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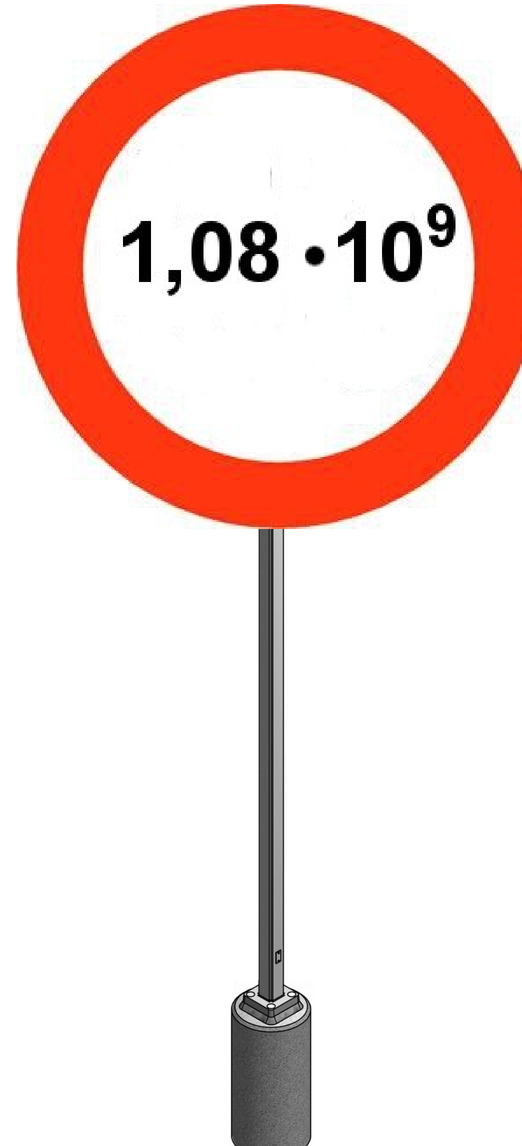
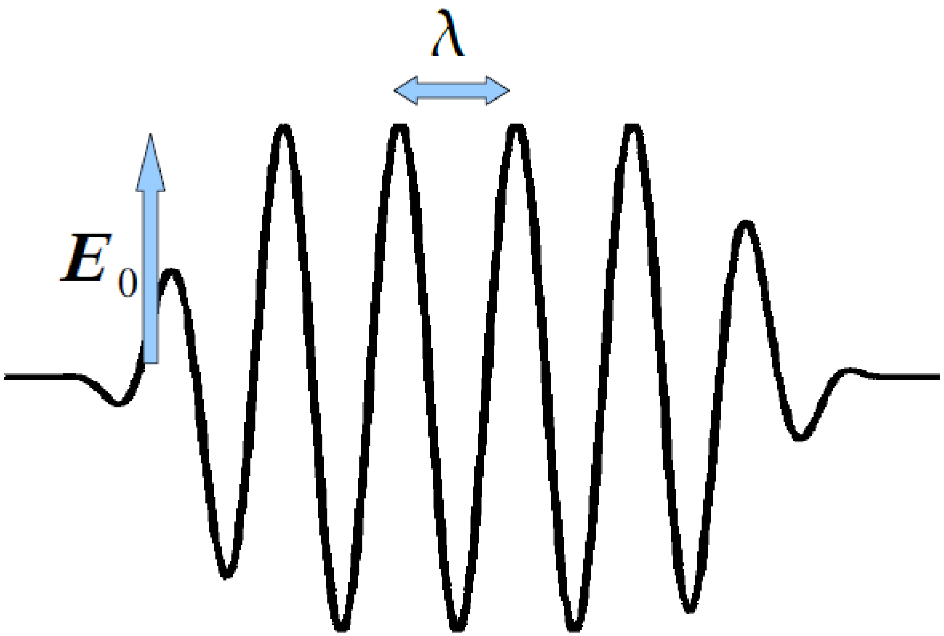
Physics in the FAST lane

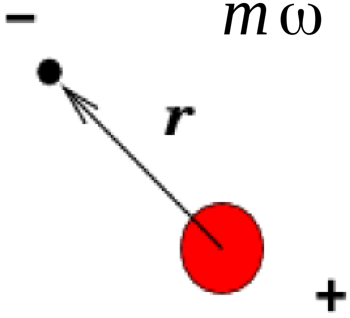


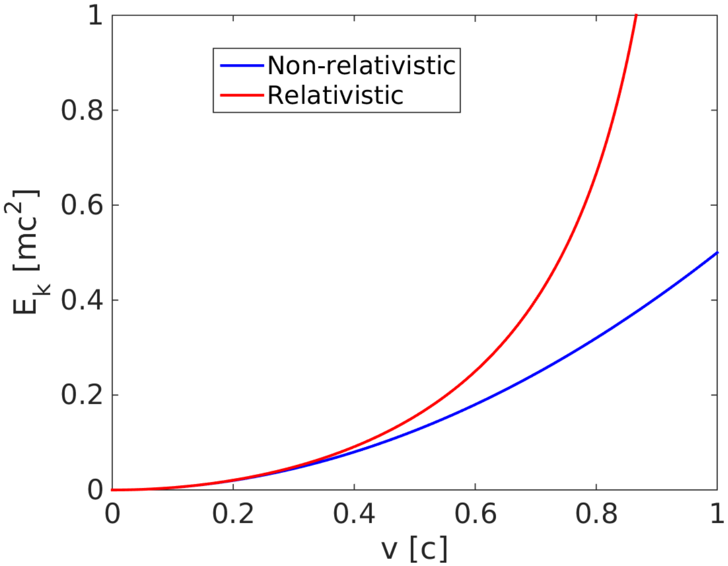
For Ladislav, Bergen December 19th

A laser pulse and a hydrogen atom



$$v \sim \frac{eE_0}{m\omega}$$





The story dates back

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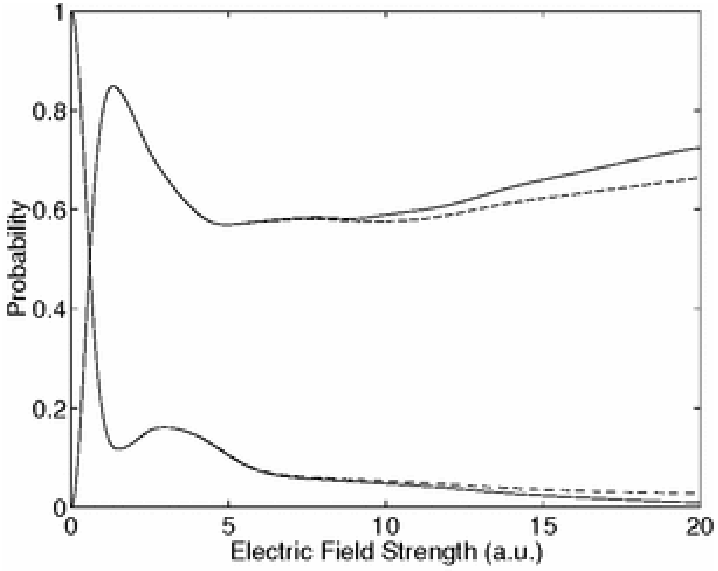
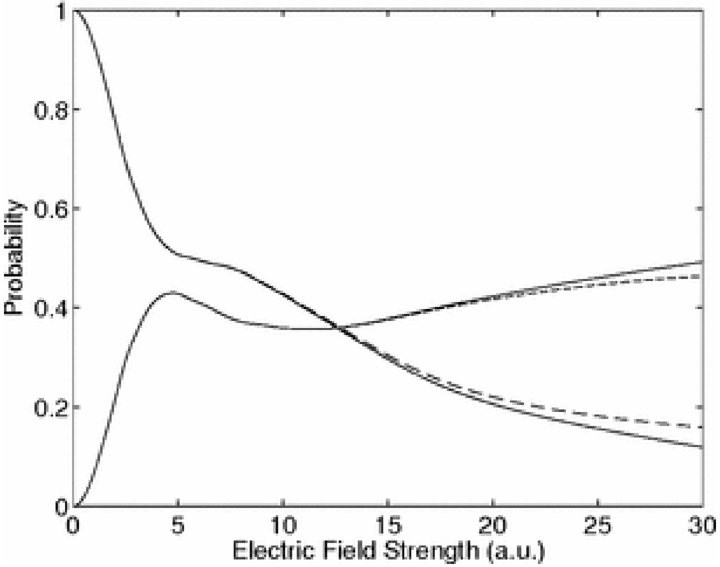
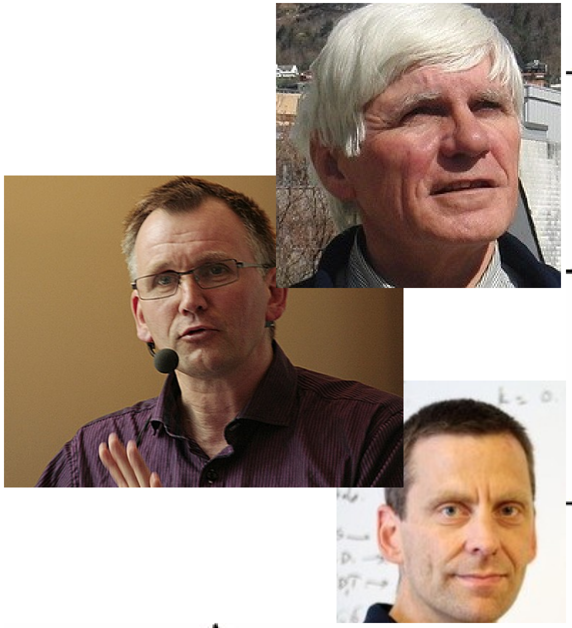
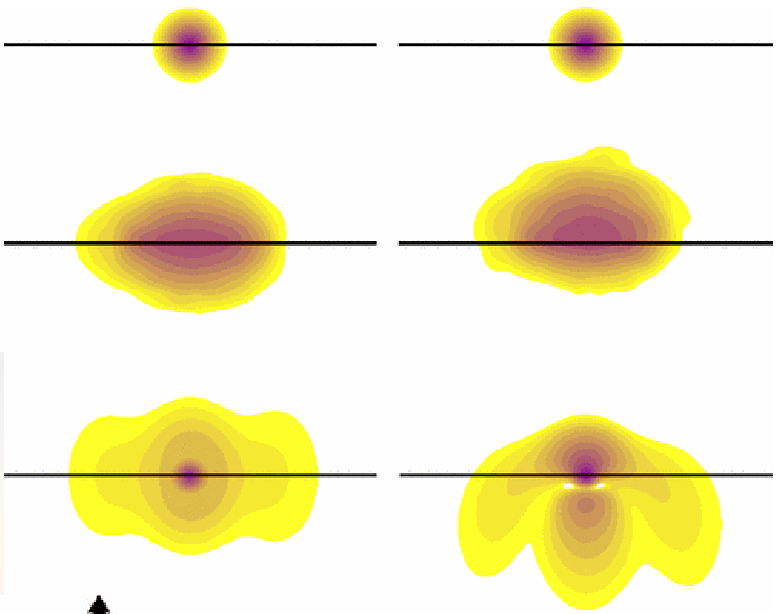
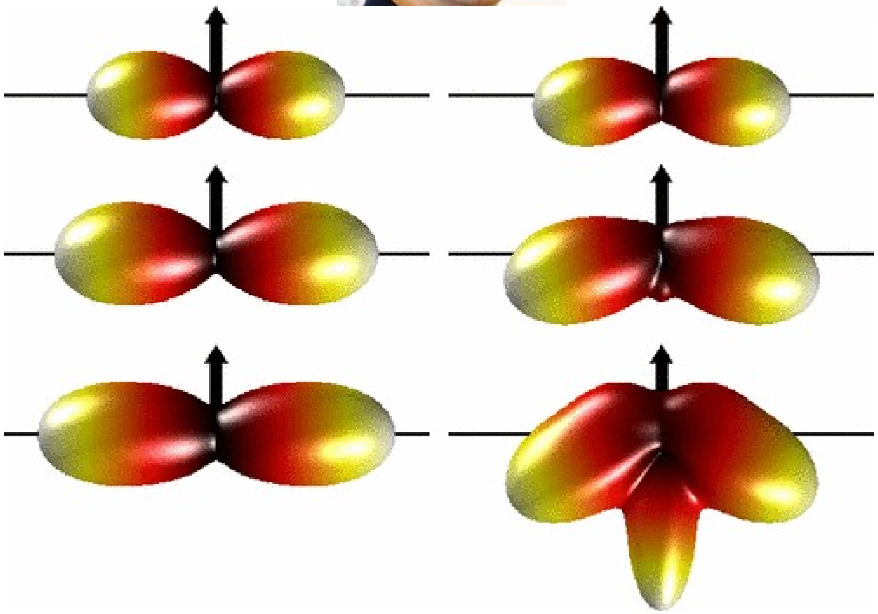




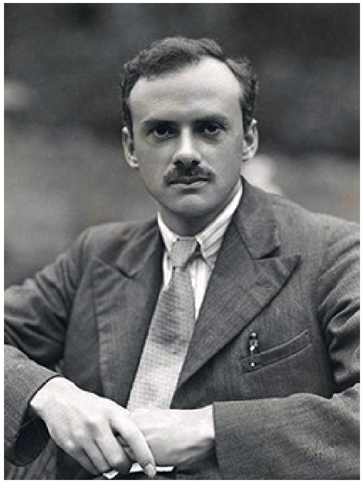
PRL **95**, 043601 (2005)







PRL **97**, 043601 (2006)



$$i\hbar\dot{\Psi}=\left[c\boldsymbol{\alpha}\cdot\left(\boldsymbol{p}+e\boldsymbol{A}\right)+V+mc^{2}\beta\right]\Psi$$

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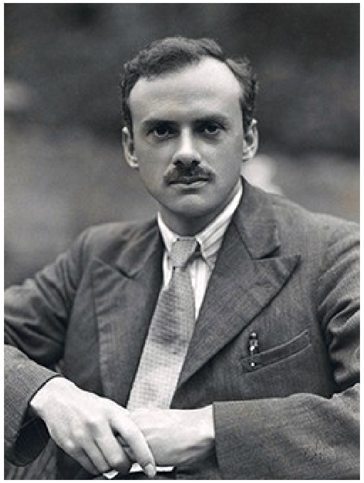

$$i\hbar\dot{\Psi}=\left[c\,\boldsymbol{\alpha}\cdot\left(\boldsymbol{p}+e\boldsymbol{A}\right)+V+mc^{2}\beta\right]\Psi$$

$$\Psi\in C^{4}$$

$$H=H_{0}+H_{I}$$

$$H_{0}=c\,\boldsymbol{\alpha}\cdot\boldsymbol{p}+V+mc^{2}\beta$$

$$H_{I}=c\,\alpha_{z}A$$

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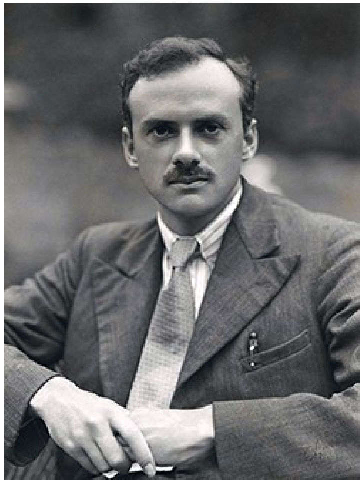

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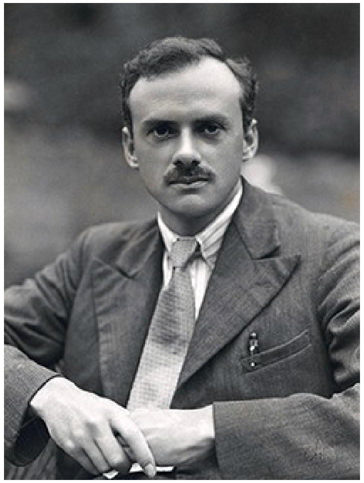
$$\boldsymbol{\alpha}=\begin{pmatrix}0 & \boldsymbol{\sigma}\\ \boldsymbol{\sigma} & 0\end{pmatrix},\sigma_{x}=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\sigma_{y}=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\sigma_{y}=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

$$\beta=\begin{pmatrix}I_{2} & 0\\ 0 & -I_{2}\end{pmatrix}$$



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Stockholm University

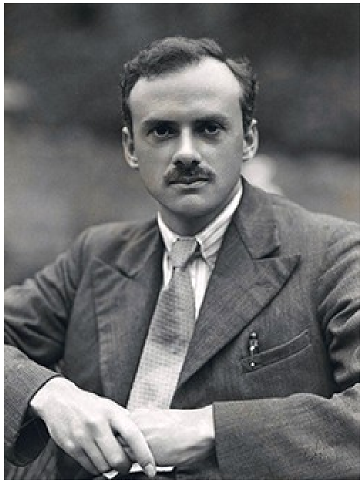
Codes for $H_0\psi_a = \varepsilon_a\psi_a$

Expand: $\Psi(t) = \Sigma_a c_a \psi_a$

ODE: $i\dot{\boldsymbol{c}} = [Diag(\varepsilon_1, \varepsilon_2, \ldots) + H']\boldsymbol{c}$

$$H'_{a,b} = c\langle\psi_a|\alpha_z A|\psi_b\rangle$$

How hard can it be?



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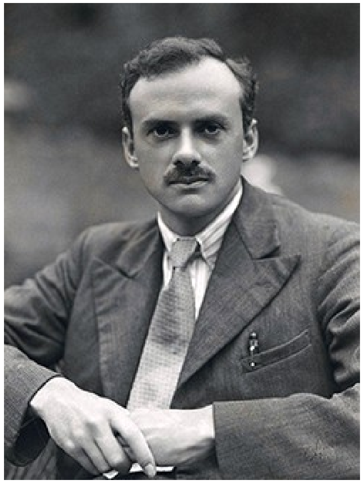
Harder than we thaught



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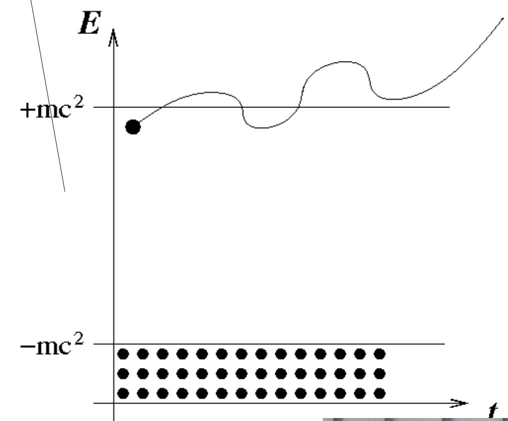

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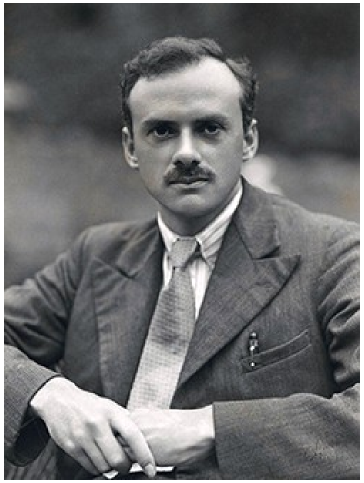

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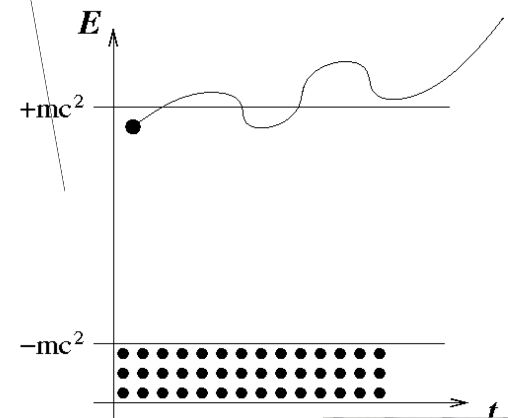

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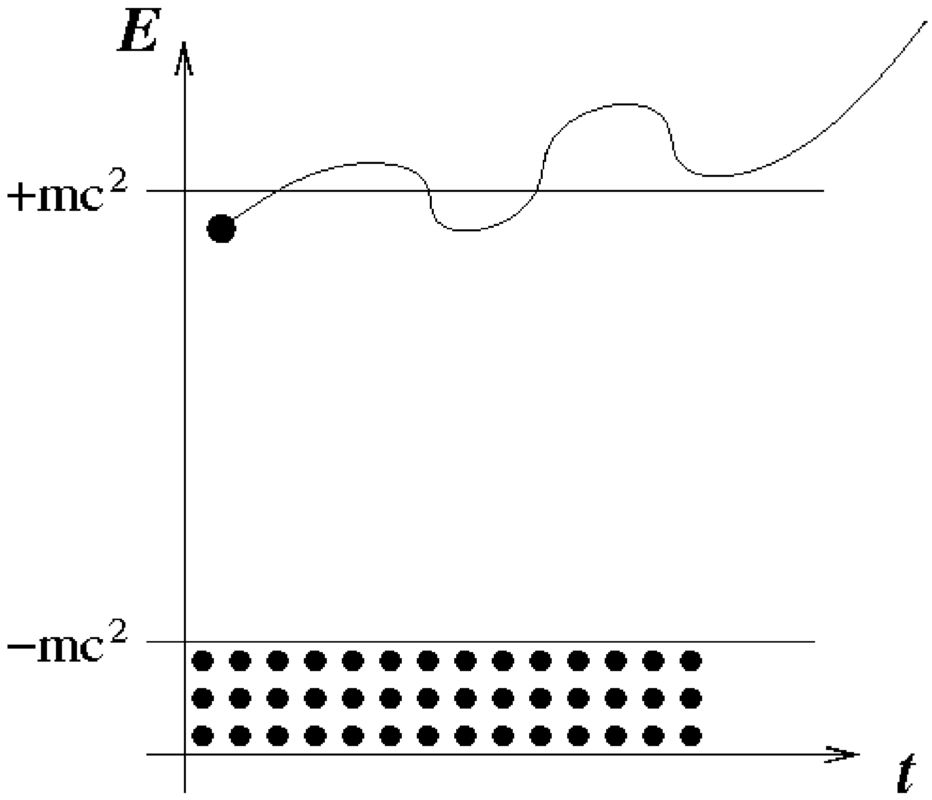
$$A(t-x/c)$$

$mc^2\beta$

The Dirac sea



$mc^2\beta$

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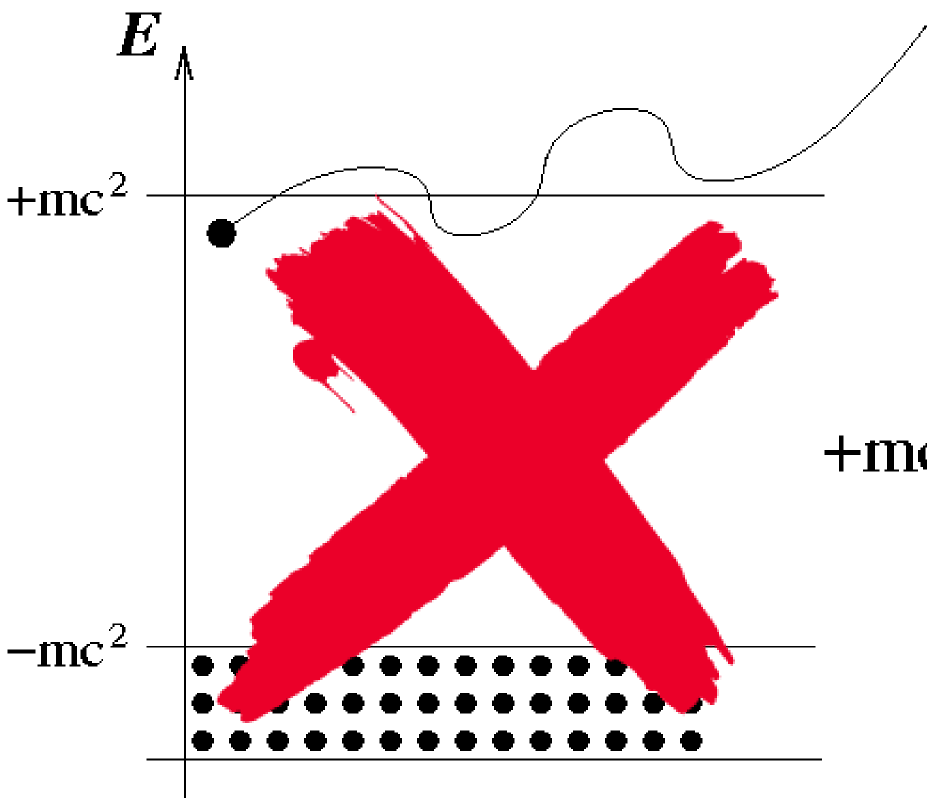
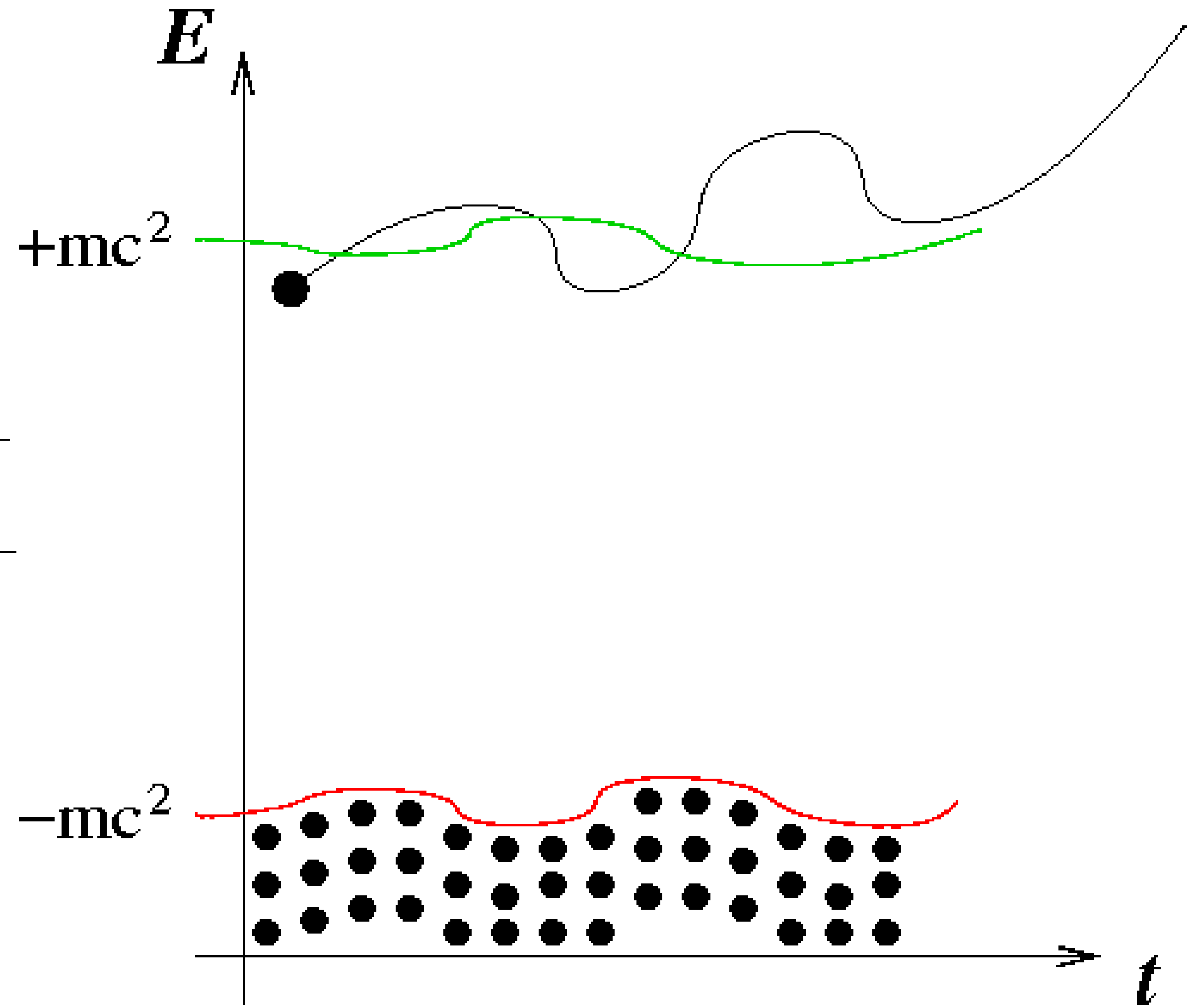
The Dirac sea isn't calm





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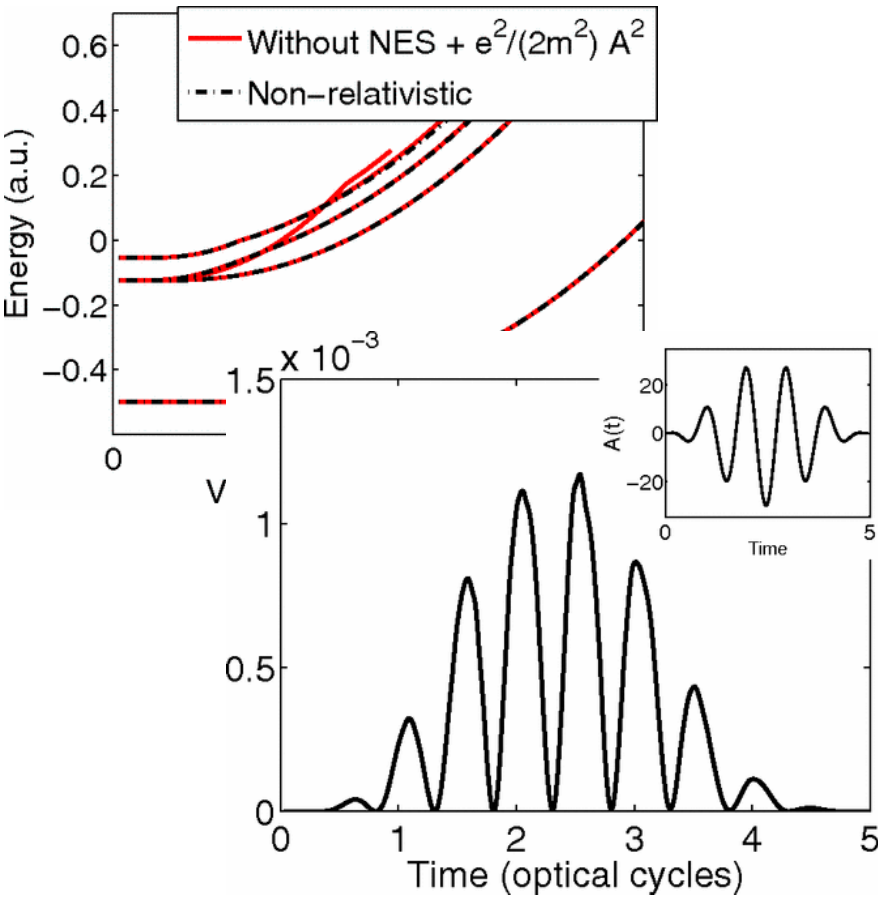
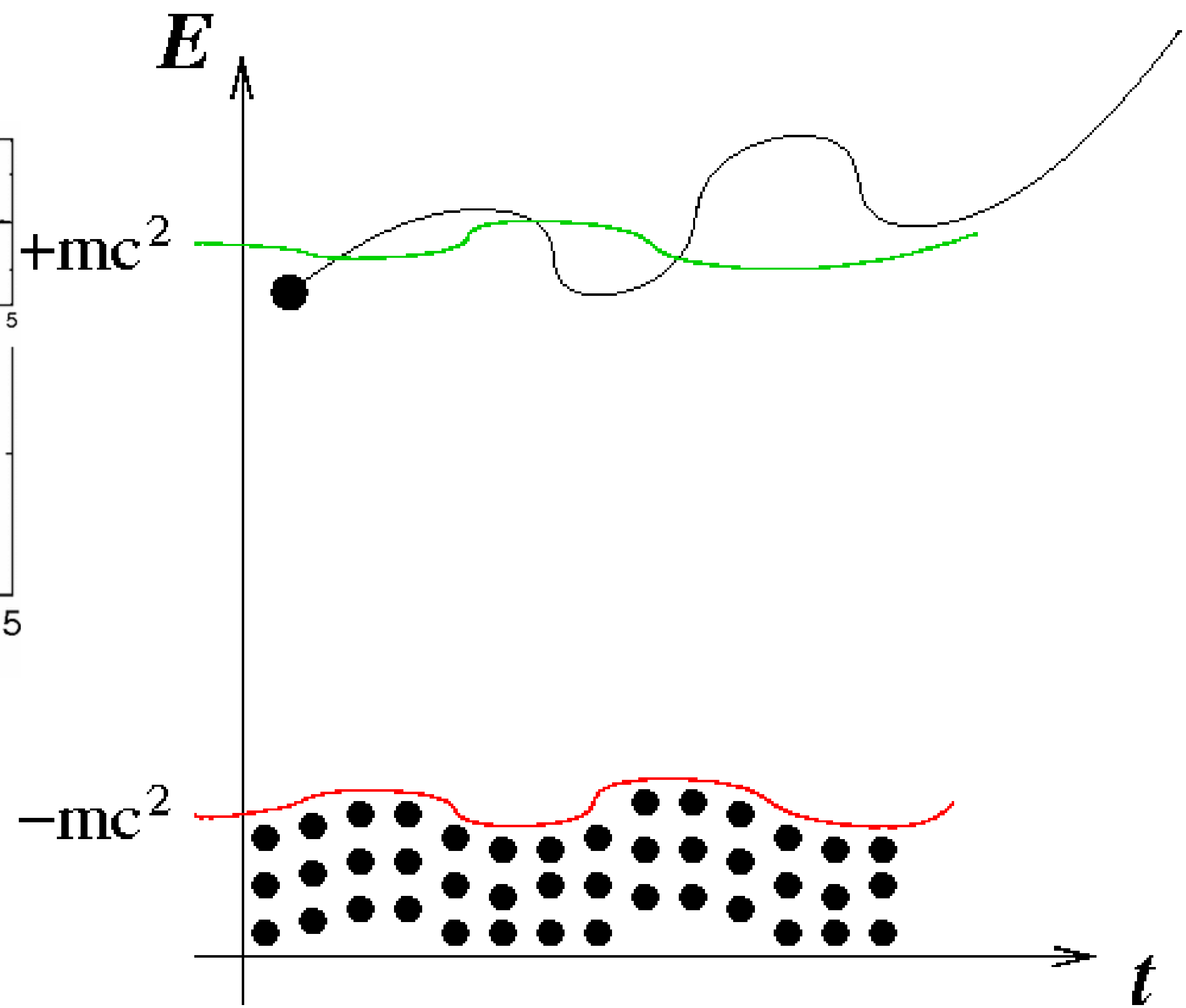


PRA **79**, 043418 (2009)



$2mc^2$ energy spliting (stiffness): *Magnus propagator*

Crank Nicolson, Runge Kutta, etc.:

Error ~ $\Psi^{(n)}\tau^n \sim H^n\tau^n, \|H\| \sim 2mc^2, \tau < \dfrac{1}{2mc^2}$

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Magnus (2nd order):

$$\Psi(t+\tau) \approx \exp\left[-i\hbar H(t+\tau/2)\tau\right]\Psi(t)$$

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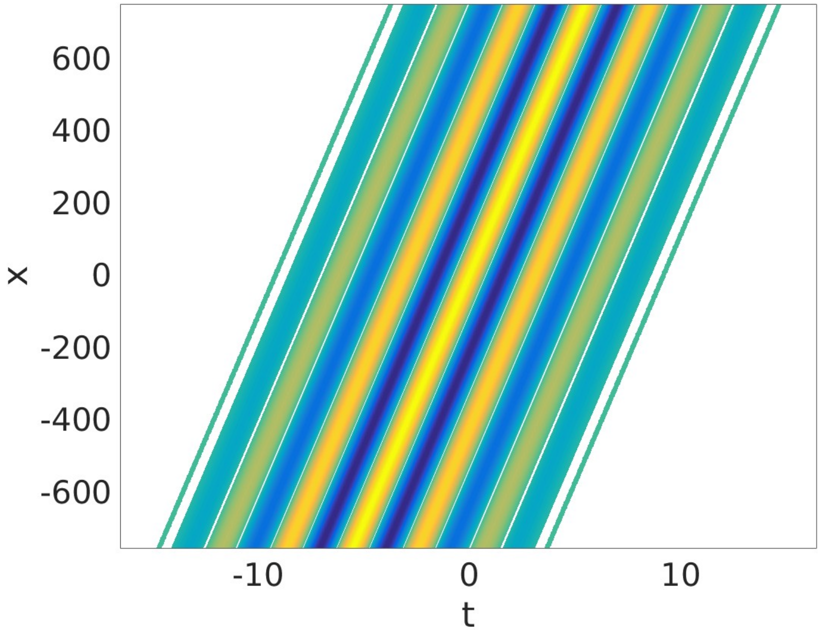
Problem: Requires diagonalization

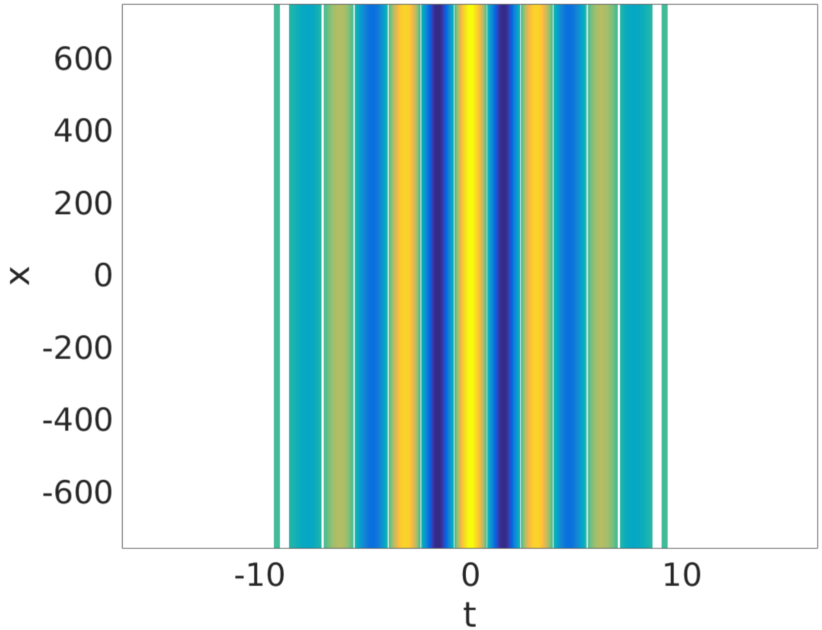
$$H'_{a,b} = c\langle\psi_a|\alpha_z A|\psi_b\rangle$$

Interaction:
Separating space and time

$$A(t - x/c)$$



Dipole approximation (not valid)



$$H'_{a,b} = c\langle \psi_a | \alpha_z A | \psi_b \rangle$$

Interaction:
Separating space and time

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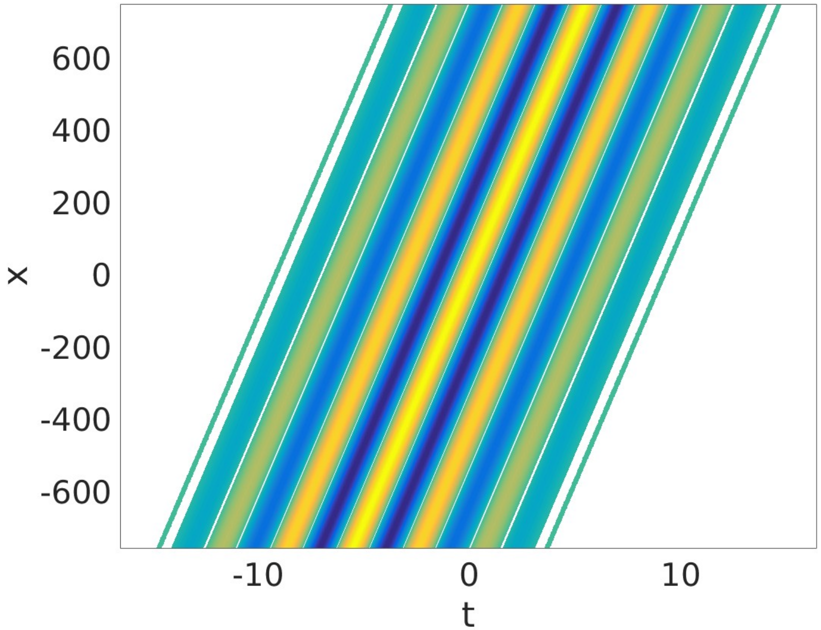
$$A(t - x/c) \approx \Sigma_{n=0}^{n_{trunc}} T_n(t)\, X_n(x)$$

$$H'_{a,b} = c\,\Sigma_n T_n(t) \langle \psi_a | \alpha_z X_n(x) | \psi_b \rangle$$



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Separating space and time

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$$H'_{a,b} = c\,\Sigma_n T_n(t) \langle \psi_a | \alpha_z X_n(x) | \psi_b \rangle$$

Taylor

Fourier

$$A \approx \Sigma_{n=0}^{n_{trunc}} \frac{1}{n!} A^{(n)}(t)(-x/c)^n$$

$$A \approx \Sigma_n a_n \exp[2\pi n i / T (t - x/c)]$$

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Separating space and time

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T equal pulselength?

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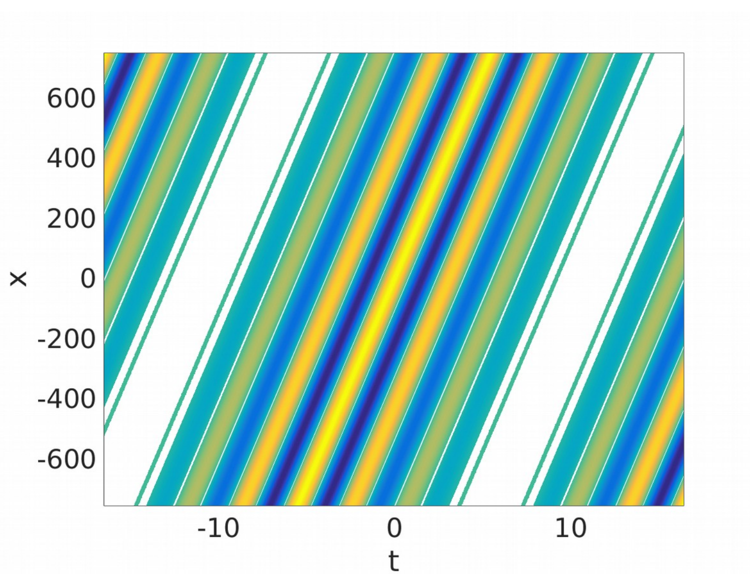
~~*T* equal r[illegible]elength?~~



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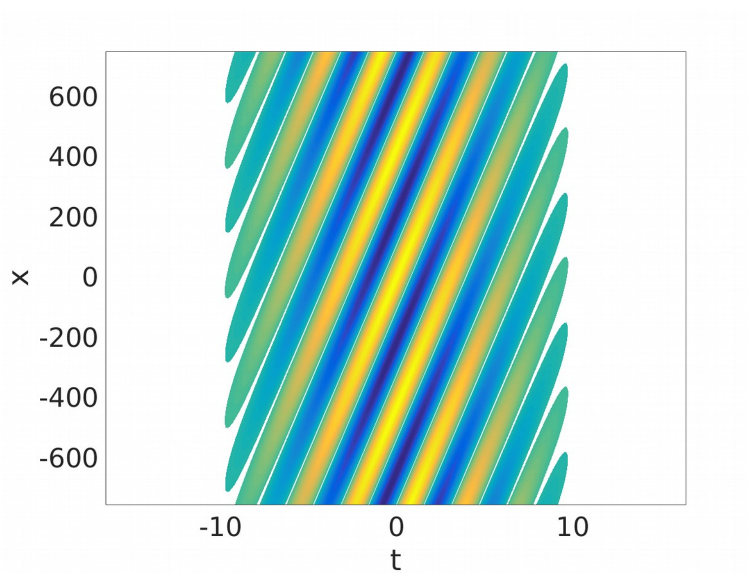

~~*T* equal wavelength?~~

$$A = f(t-x/c)\sin(\omega(t-x/c)) \rightarrow f(t)\sin(\omega t - kx)?$$

Interaction:
Separating space and time

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$$A(t-x/c)\approx\Sigma_{n=0}^{n_{trunc}}T_n(t)\,X_n(x)$$

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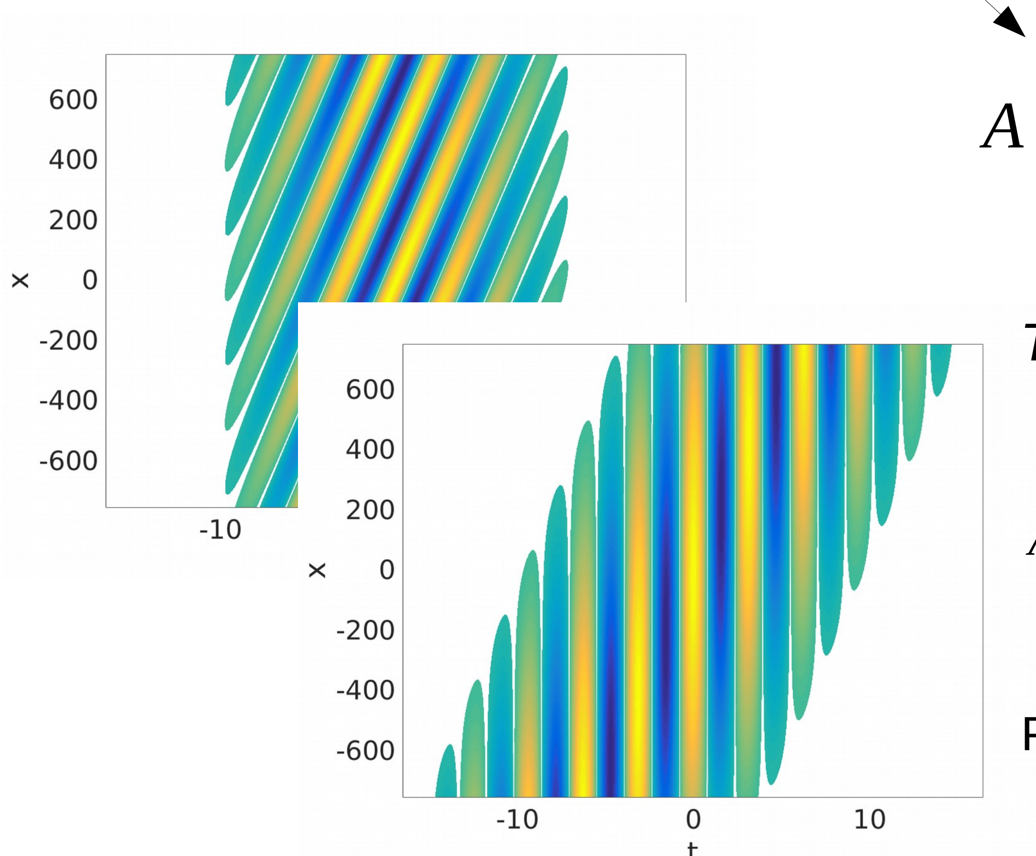
Fourier

$$A\approx\Sigma_n a_n\exp[2\pi n i/T(t-x/c)]$$



~~*T* equal r[illegible]elength?~~

$$A=f(t-x/c)\sin(\omega(t-x/c))\rightarrow f(t)\sin\cancel{[illegible]\,t-kx})?$$

$$\rightarrow f(t-x/c)\sin(\omega t)$$

PRA **93**, 053411 (2016)

Interaction:
Separating space and time

$$A(t-x/c)\approx\Sigma_{n=0}^{n_{trunc}}T_n(t)X_n(x)$$

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$$A\approx\Sigma_{n=0}^{n_{trunc}}\frac{1}{n!}A^{(n)}(t)(-x/c)^n$$

Fou

$$A\approx\Sigma_{\ldots}\ldots\mathrm{xp}\ldots\pi ni/T(t-x/c)]$$

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Separating space and time

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$$A\approx\Sigma_{n=0}^{n_{trunc}}\frac{1}{n!}A^{(n)}(t)(-x/c)^n$$

Fou

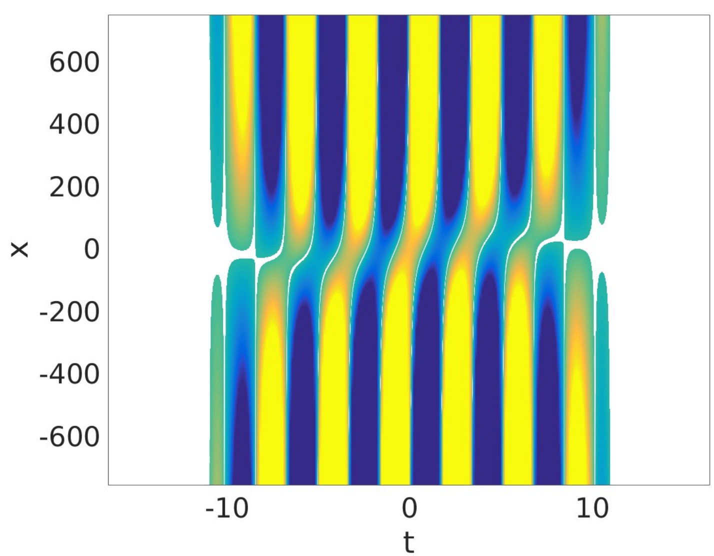
$$A\approx\Sigma_n \ldots \exp[\ldots\pi n i/T(t-x/c)]$$

For the TDSE:

1st order will do:)

Førre, Simonsen, PRA **90**, 053411 (2014)

Alas...



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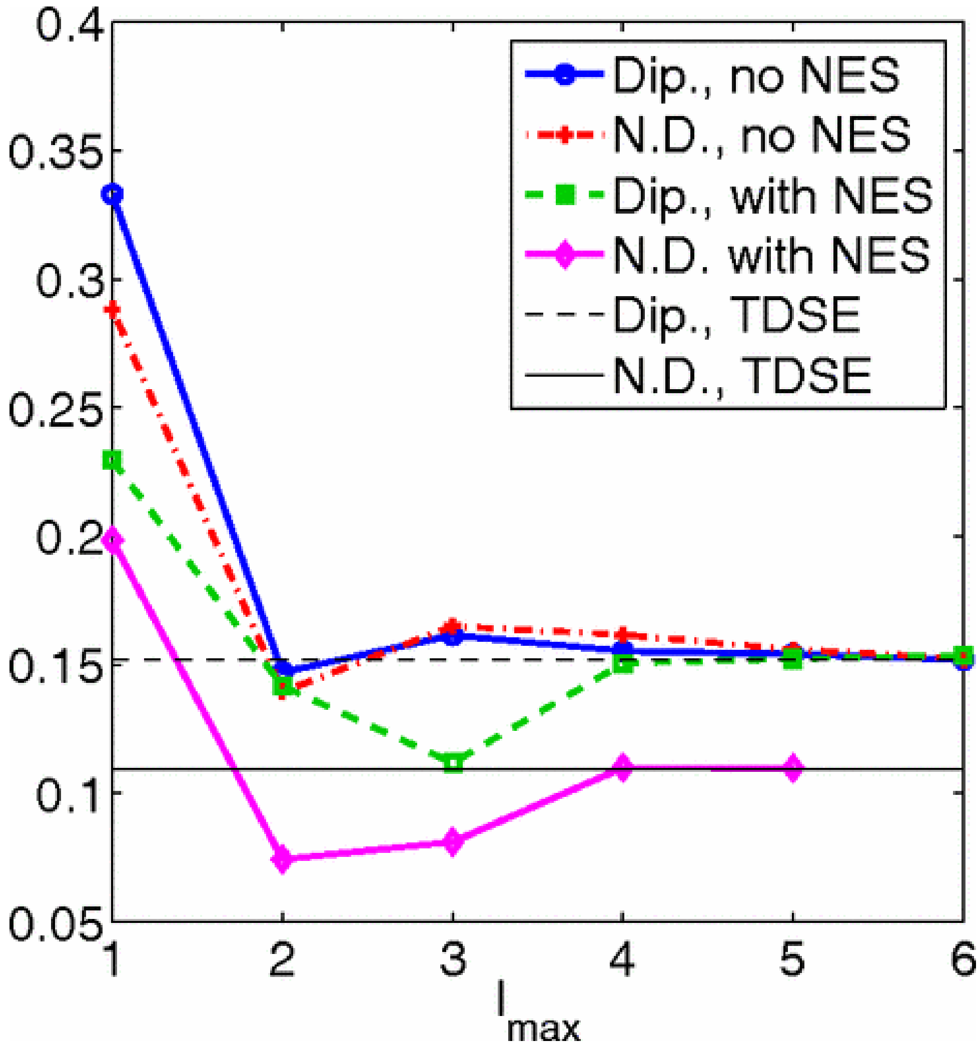
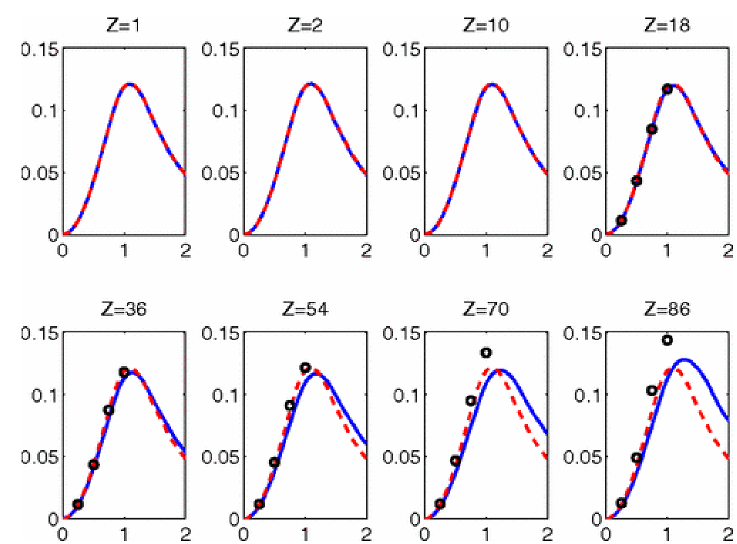


ω=2 a.u. ~ 33 eV
E_0=30 a.u. ~ $3\cdot10^{19}$ W/cm^2

PRA **79**, 043418 (2009)



2013: Enter Tor Kjellsson

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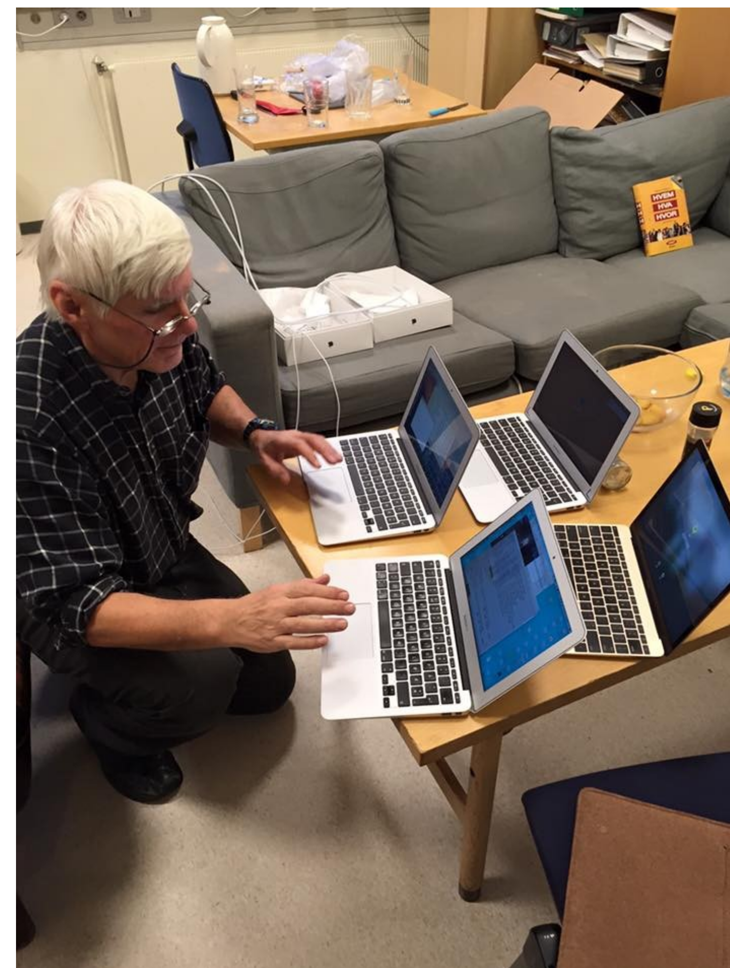
Tor's implementation:

Roughest calculation: 1536 CPUs running for several days.
Only 29% overhead!

Number of states: 1902594
Non-zero elements: 386597830910 (3.02 TB memory)
Reduced elements : 3907655071 (30.5 GB memory)

5th order in x, $l_{max}=30$, *500 splines per symmetry* ($r_{max}=150$ a.u.), $dt=10^{-3}$ a.u.

Much effort spent om optimizing memory usage!



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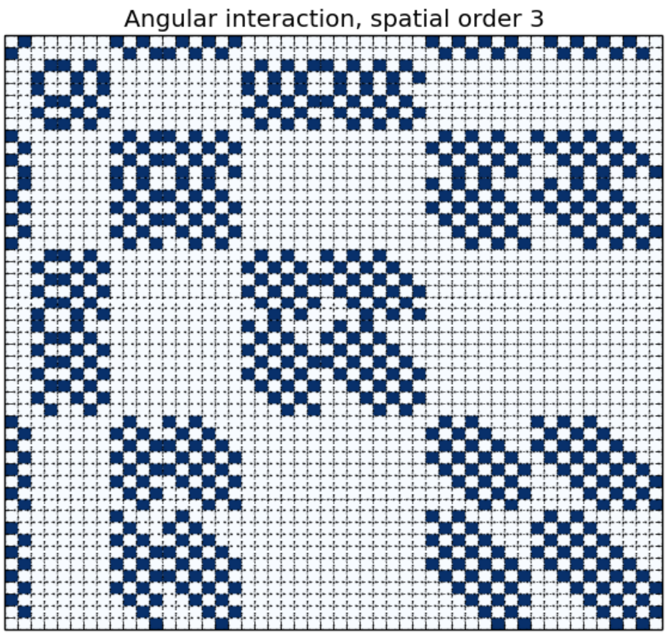
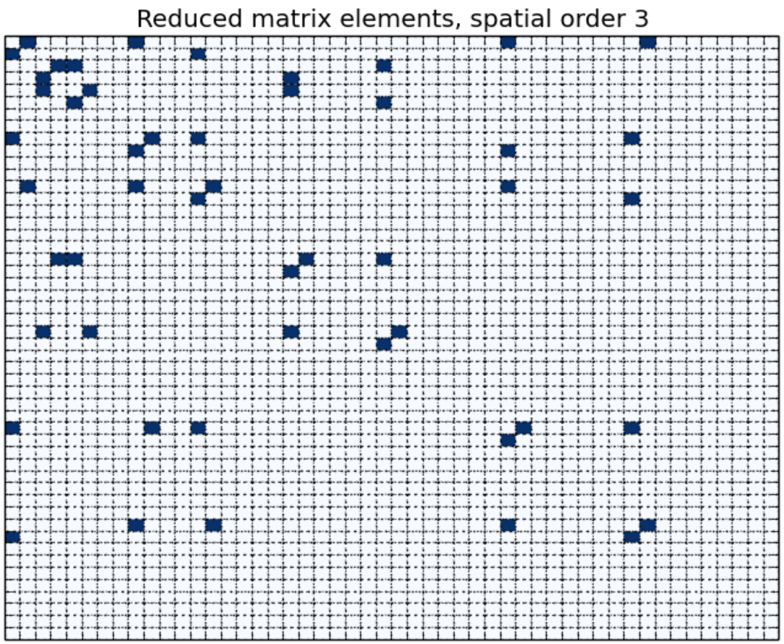
$$\alpha_z x^n, n = 0,1,2,3$$





$2mc^2$ energy spliting (stiffness): *Magnus propagator,* revisited

$$\Psi(t+\tau) \approx \exp[-i\hbar H(t+\tau/2)\tau]\Psi(t)$$

Problem: Requires diagonalization

Solution: Exponentiate approximately within a *Krylov* subspace:

$$K_m = Span\{H^k \Psi, k=0,\ldots,m\}$$

$$m \sim 50 \ll 2\cdot 10^6$$

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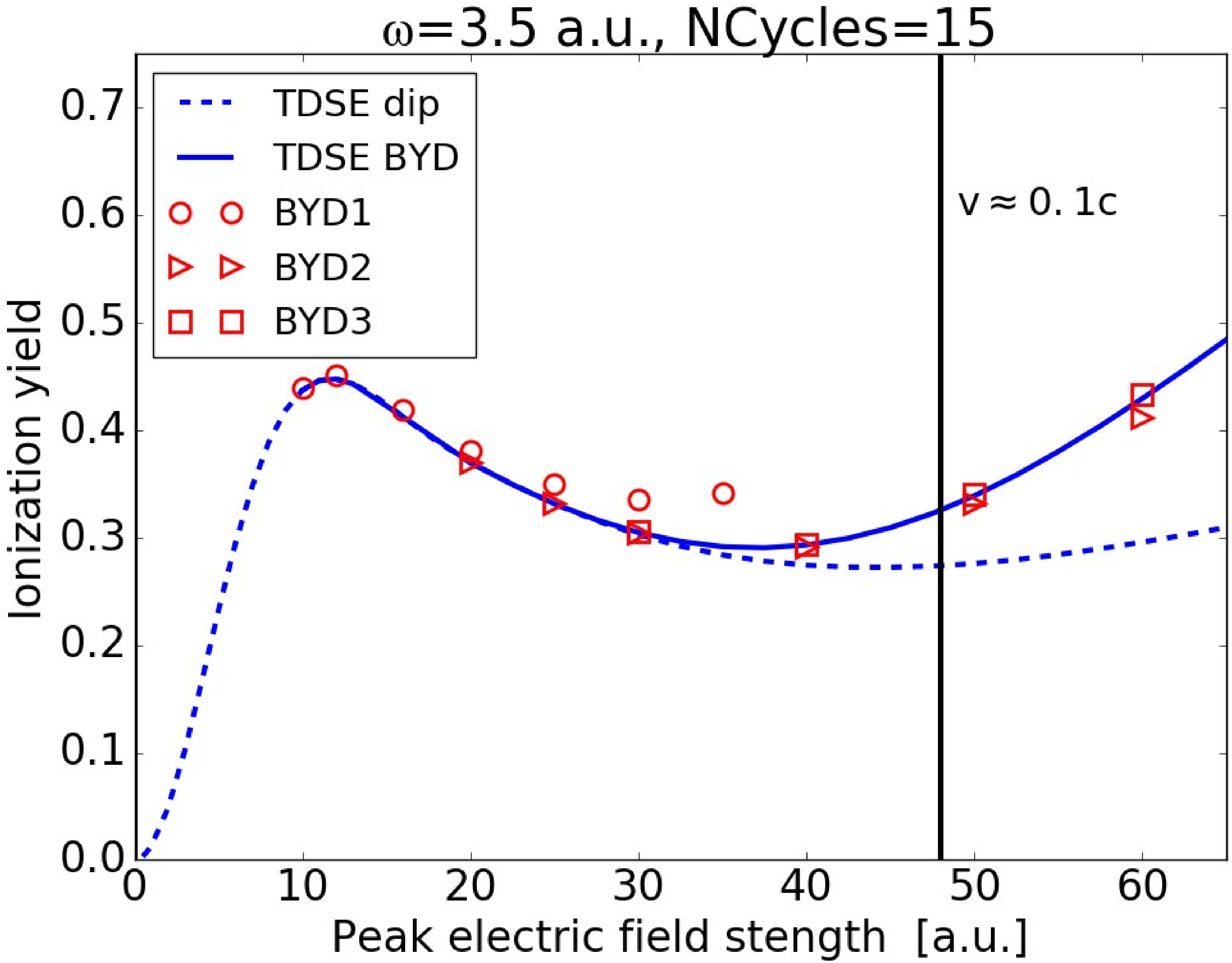

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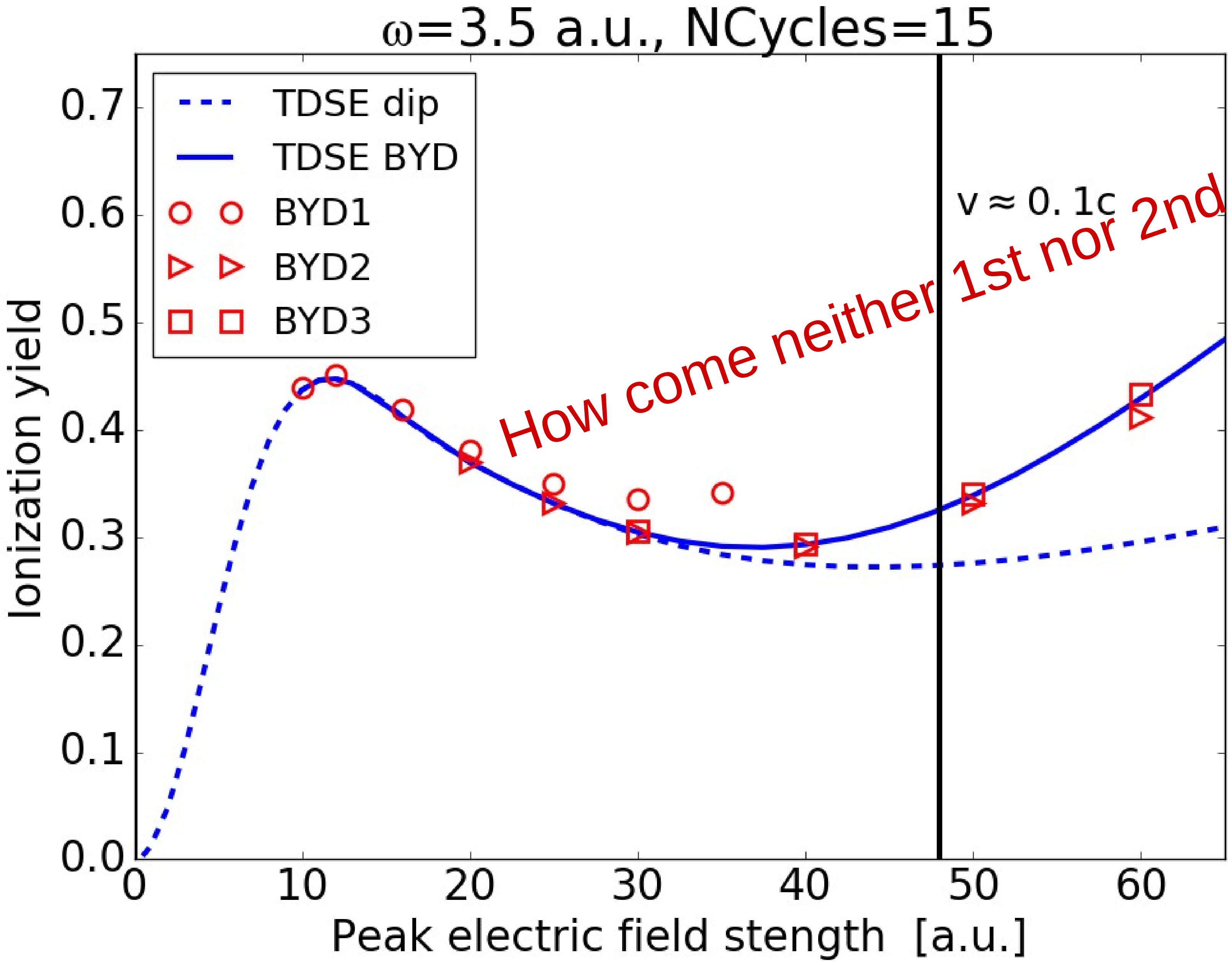

How come neither 1st nor 2nd order will do?

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Implicit inclusion of diamagnetic term

$$\Psi = \begin{pmatrix} \Psi_F \\ \Psi_G \end{pmatrix}$$

Postitive energy: $\Psi_F \sim c\,\Psi_G$

$$V\,\Psi_F + c\,\boldsymbol{\sigma}\cdot\left(e\,\boldsymbol{A} + \boldsymbol{p}\right)\Psi_G = i\hbar\,\dot{\Psi}_F$$

$$c\,\boldsymbol{\sigma}\cdot\left(e\,\boldsymbol{A} + \boldsymbol{p}\right)\Psi_F + \left(V - 2mc^2\right)\Psi_G = i\hbar\,\dot{\Psi}_G$$

Implicit inclusion of diamagnetic term

$$\Psi = \begin{pmatrix} \Psi_F \\ \Psi_G \end{pmatrix}$$ Postitive energy: $\Psi_F \sim c\,\Psi_G$

$$V\,\Psi_F + c\,\boldsymbol{\sigma}\cdot\left(e\,\boldsymbol{A}+\boldsymbol{p}\right)\Psi_G = i\hbar\,\dot{\Psi}_F$$

$$c\,\boldsymbol{\sigma}\cdot\left(e\,\boldsymbol{A}+\boldsymbol{p}\right)\Psi_F + \left(V-2mc^2\right)\Psi_G = i\hbar\,\dot{\Psi}_G$$

2mc² dominates: $\Psi_G \approx \frac{1}{2mc^2}\boldsymbol{\sigma}\cdot\left(e\,\boldsymbol{A}+\boldsymbol{p}\right)\Psi_F$

Implicit inclusion of diamagnetic term

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Implicit inclusion of diamagnetic term

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With $A \approx A(t) - \frac{x}{c} A'(t)$ (1st order expansion)

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Should effectively cancel 2nd order term

Førre, Simonsen, PRA **90**, 053411 (2014)

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Must include higher orders of *x*

*Smarter: Use **propagation gauge** for TDDE*

Førre, Simonsen, PRA **93**, 013423 (2016)

Relativistic?

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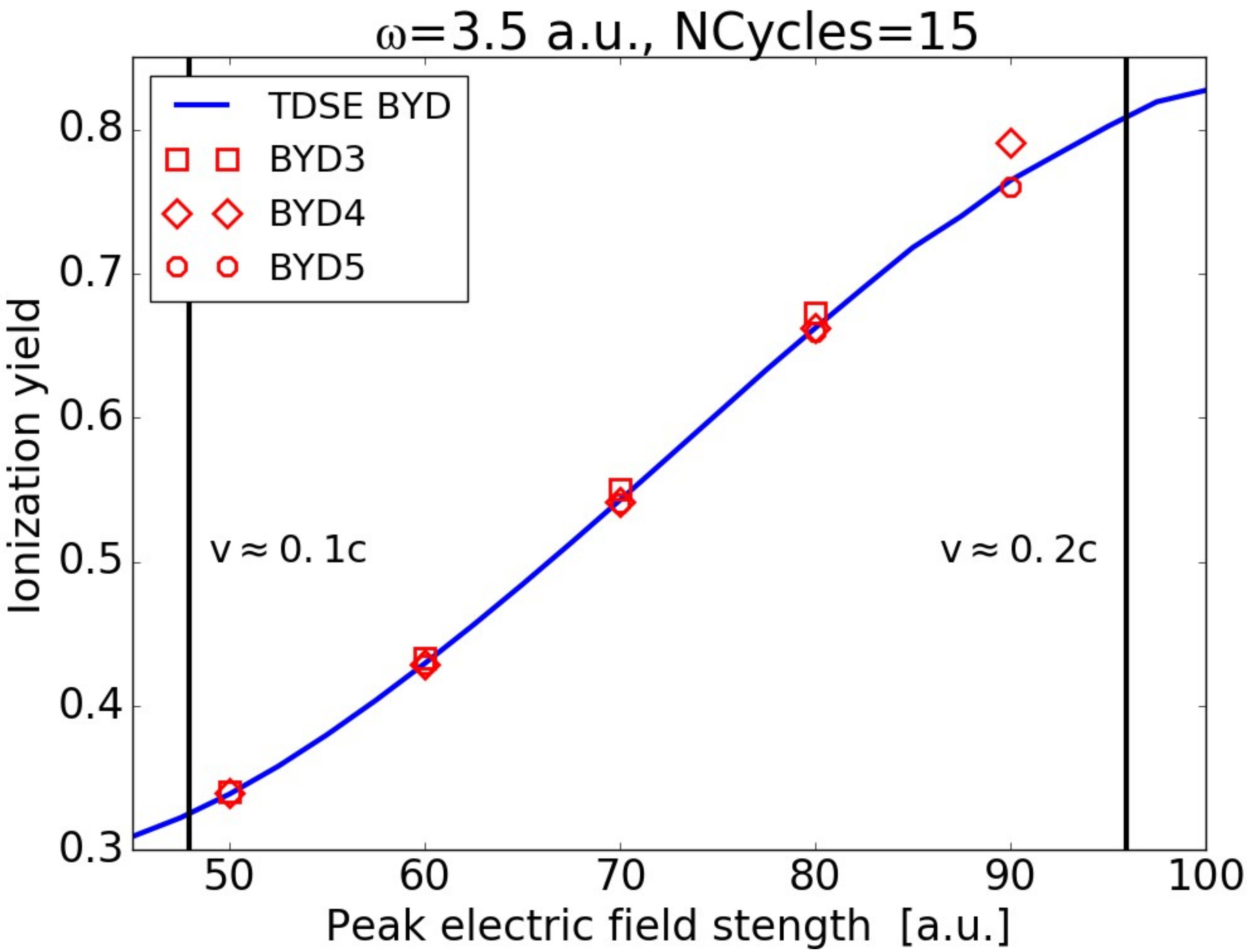
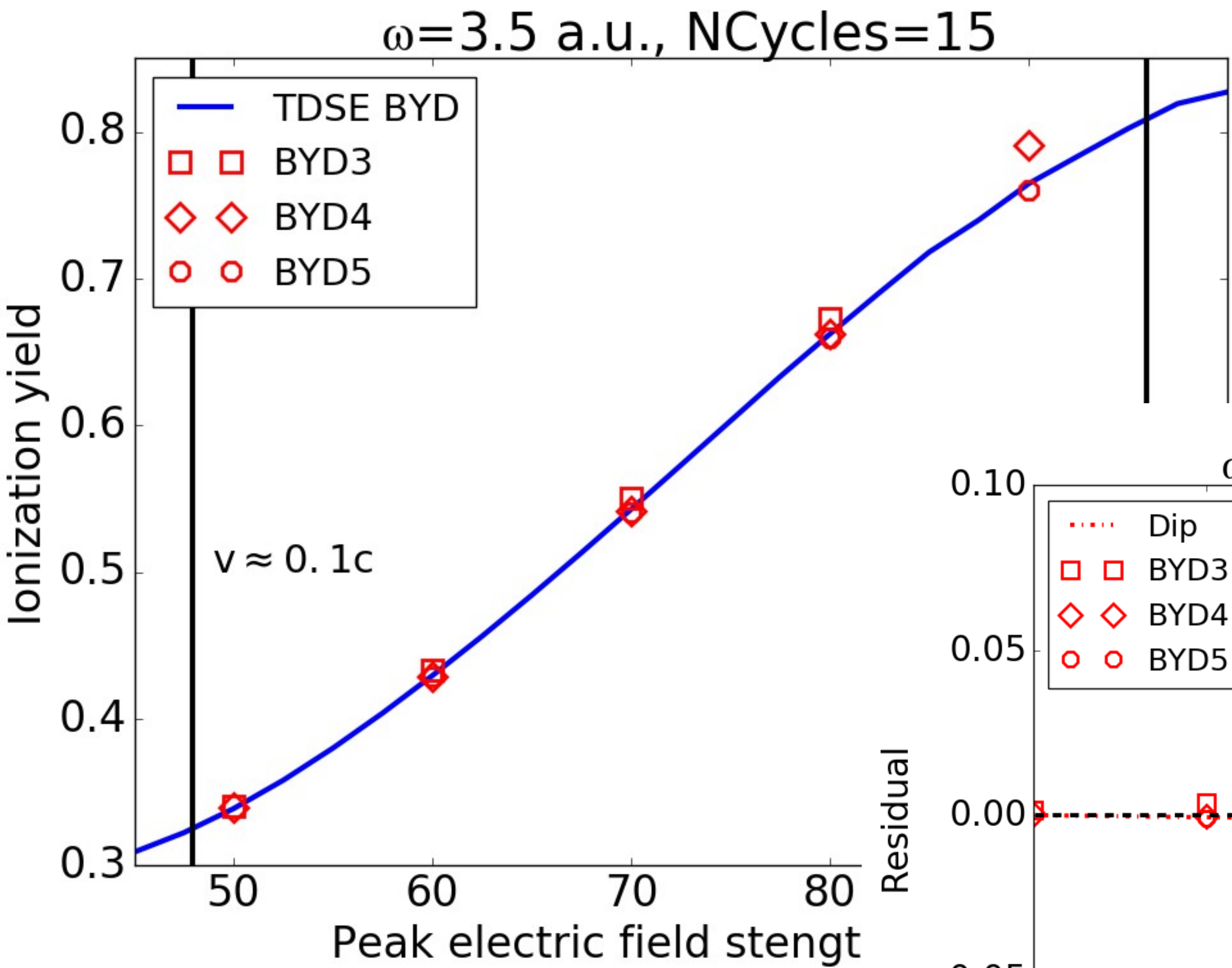
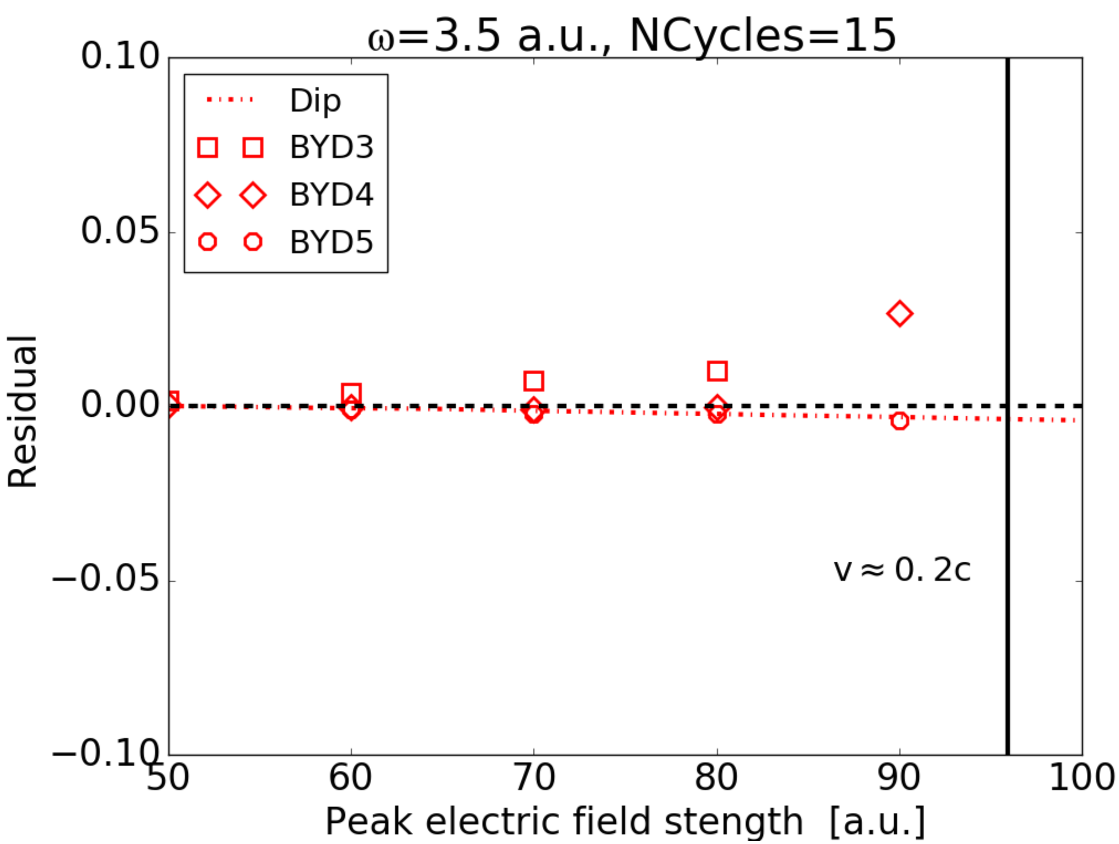


Relativistic?





Relativistic?

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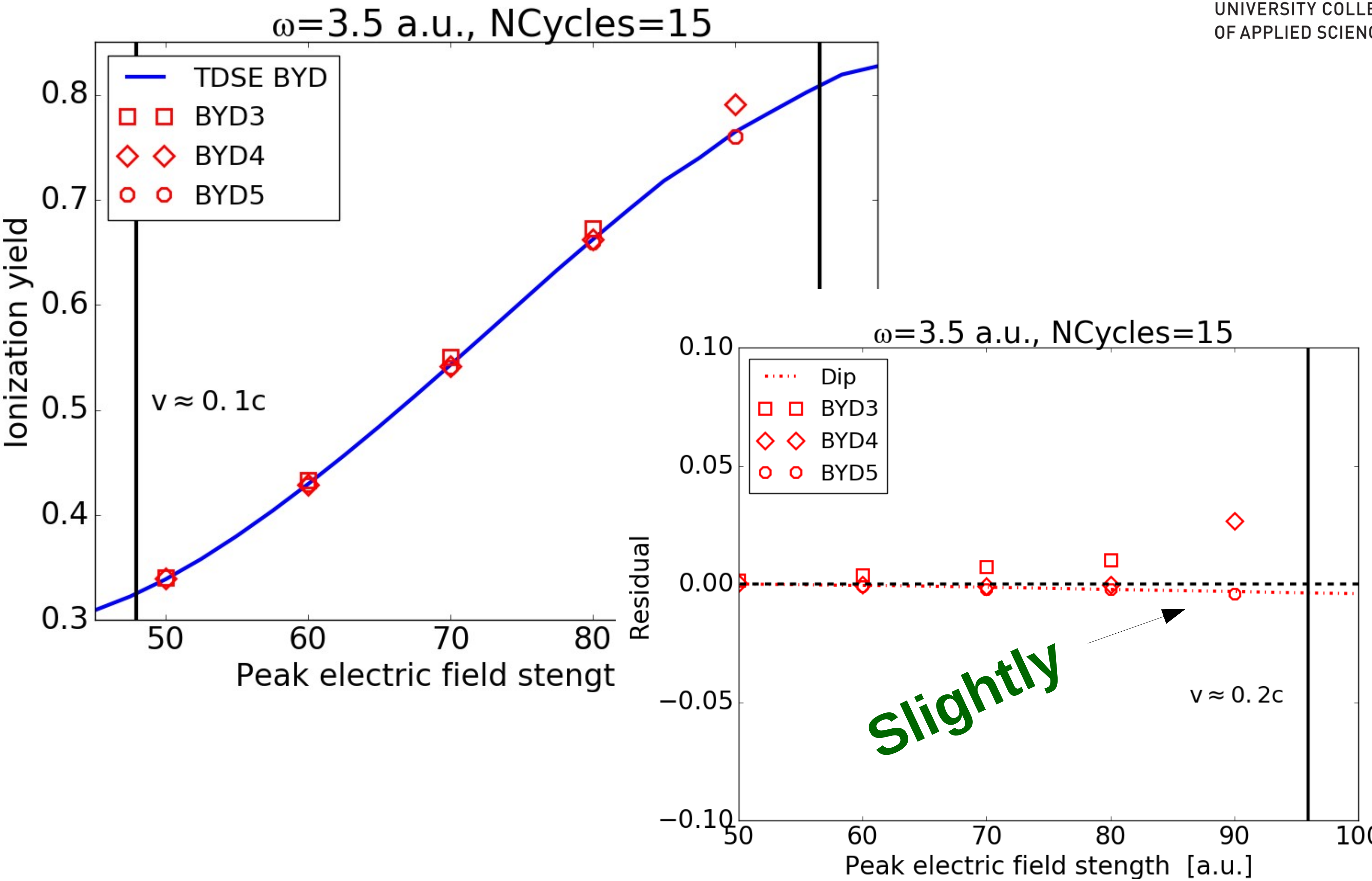

Slight shift downwards: How come?

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Initiall guess: Increased relativistic intertia

Model: $$m \rightarrow \frac{m}{\sqrt{1-(v/c)^2}}, \quad v=\frac{e}{m}A(t)$$

TDSE (dipole approx.)

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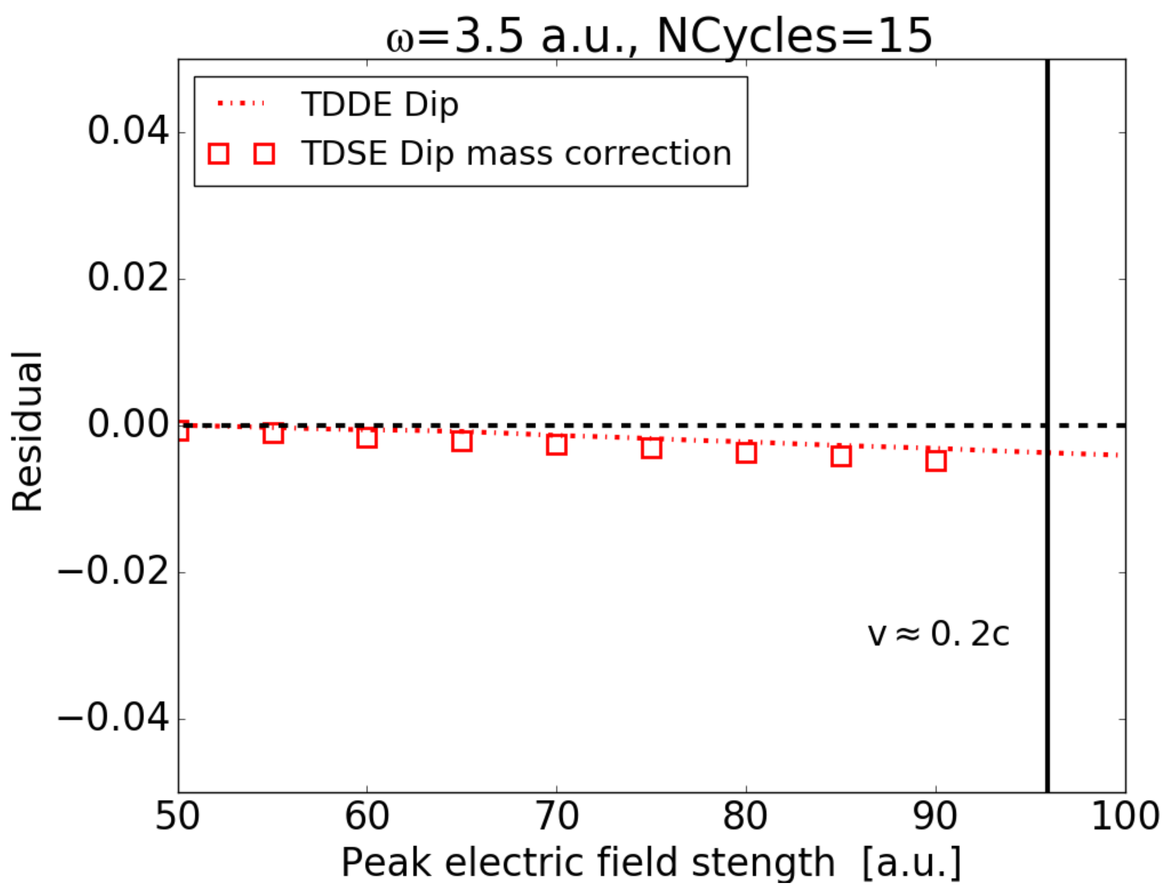
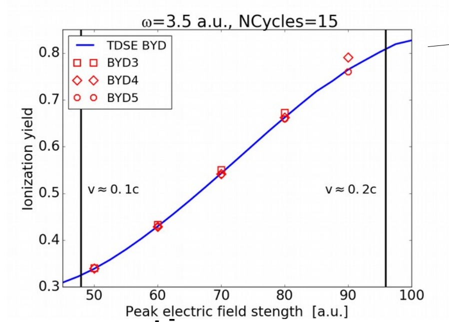
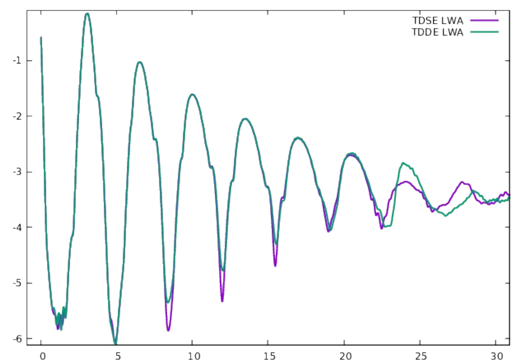


What's next?

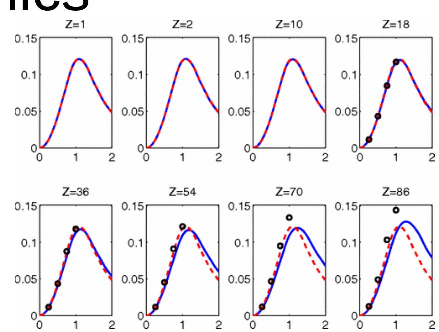


Push things forward within the propagation gauge



Study photoelectron spectra

High *Z*: Rel. structure vs. rel. dynamics



Study spin-dynamics;
TDPE vs. TDDE

$$\frac{e\hbar}{2m}\boldsymbol{\sigma}\cdot\boldsymbol{B}(t)$$

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Gratulerar!

$$\Psi(t) = \sum_{n,j,m,\kappa} c_{n,j,m,\kappa}(t)\,\psi_{n,j,m,\kappa}(\mathbf{r}) \quad , \tag{21}$$

with

$$\psi_{n,j,m,\kappa}(\mathbf{r}) = \begin{pmatrix} F_{n,j,m,\kappa}(\mathbf{r}) \\ G_{n,j,m,\kappa}(\mathbf{r}) \end{pmatrix} \quad , \tag{22}$$

where

$$\begin{pmatrix} F_{n,j,m,\kappa}(\mathbf{r}) \\ G_{n,j,m,\kappa}(\mathbf{r}) \end{pmatrix} = \frac{1}{r}\begin{pmatrix} P_{n,\kappa}(r)X_{\kappa,j,m}(\Omega) \\ iQ_{n,\kappa}(r)X_{-\kappa,j,m}(\Omega) \end{pmatrix} \quad . \tag{23}$$

Here $\kappa = l$ for $j = l - 1/2$ and $\kappa = -(l+1)$ for $j = l + 1/2$, and $X_{\kappa,j,m}$ represents the spin-angular part which has the analytical form

$$X_{\kappa,j,m} = \sum_{m_s,m_l} \langle l_\kappa, m_l; s, m_s | j, m\rangle Y^{l_\kappa}_{m_l}(\theta,\phi)\chi_{m_s} \quad , \tag{24}$$

where $Y^{l_\kappa}_{m_l}(\theta,\phi)$ is a spherical harmonic and χ_{m_s} is an eigenspinor. The radial components $P_{n,\kappa}(r)$ and $Q_{n,\kappa}(r)$ are expanded in B-splines [24];

$$P_{n,\kappa}(r) = \sum_i a_i B^{k_1}_i(r) \quad , \quad Q_{n,\kappa}(r) = \sum_j b_j B^{k_2}_j(r). \tag{25}$$

$$H_{B\tilde{B}}(t) = \sum_{i,p} a_i(t)\langle n\kappa jm|\alpha_z x^p|\tilde{n}\tilde{\kappa}\tilde{j}\tilde{m}\rangle. \tag{30}$$

Working in the eigenbasis of H_0, we may compute these couplings using angular momentum theory by first expressing the operators in terms of spherical tensor operators [26]. For x^p, these are spherical harmonics Y^λ_μ;

$$x^n = \sum_i c_i r^n Y^{\lambda_i}_{\mu_i} \quad , \tag{31}$$

while $\sigma_z = \sigma^1_0$ is a component of a rank-1 spherical tensor operator. The couplings in Eq. (30) are now given by summing up terms factored in a radial part and spin-angular part:

$$\begin{aligned} &\langle n\kappa jm|\alpha_z r^\gamma Y^\lambda_\mu|\tilde{n}\tilde{\kappa}\tilde{j}\tilde{m}\rangle = \\ &i\int_r \Big[P^*_{n\kappa}(r)r^\gamma Q_{\tilde{n}\tilde{\kappa}}(r)\langle\kappa jm|\sigma^1_0 Y^\lambda_\mu|\text{-}\tilde{\kappa}\tilde{j}\tilde{m}\rangle - \\ &Q^*_{n\kappa}(r)r^\gamma P_{\tilde{n}\tilde{\kappa}}(r)\langle\text{-}\kappa jm|\sigma^1_0 Y^\lambda_\mu|\tilde{\kappa}\tilde{j}\tilde{m}\rangle\Big]\,dr \end{aligned} \tag{32}$$

$$\sigma_0^1 Y_\mu^\lambda = \sum_{K=|\lambda-1|}^{\lambda+1} \langle 10;\lambda\mu|KQ\rangle \left\{\boldsymbol{\sigma}^1 \mathbf{Y}^\lambda\right\}_Q^K \ , \quad Q=\mu \quad .$$

With this choice the spin-angular part may be computed as:

$$\langle \kappa j m|\sigma_0^1 Y_\mu^\lambda|\tilde{\kappa}\tilde{j}\tilde{m}\rangle = \sum_{K=|\lambda-1|}^{\lambda+1} (-1)^{\lambda-1-Q} \sqrt{2K+1} \\ \times \begin{pmatrix} 1 & \lambda & K \\ 0 & \mu & -\mu \end{pmatrix} \langle \kappa j m| \left\{\boldsymbol{\sigma}^1 \mathbf{Y}^\lambda\right\}_Q^K |\tilde{\kappa}\tilde{j}\tilde{m}\rangle \quad . \tag{33}$$

The Wigner-Eckart theorem can be applied to the matrix element of the combined operator $\left\{\boldsymbol{\sigma}^1 \mathbf{Y}^\lambda\right\}_Q^K$:

$$\langle \kappa j m| \left\{\boldsymbol{\sigma}^1 \mathbf{Y}^\lambda\right\}_Q^K |\tilde{\kappa}\tilde{j}\tilde{m}\rangle = \\ (\text{-}1)^{j-m} \begin{pmatrix} j & K & \tilde{j} \\ -m & Q & \tilde{m} \end{pmatrix} \times \langle j|| \left\{\boldsymbol{\sigma}^1 \mathbf{Y}^\lambda\right\}^K ||\tilde{j}\rangle \tag{34}$$

with the reduced matrix element given by:

$$\langle j|| \left\{\boldsymbol{\sigma}^1 \mathbf{Y}^\lambda\right\}^K ||\tilde{j}\rangle = \sqrt{(2j+1)(2K+1)(2\tilde{j}+1)} \\ \times \langle s||\boldsymbol{\sigma}^1||\tilde{s}\rangle\langle l||\mathbf{Y}^\lambda||\tilde{l}\rangle \begin{Bmatrix} l & \tilde{l} & 1 \\ s & \tilde{s} & \lambda \\ j & \tilde{J} & K \end{Bmatrix} \quad . \tag{35}$$

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