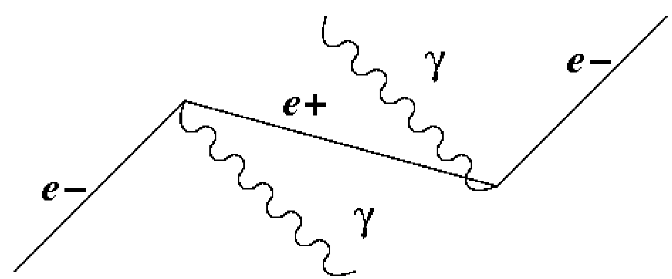
Non-relativistic

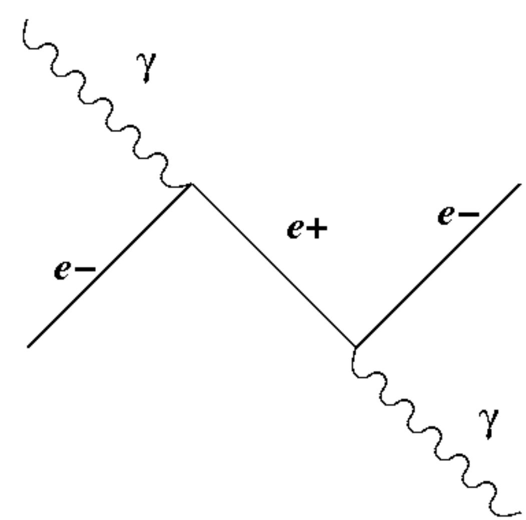
$$H_I = \mathbf{A} \cdot \mathbf{p} + \frac{1}{2} A^2$$



Relativistic

$$H_I = c\mathbf{A} \cdot \boldsymbol{\alpha}$$





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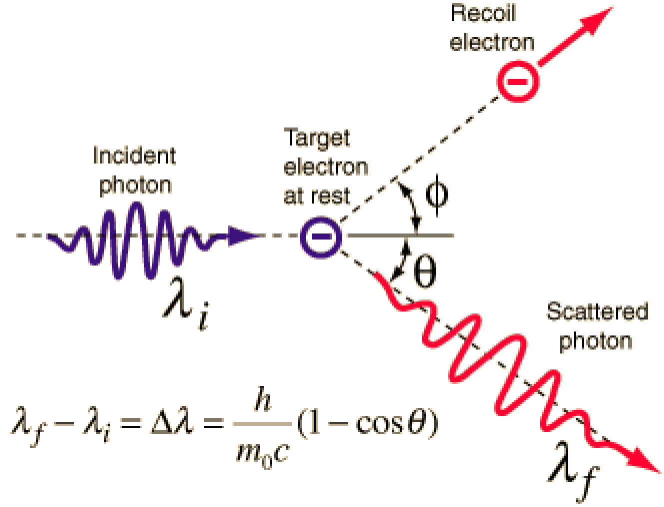
Thomson scattering



Non-relativistic

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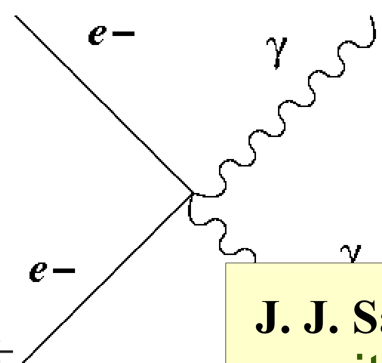

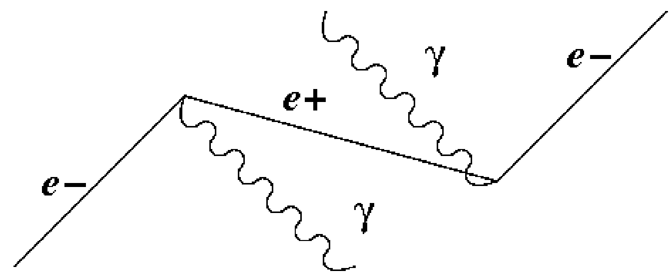

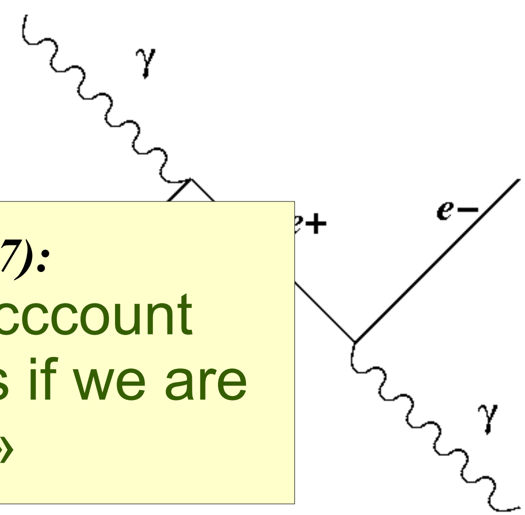

J. J. Sakurai, in «*Advanced Quantum Mechanics*» (1967):
«... it is absolutely necessary to take into acccount transitions involving *negative-energy* states if we are to obtain the correct *nonrelativistic* results.»

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The equation

$$i\dot{\Psi} = [H_0 + H_I(t)]\Psi$$

$$H_0 = c\mathbf{p}\cdot\boldsymbol{\alpha} - \frac{Z}{r} + c^2\beta$$

$$H_I = c\mathbf{A}\cdot\boldsymbol{\alpha}$$

Assumed:

-Point nucleus

-Separability of two particle-problem (infinite nuclear mass)

-No retardation effects in the Coulomb interaction

-Not quantized photon field

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The equation

$$i\dot{\Psi} = [H_0 + H_I(t)]\Psi$$

$$H_0 = c\mathbf{p}\cdot\boldsymbol{\alpha} - \frac{Z}{r} + c^2\beta$$

$$H_I = c\mathbf{A}\cdot\boldsymbol{\alpha}$$

Relativistic effects:

-High nuclear charge *(structure)*

-Intense field, high photon energy *(dynamics)*

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Expansion

$$\Psi(t) = \sum_a c_a(t)\psi_a(\mathbf{r})$$

$$H_0\psi_a(\mathbf{r}) = \varepsilon_a\psi_a(\mathbf{r})$$

$$a = (n, \kappa, j, m)$$

$$\psi_{n,\kappa,j,m}(\mathbf{r}) = \frac{1}{r}\begin{pmatrix} P_{n,\kappa}(r)X_{\kappa,j,m} \\ iQ_{n,\kappa}(r)X_{-\kappa,j,m} \end{pmatrix}$$

$$\kappa \equiv \begin{cases} l, & j = l - 1/2 \\ -(l+1), & j = l + 1/2 \end{cases}$$

$$X_{\kappa,j,m} \equiv \sum_{m_l,m_s} \langle l_\kappa, m_\kappa, s = 1/2, m_s | j, m\rangle Y_{l_\kappa,m_l}(\hat{\mathbf{r}})\chi_{m_s}$$

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S. Salomonson and P. Öster, Phys. Rev. A **40**, 5548 (1989)

Expansion

$$\Psi(t) = \sum_a c_a(t)\psi_a(\mathbf{r})$$

$$H_0\psi_a(\mathbf{r}) = \varepsilon_a\psi_a(\mathbf{r})$$

Diagonal

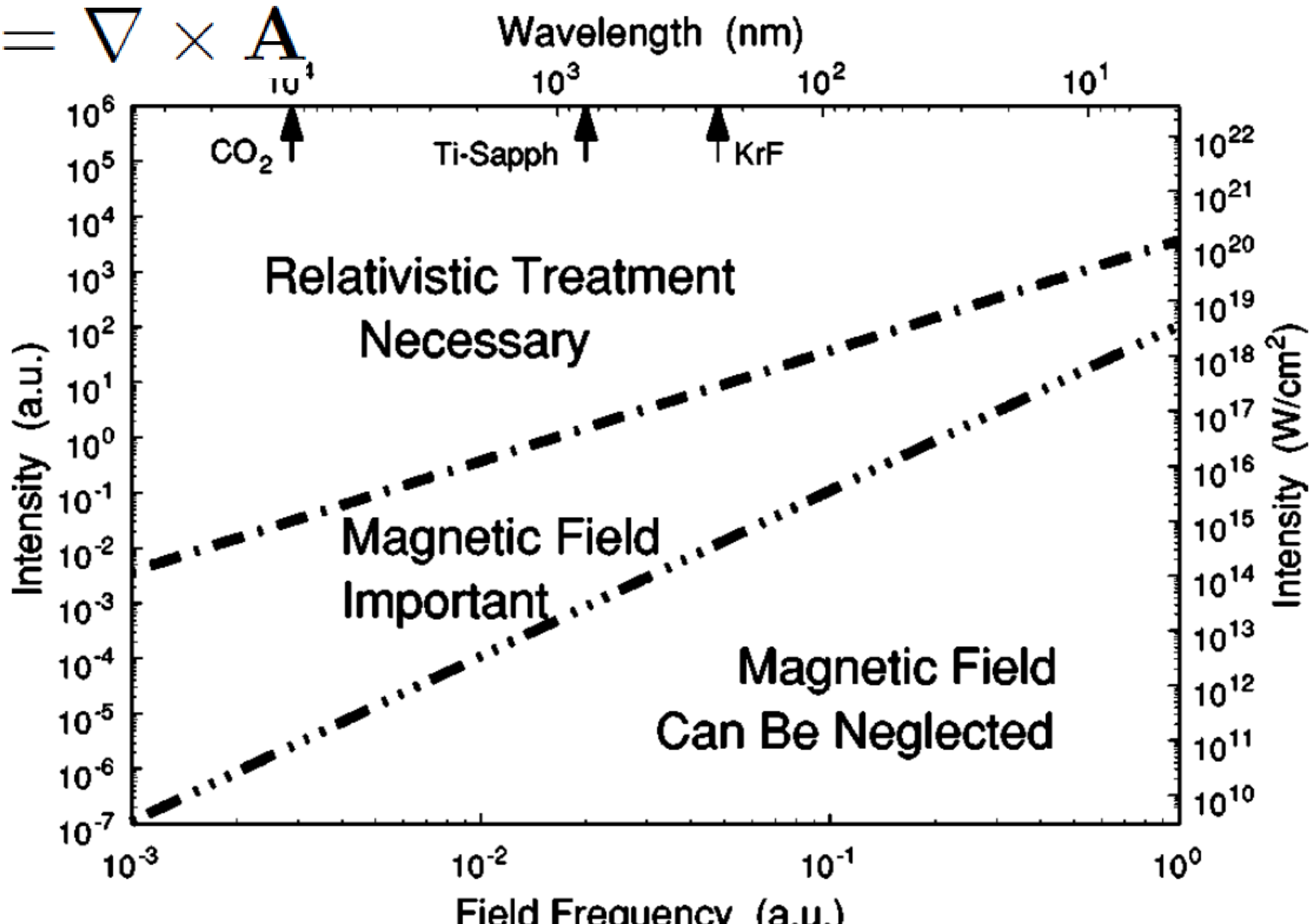
$$[H_I]_{a,b} = c\,\langle\psi_a|A_z(x,t)\alpha_z|\psi_b\rangle$$

The field

$$\mathbf{A} = \mathbf{e}_z A(t - x/c)$$

$$\mathbf{E} = -\dot{\mathbf{A}}, \quad \mathbf{B} = \nabla \times \mathbf{A}$$

Dipole approximation?



H. R. Reiss, Phys. Rev. A **63**, 013409 (2000)

In order not ha have to calculate new couplings at each time:

$$[H_I]_{a,b} = c \, \langle \psi_a | A_z(x,t) \alpha_z | \psi_b \rangle$$

$$A(t - x/c) \approx \sum_{\Omega} a_{\Omega} \exp[i\Omega(t - x/c)] = \sum_{\Omega} a_{\Omega} \exp(i\Omega t) \exp(-i\Omega x/c)$$

$$\exp(\pm i\mathbf{K} \cdot \mathbf{r}) = 4\pi \sum_{\lambda,\mu} (\pm i)^{\lambda} \underbrace{j_{\lambda}(Kr)}_{\text{Radial part}} \underbrace{Y^{*}_{\lambda,\mu}(\hat{\mathbf{k}}) Y_{\lambda,\mu}(\hat{\mathbf{r}})}_{\text{Angular part}}$$

$$H_I(t) = \sum_{\Omega} e^{i\Omega t} H_I^{\Omega}, \quad \dot{H}_I^{\Omega} \equiv 0$$

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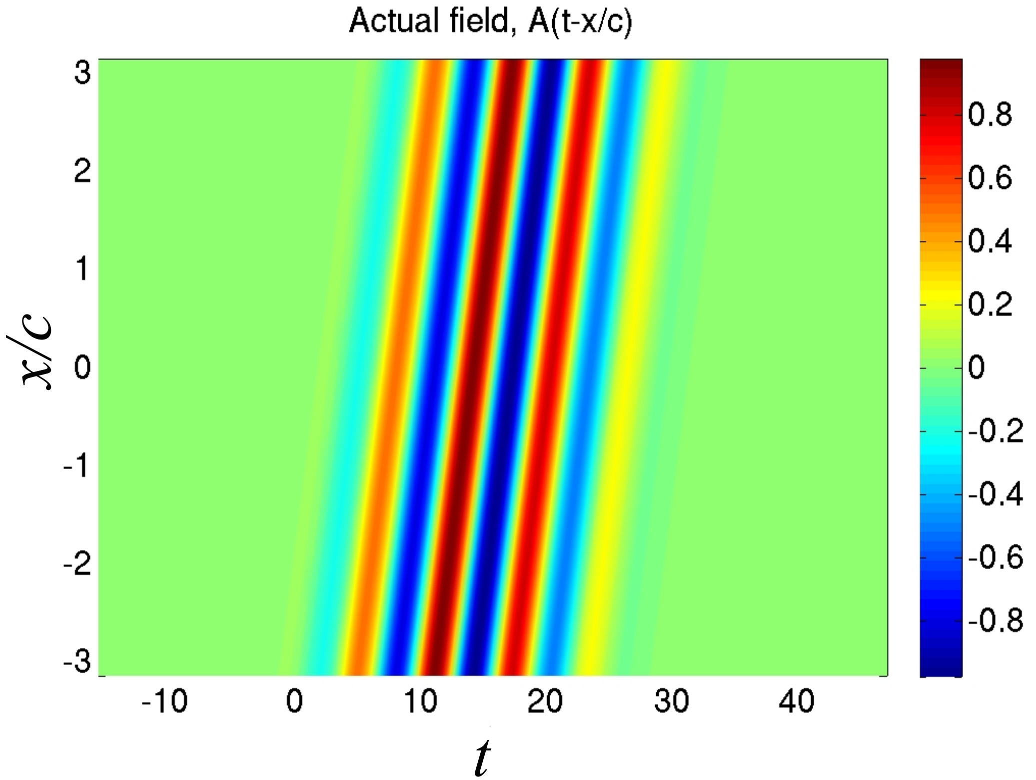

$$\eta \equiv t - x/c$$

$$A(\eta) = \begin{cases} A_0 \sin^2\left(\frac{\pi}{T}\eta\right)\sin(\omega\eta), & 0 < \eta < T \\ 0 & \text{otherwise} \end{cases}$$

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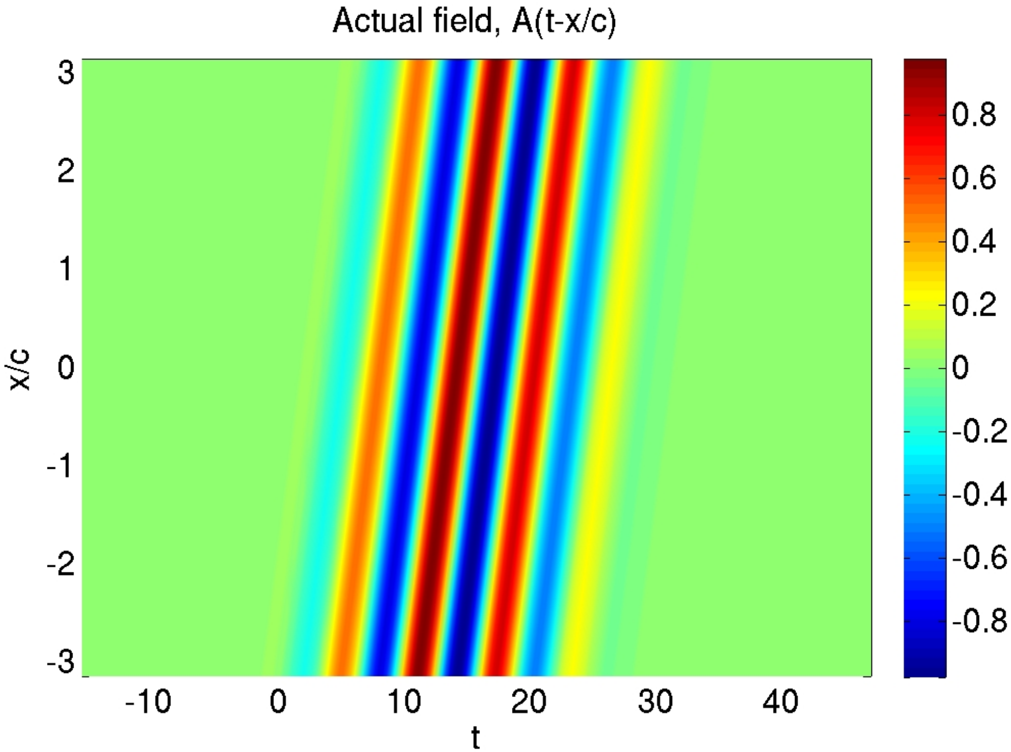

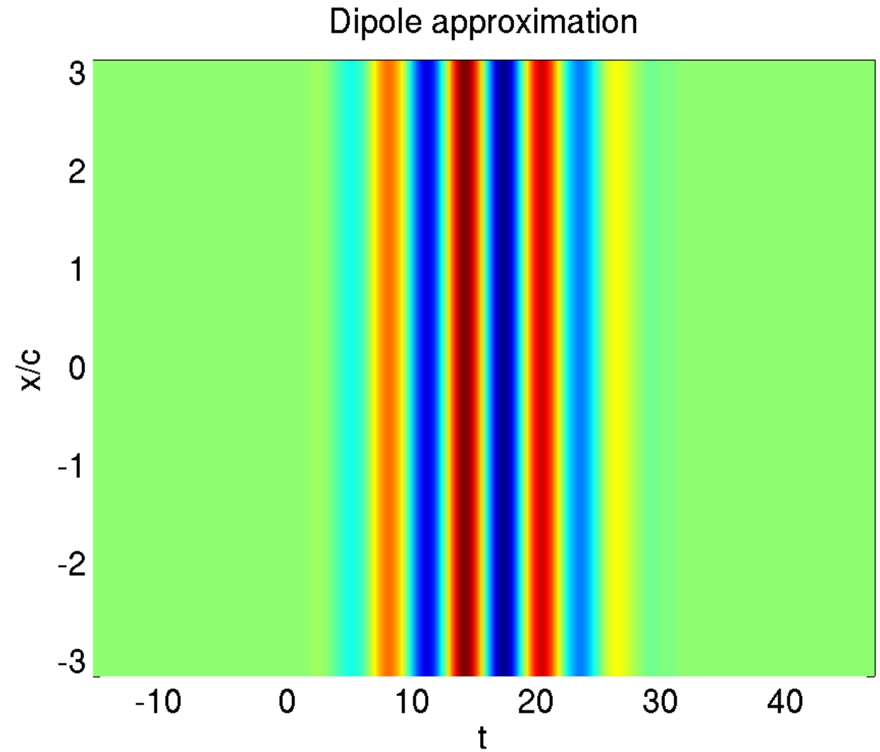

$$A(\eta) \approx A(t)$$

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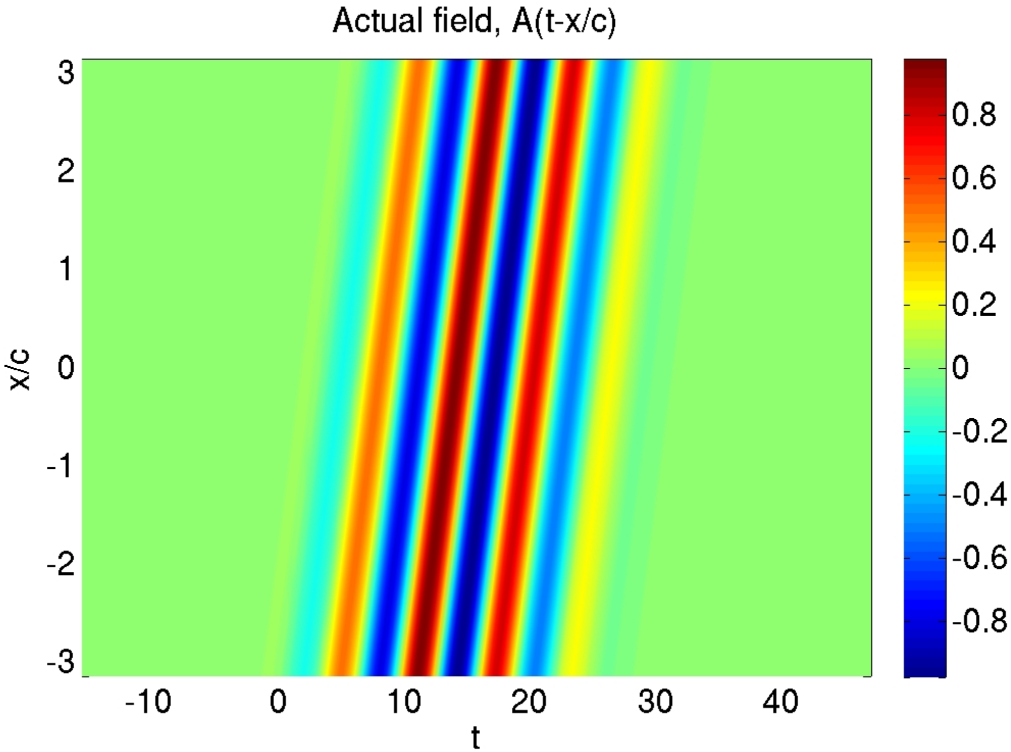
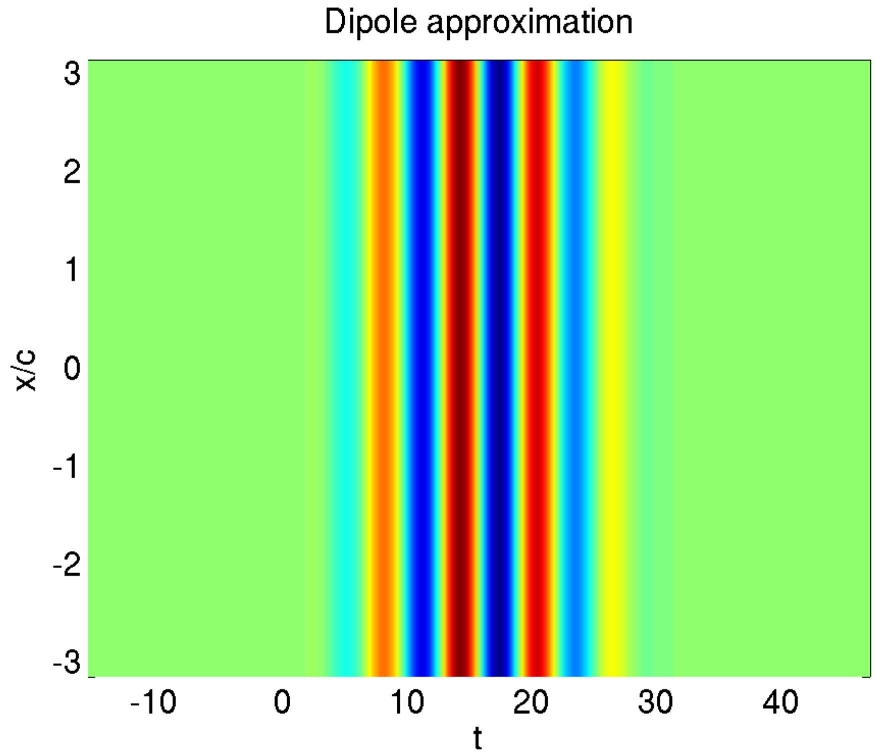
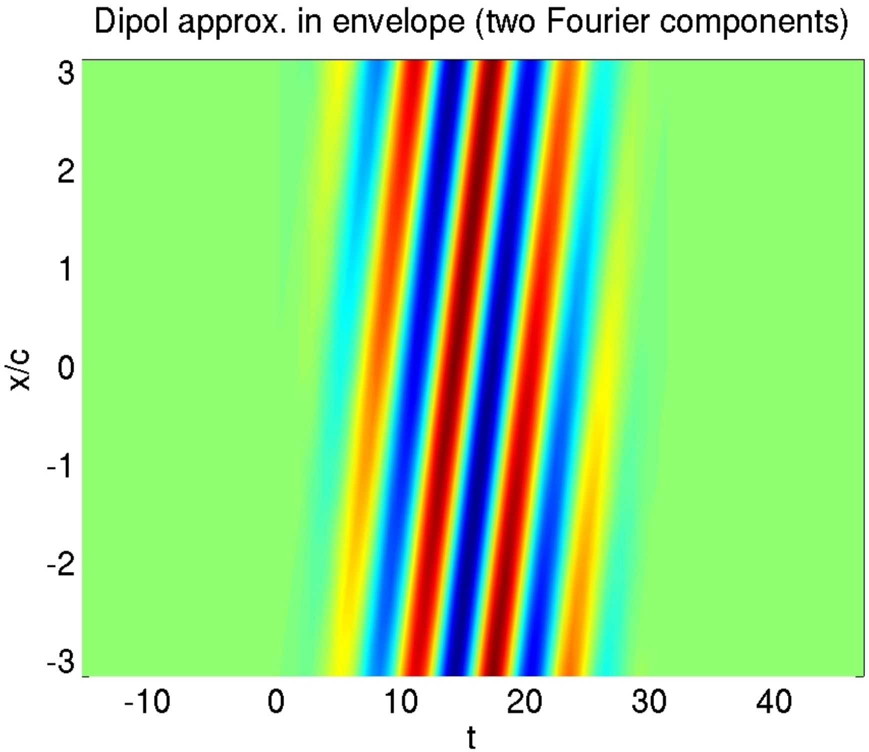
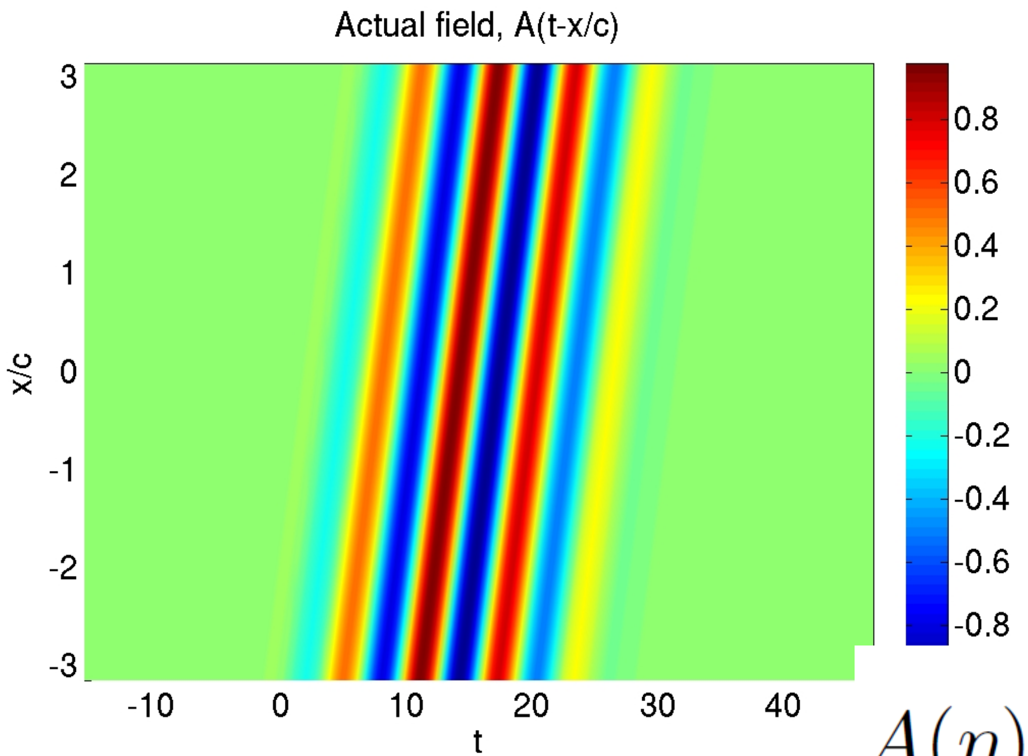
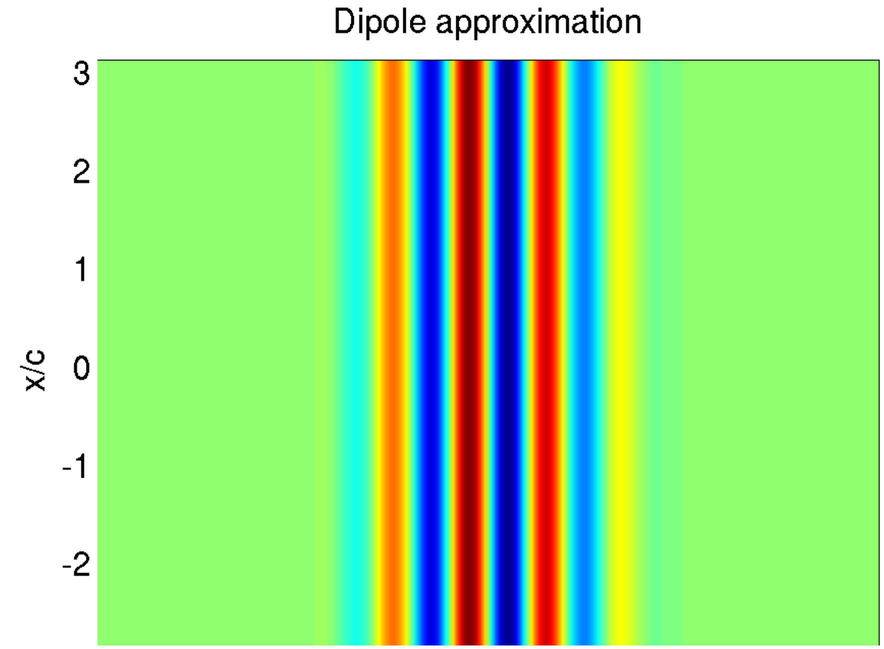




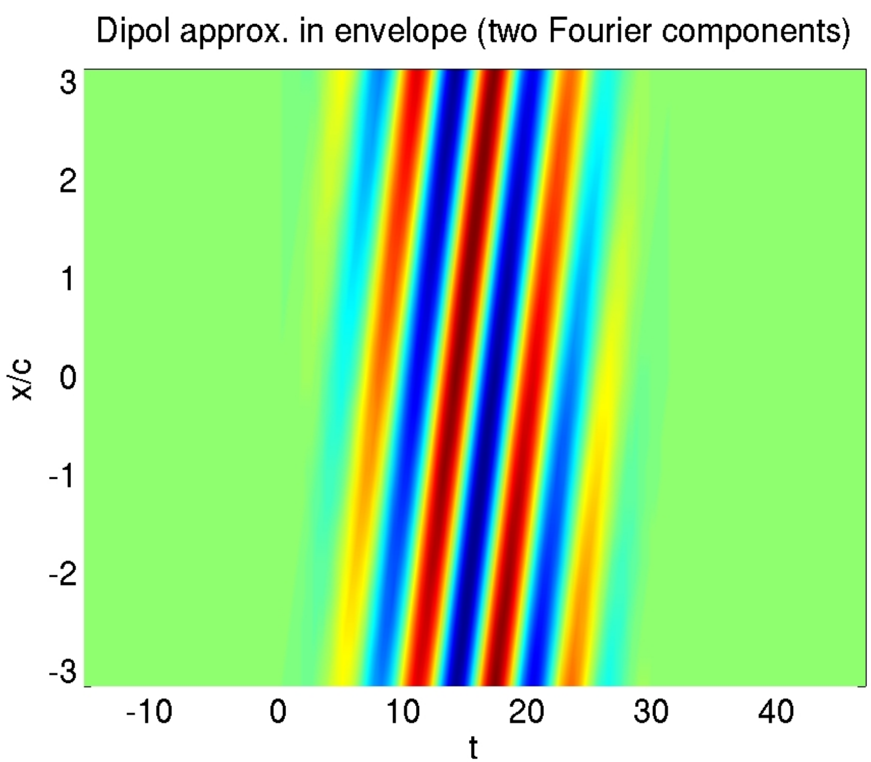


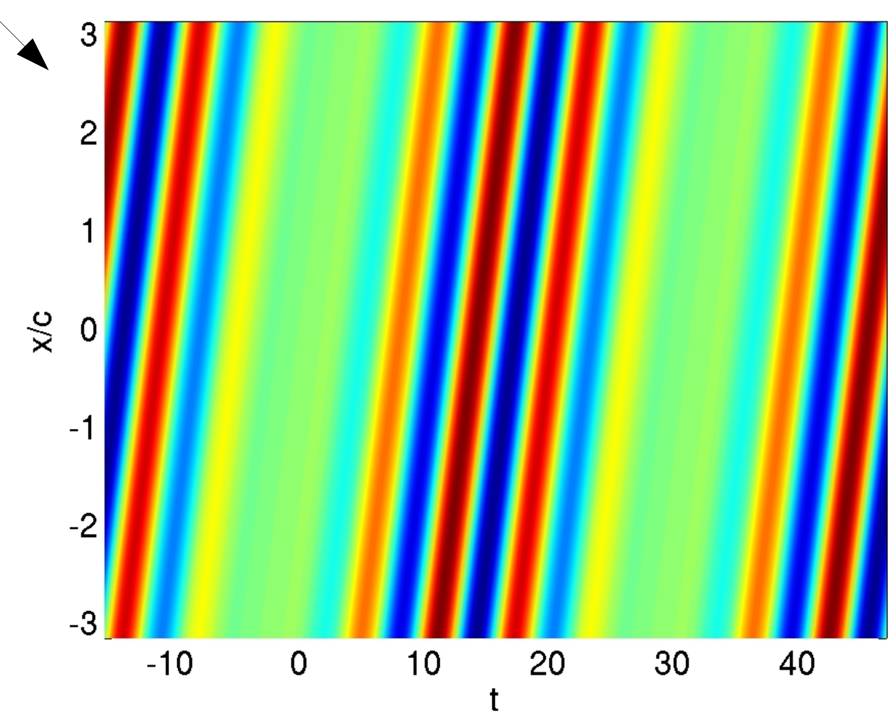
$$A(\eta) \approx A_0 \sin^2\left(\frac{\pi}{T}t\right) \sin(\omega\eta), \ 0 < t < T$$



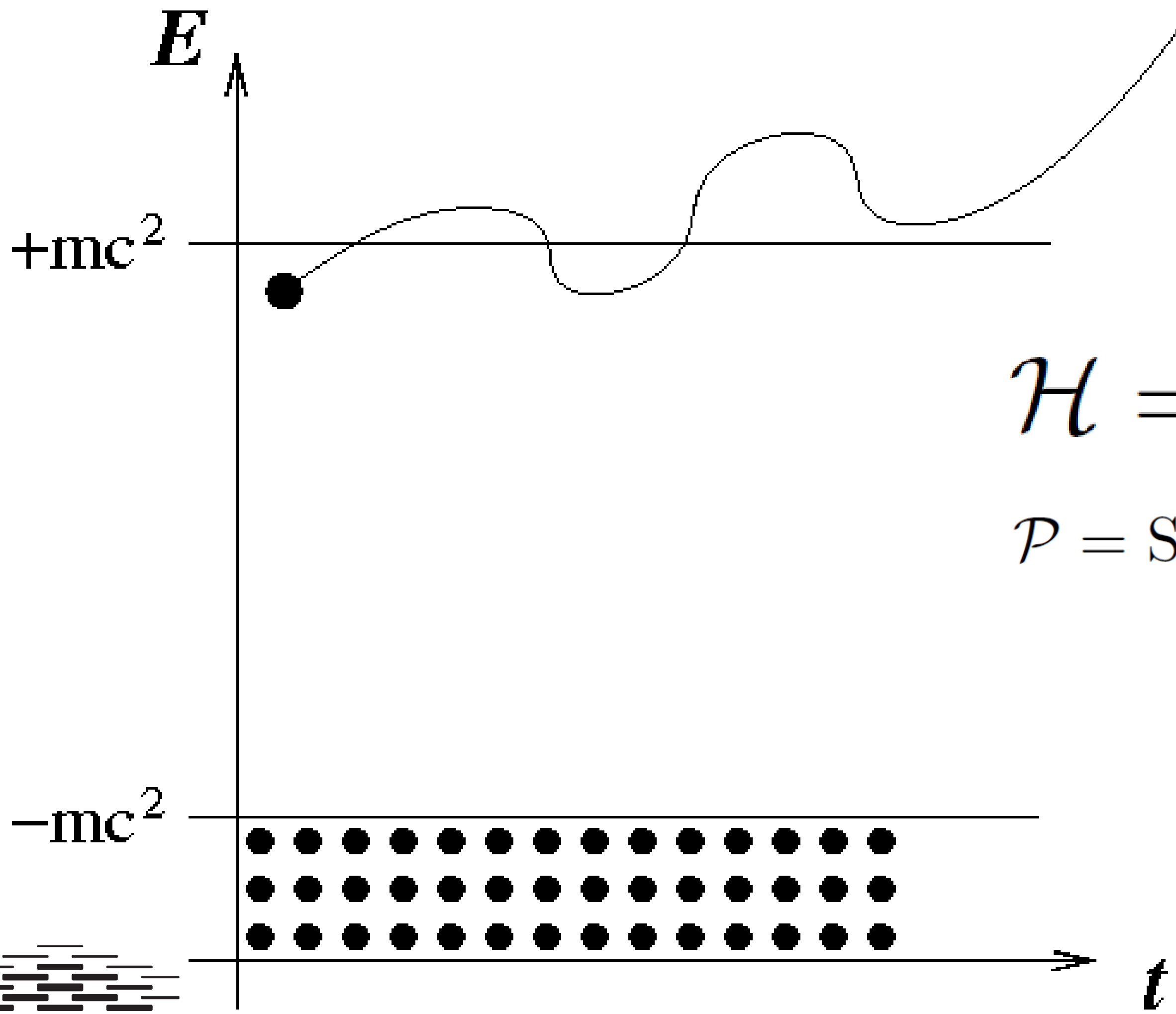


$$A(\eta) \approx A_0 \sin^2\left(\frac{\pi}{T}\eta\right) \sin(\omega\eta), \ \forall\eta$$





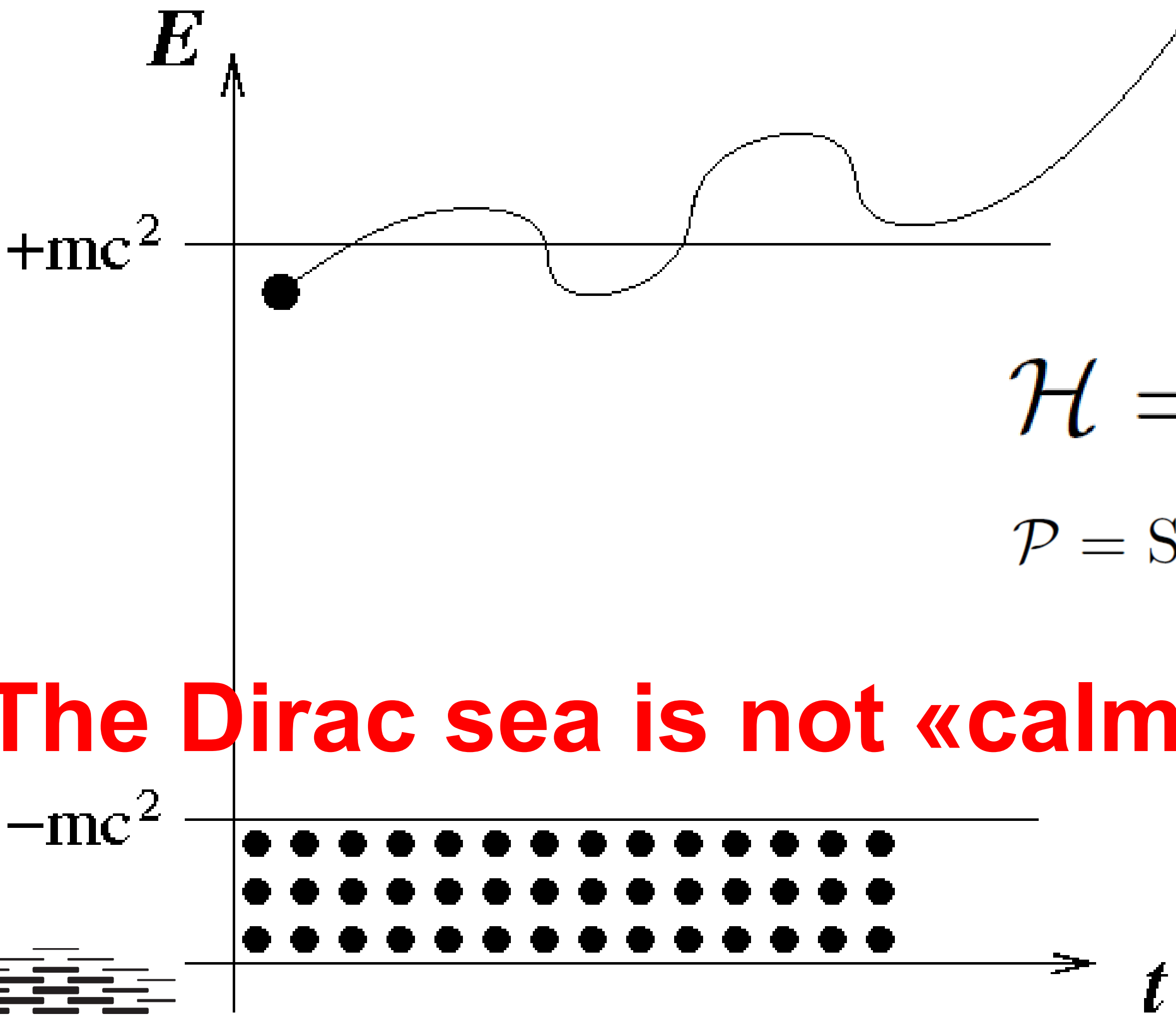
The Dirac sea



$$\mathcal{H} = \mathcal{P} \otimes \mathcal{Q}$$

$$\mathcal{P} = \mathrm{Span}\{\psi_a | H\psi_a = \varepsilon_a \psi_a \wedge \varepsilon_a > 0\}$$

The Dirac sea



$$\mathcal{H} = \mathcal{P} \otimes \mathcal{Q}$$

$$\mathcal{P} = \mathrm{Span}\{\psi_a | H\psi_a = \varepsilon_a \psi_a \wedge \varepsilon_a > 0\}$$

The Dirac sea is not «calm»

$$\dot{\mathcal{P}}, \dot{\mathcal{Q}} \neq 0$$

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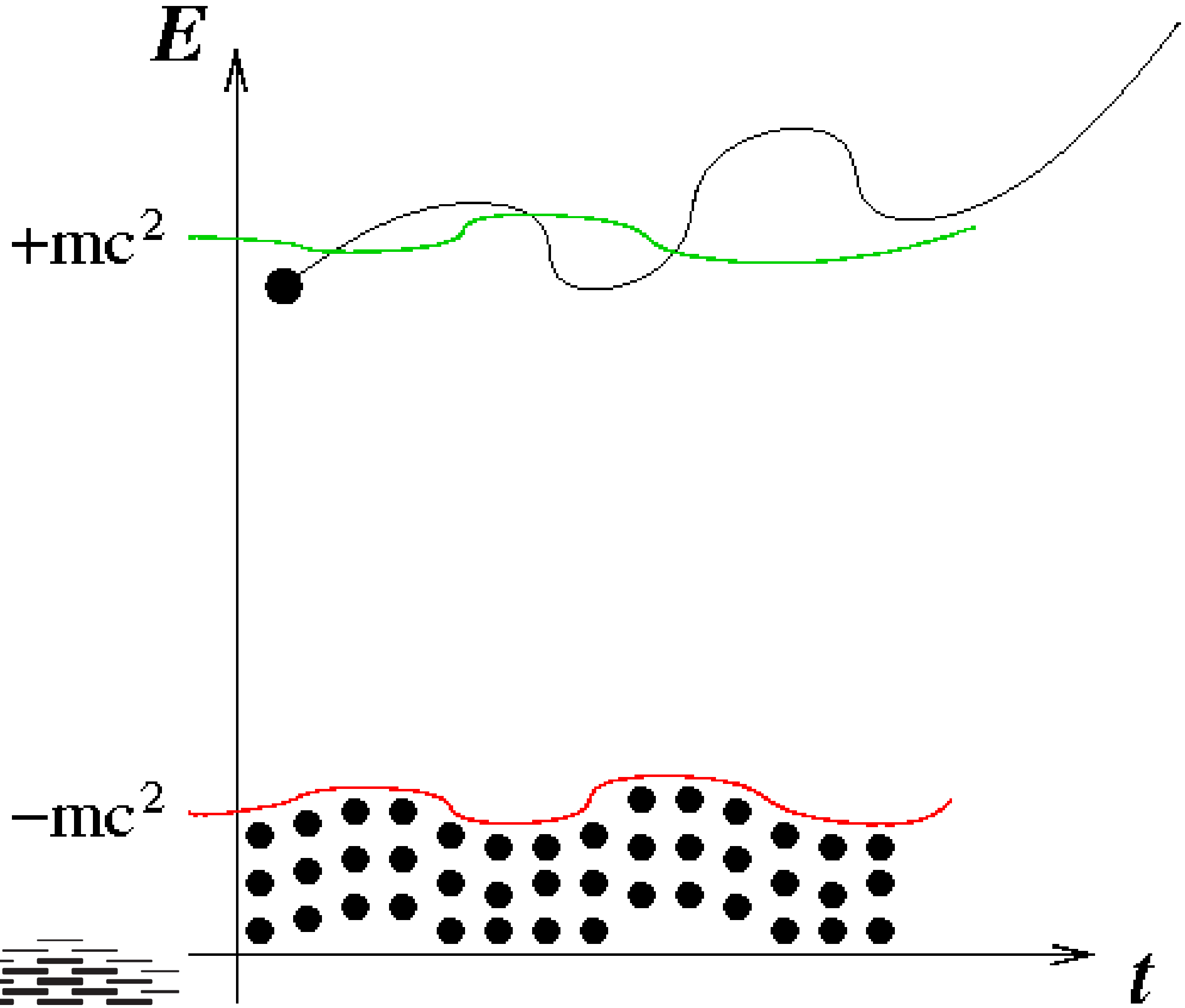
The Dirac sea



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The propagator

$$\Psi(t+\Delta t) = \exp[-iH(t)\Delta t]\,\Psi(t) + \mathcal{O}(\Delta t^2)$$

Advantage: Does not suffer from the restriction $\Delta t \ll c^{-2}$

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The propagator

$$\Psi(t+\Delta t) = P(t+\Delta t)\exp[-iH(t)\Delta t]\,\Psi(t) + \mathcal{O}(\Delta t^2)$$

Projection onto the subspace $\mathcal{P}(t+\Delta t)$.

Advantage: Does not suffer from the restriction $\Delta t \ll c^{-2}$

Disdvantage: Full diagonalization of the Hamiltonian needed for each *t.*

-Expensive.

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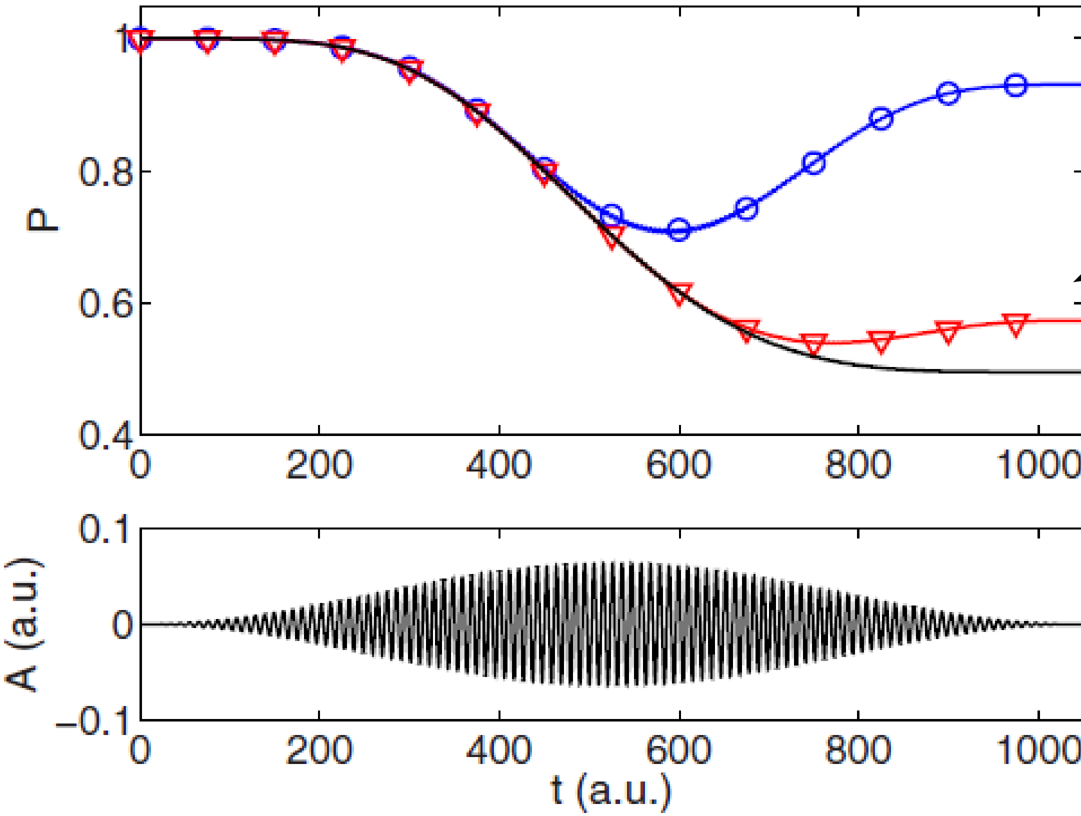
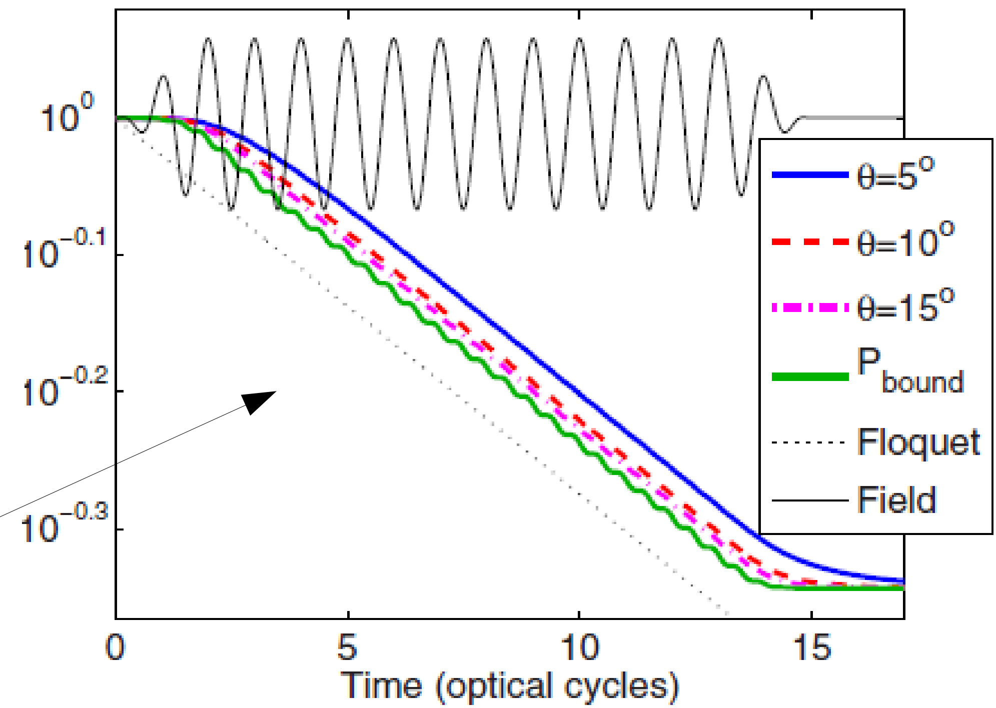
Complex scaling: $r \rightarrow re^{i\theta}$



50 states

100 states

20 states, θ=20°



$$\frac{d}{dt}\left|\mathbf{c}(t)\right|^2 \leq 0$$

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J. Bengtsson, E. Lindroth, S. S., Phys. Rev. A **78**, 032502 (2008)

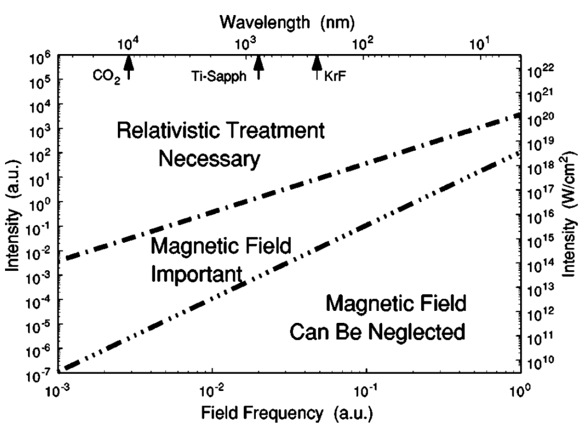
Does the distinction between $\mathcal{P}(0)$ and $\mathcal{P}(t)$ really matter?

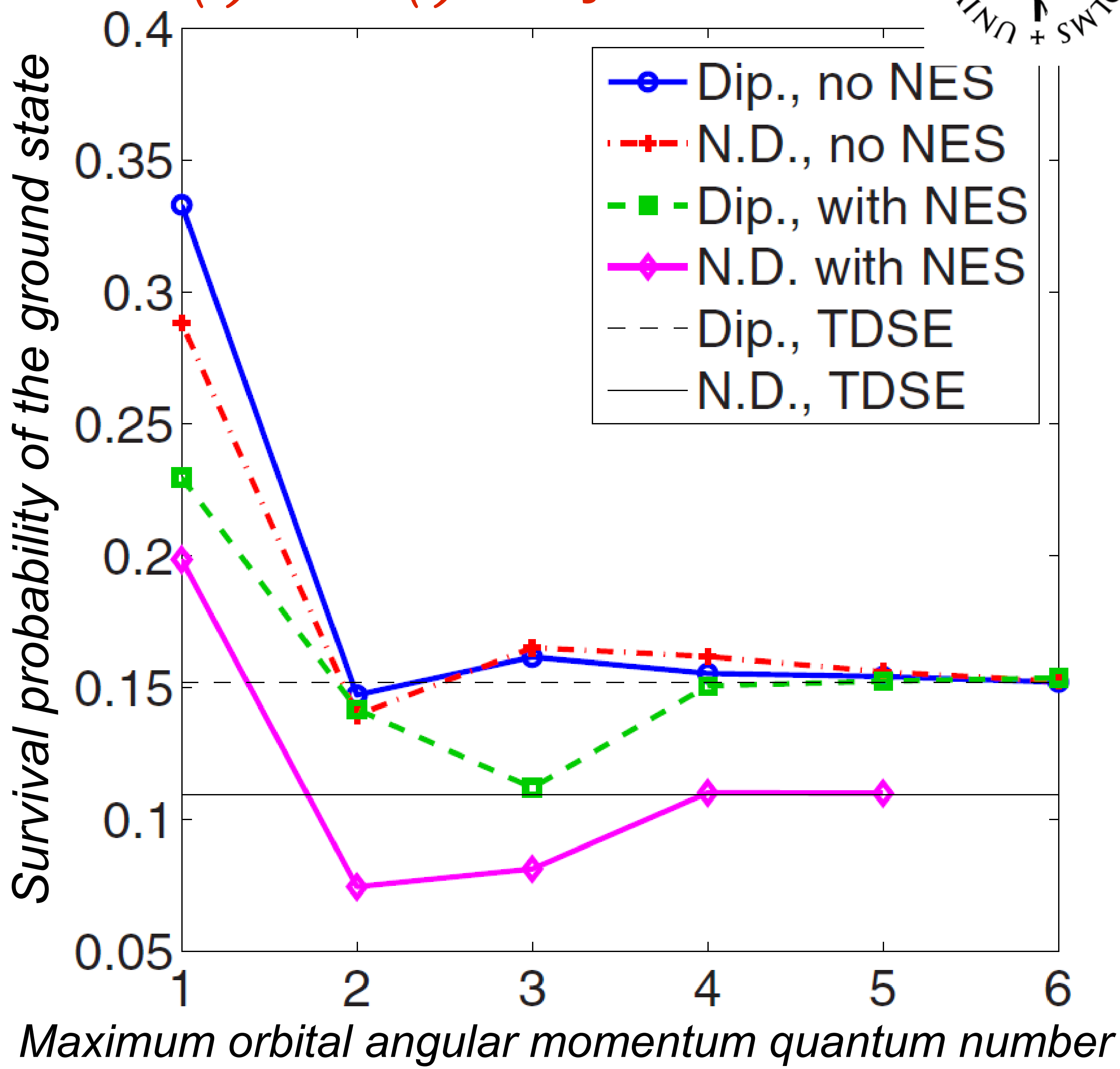
The negative energy states of H_0 do not necessarily coincide with the negative energy states of $H(t)$.

But does this actually make a difference in practice?

Does the distinction between $\mathcal{P}(0)$ and $\mathcal{P}(t)$ really matter?

Yes, it does





S. S., E. Lindroth, J. Bengtsson, Phys. Rev. A **79**, 043418 (2009)

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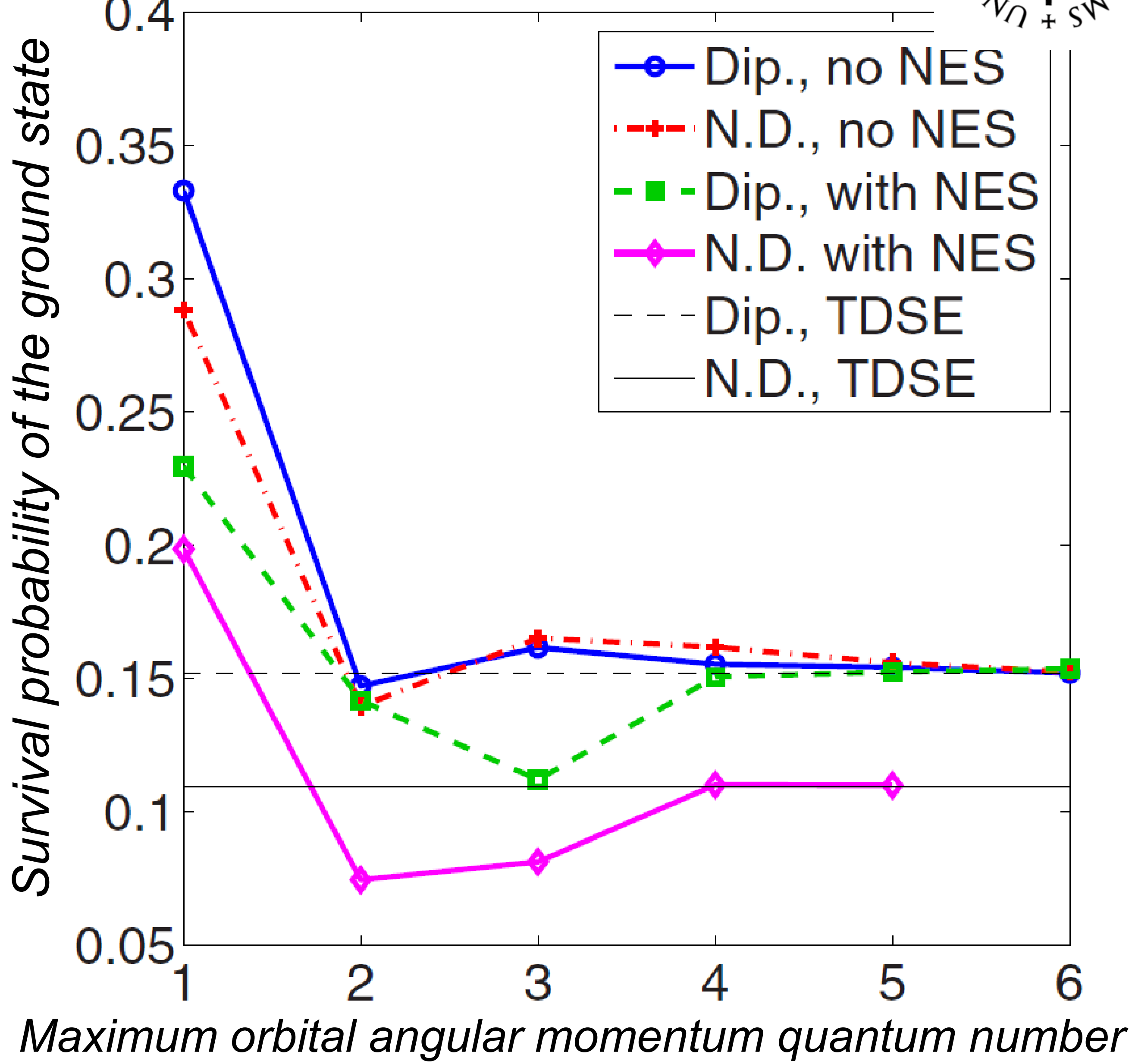
Does the distinction between $\mathcal{P}(0)$ and $\mathcal{P}(t)$ really matter?

Yes, it does

TDSE:
Non-dipole correction comes from dia-magnetic term, $\frac{1}{2} A^2$



S. S., E. Lindroth, J. Bengtsson, Phys. Rev. A **79**, 043418 (2009)

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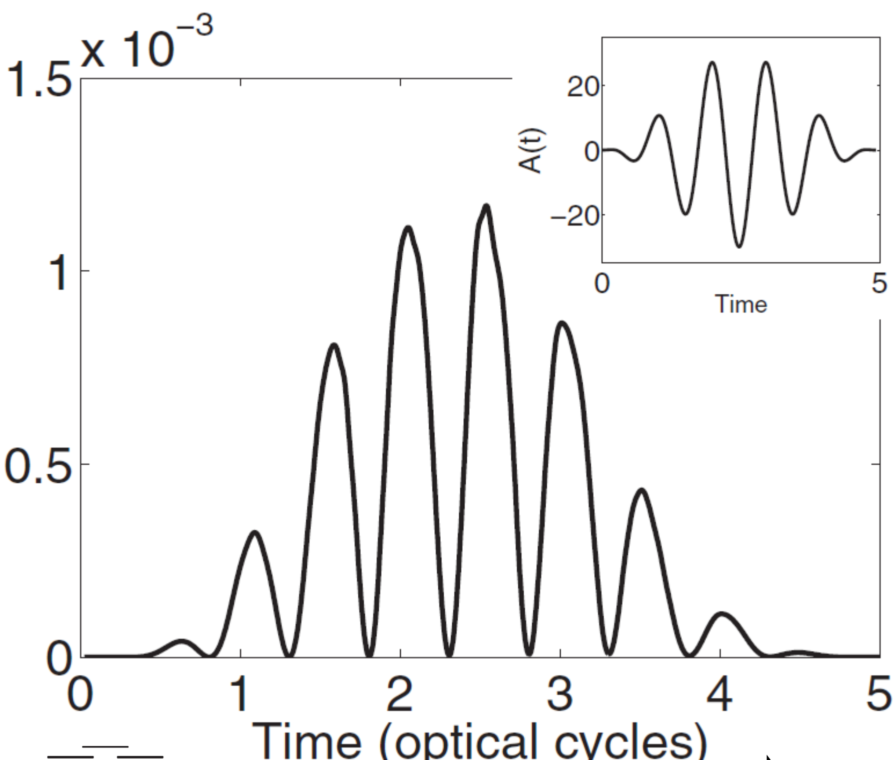

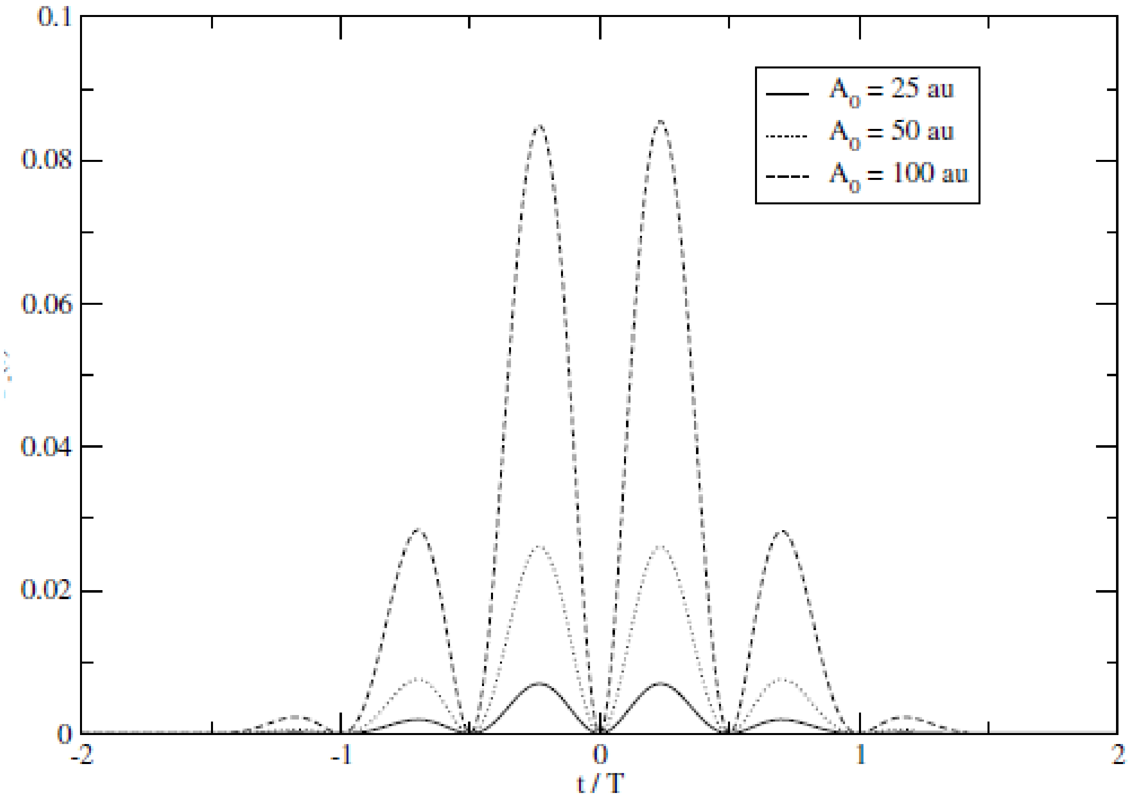

M. Boca, V. Florescu, Eur. Phys. J. D **46**, 15 (2008)

S. S., E. Lindroth, J. Bengtsson, Phys. Rev. A **79**, 043418 (2009)

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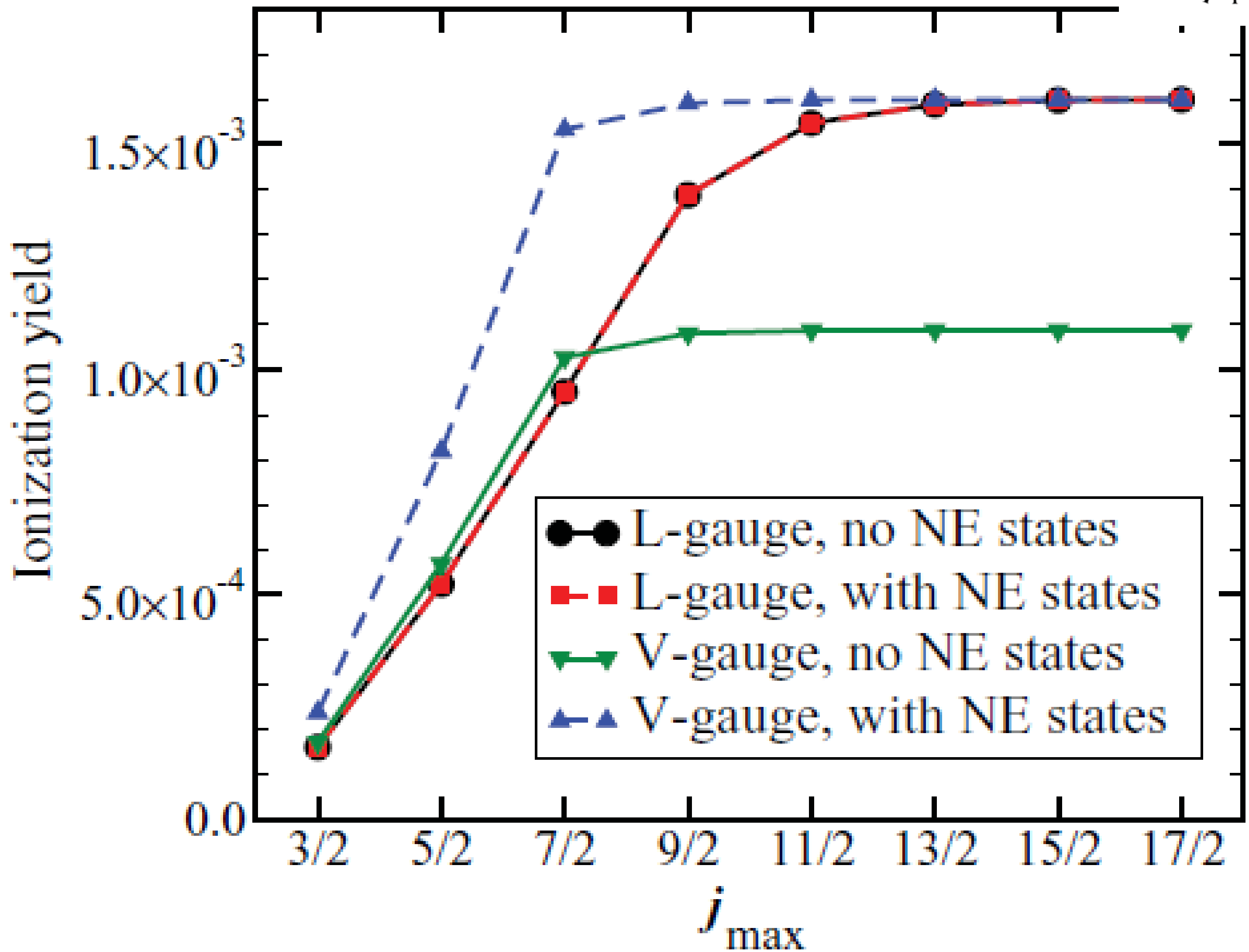
Does the distinction between $\mathcal{P}(0)$ and $\mathcal{P}(t)$ really matter?

Yes, it does,

however, the importance is gauge-dependent



Y. V. Vanne, A. Saenz, Phys. Rev. A **85**, 033411 (2012)

S. S., E. Lindroth, J. Bengtsson, Phys. Rev. A **79**, 043418 (2009)

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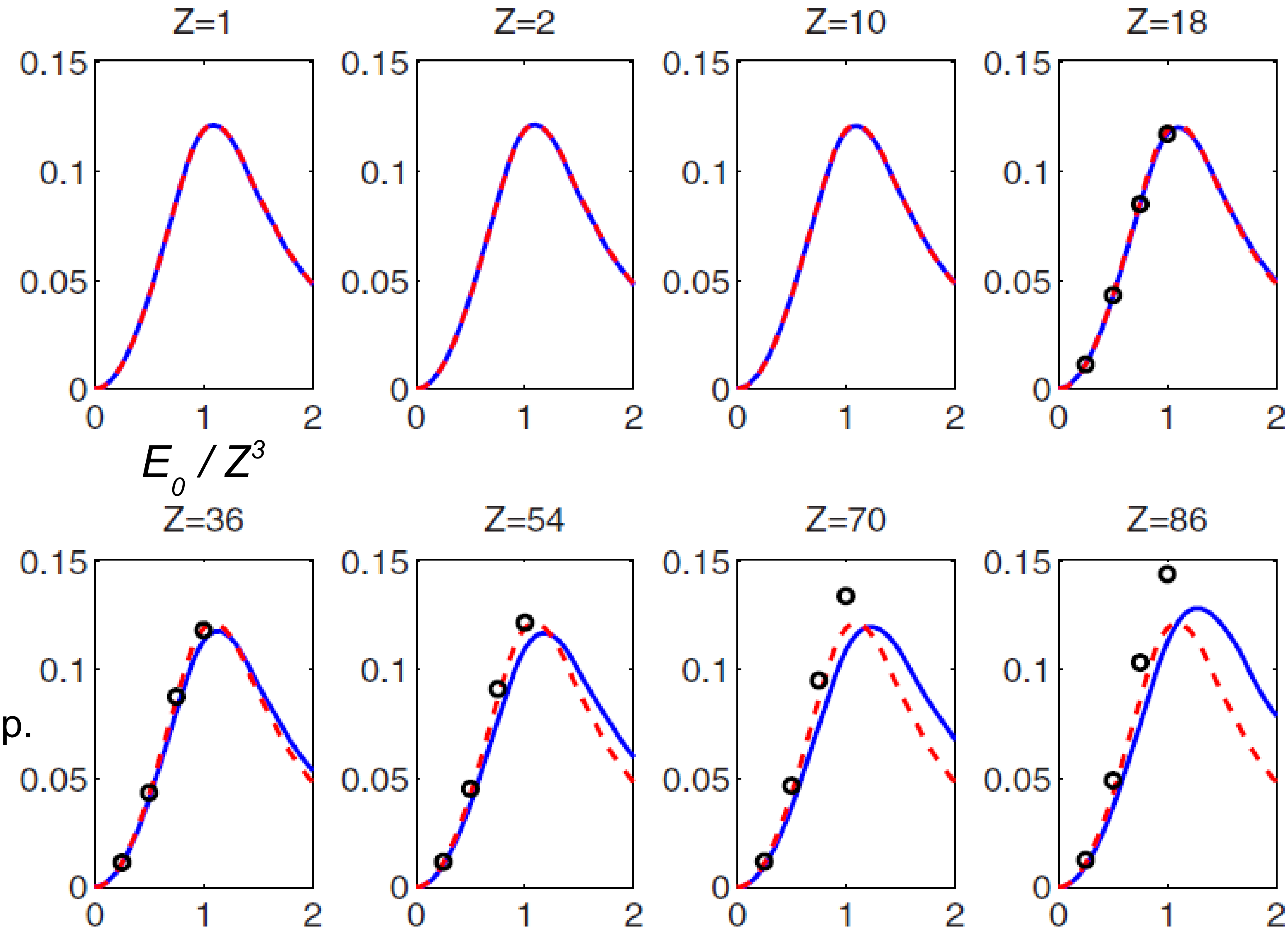
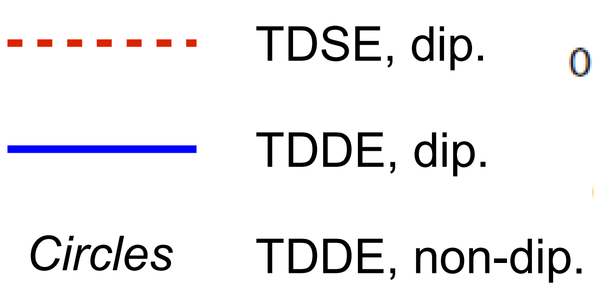
Relativistic effects due to modified structure

$$
\begin{aligned}
\tilde{t} &= Z^2 t \\
\tilde{\mathbf{r}} &= Z\mathbf{r} \\
\tilde{E}_0 &= E_0/Z^3 \\
\tilde{\omega} &= \omega/Z^2
\end{aligned}
$$

Ionization rates





S. S., E. Lindroth, J. Bengtsson, Phys. Rev. A **79**, 043418 (2009)

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In summary

-Method for solving TDDE for (3D) hydrogen-like systems exposed to laser pulses

Fourier/ multipole expansion of external field

Complex scaling

Projection

-Seen that negative energy states of H_0 are crucial (in general)

Depends on gauge and number of photons

-Calculated ionization rates for inceasing nuclear charge

Atomic stabilization

Things to improve on

-Alternatives to full diagonalization of $H(t)$

Necessary in order to exponentiate the Hamiltonian and distinguish between $\mathcal{P}(t)$ and $\mathcal{Q}(t)$?

Methods based on Krylov sub-spaces?

Higher order Magnus-type propagator?

-Parallel implementation?

-Going further beyond the dipole approximation for the field

Higher order Fourier expansion?

Other ways of implementation?

-Length gauge implementation instead?

$$H_I = zE(\eta) + c\alpha_x z\mathbf{B}(\eta) \cdot \mathbf{e}_y$$

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Statoil

We are sorry (at least many of us)

$$\Psi(t+\Delta t) - e^{-iH(t)\Delta t}\Psi(t) = \frac{i}{2}\Delta t^2 \dot{H}_I\,\Psi(t) + \mathcal{O}(\Delta t^3)$$

Runge-Kutta, Leapfrog, Crank-Nicolson:

$$\Psi(t+\Delta t) - \Psi_{\mathrm{scheme}}(t+\Delta t) = C\Delta t^n \frac{\partial^n}{\partial t^n}\Psi(t) + \mathcal{O}(\Delta t^{n+1})$$

$$H^n\Psi(t)$$

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M. Hochbruck, C. Lubich, SIAM Journal of Numerical Analysis **41**, 945 (2003)

$$\langle\psi_a^+|\alpha|\psi_b^+\rangle \sim \begin{pmatrix} L_a^* & S_a^* \end{pmatrix} \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \begin{pmatrix} L_b \\ S_b \end{pmatrix} \sim (L_a^*|\sigma|S_b) + (S_a^*|\sigma|L_b)$$

$$\langle\psi_a^+|\alpha|\psi_b^-\rangle \sim \begin{pmatrix} L_a^* & S_a^* \end{pmatrix} \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \begin{pmatrix} S_b \\ L_b \end{pmatrix} \sim (L_a^*|\sigma|L_b) + (S_a^*|\sigma|S_b)$$

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