

Quantum relativistic dynamics and QED effects in multi-center systems

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Heidelberg, July 22nd 2015

Outline

1 Pair production in multi-center systems

- Pair creation mechanisms
- Model description
- Pair production in inhomogeneous field
- Numerical results for pair production
 - Position of resonances and pair production
 - Total Rate: REPP and ECEPP

2 Numerical solution of the Dirac equation

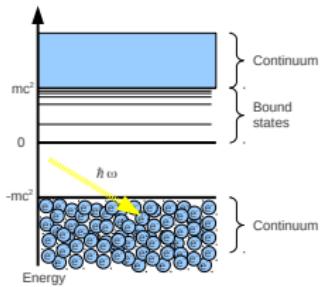
- Dirac equation description
- Balance principles
- Numerical results: time-independent
- Time-dependent generalization

3 Conclusion

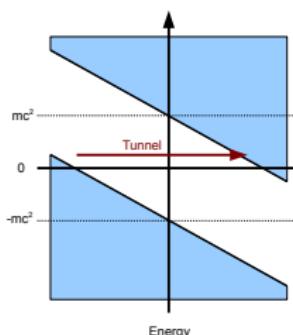
Pair production in multi-center systems

Pair creation mechanisms with an external field

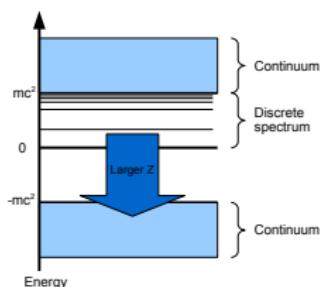
Photon Excitation



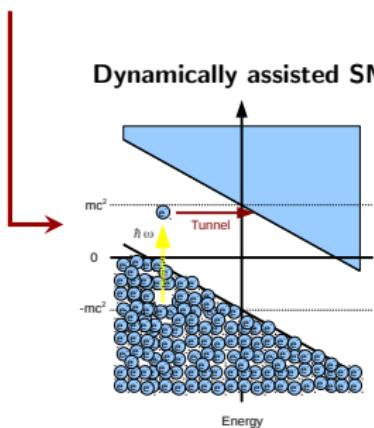
Schwinger's process



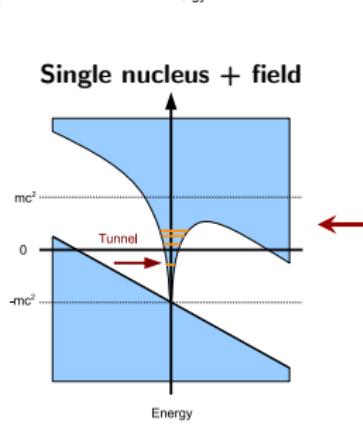
Heavy nuclei “plunging”



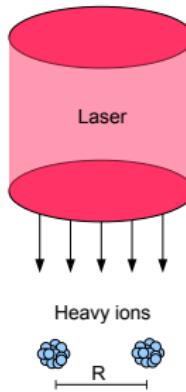
Dynamically assisted SM



Single nucleus + field



Two-center systems (diatomic “molecule”)



Questions?

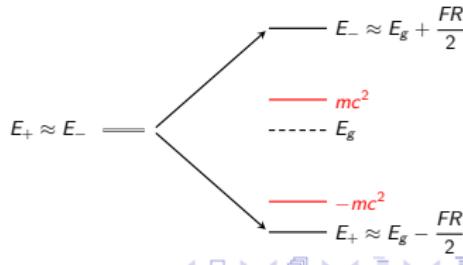
- Can we use effects similar from non-relativistic ionization of molecules to enhance pair production (CREI)?
 - Stark effect at large inter-nuclei distance:

$$\Delta E_{\text{Stark}} \approx \pm \frac{FR}{2} \approx 2mc^2$$

Use Stark's effect to “plunge” in the Dirac sea

- $R \approx 10.$ a.u.
 - $mc^2 \approx 18769.$ a.u.
 - $E_g^{U^{91+}} \approx 13908.$ a.u.

$$I \approx 1.5 \times 10^{24} \text{ W/cm}^2$$



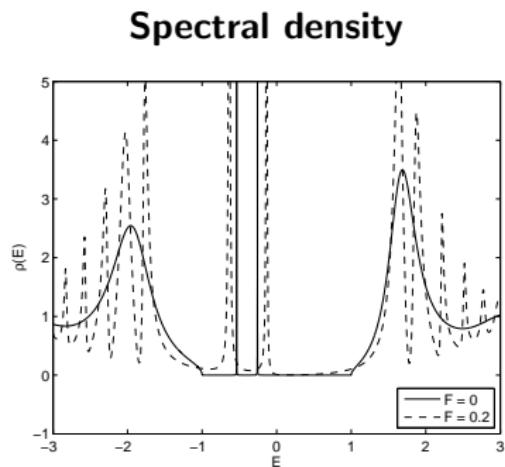
Simple model description

- (Very) Simple toy model
 - ➊ 1-D model
 - ➋ Nuclei potential: delta function wells

$$V_{\text{nucl.}}(s) = -g \sum_{i=1}^{N_{\text{nuc}}} \delta(x - R_i)$$

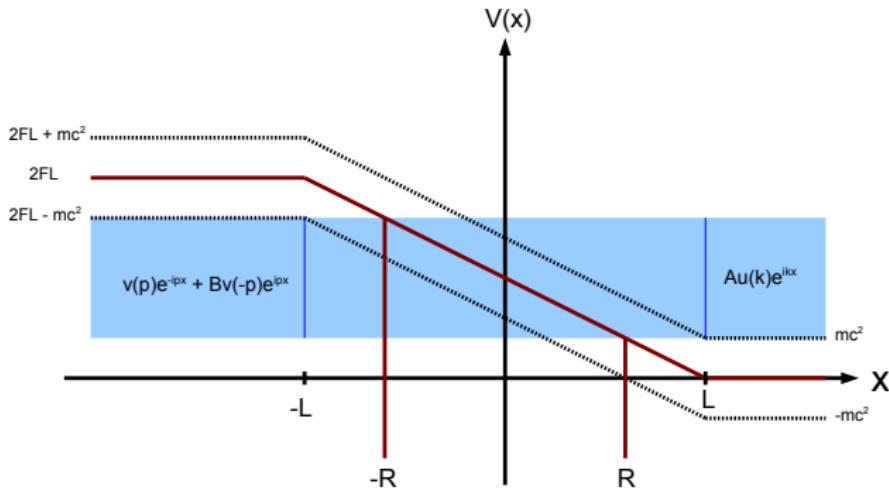
$$g \approx 0.8 = U^{91+}$$

- ➌ Laser electric field: static (adiabatic limit) $V_{\text{field}}(x) = -Fx$



Position of resonances → WTK

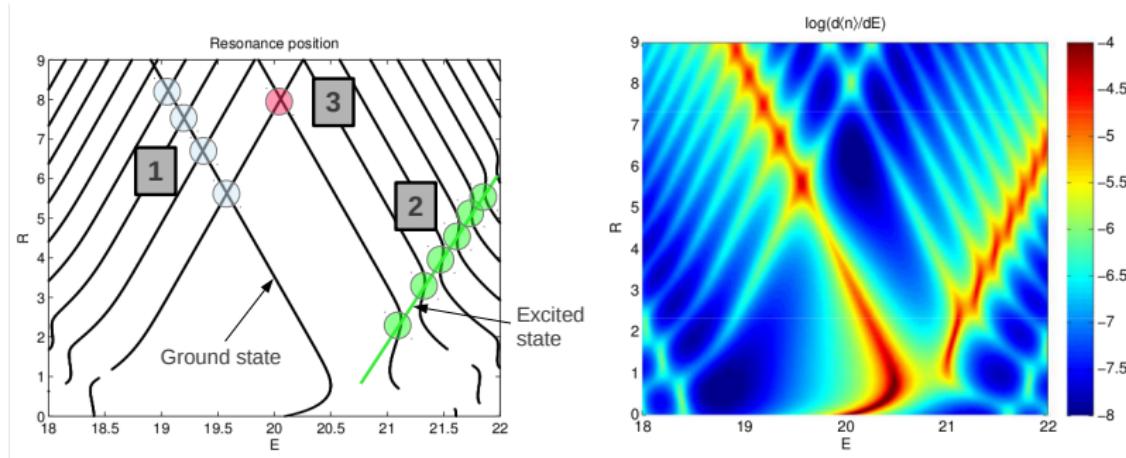
Pair production = Transmission-reflection problem



$$\frac{d\langle n \rangle}{dt dE} = \frac{1}{2\pi} |A(E)|^2, \quad E \in \Omega_{\text{Klein}}$$

$$\frac{d\langle n \rangle}{dt} = \frac{1}{2\pi} \int_{\Omega_{\text{Klein}}} dE |A(E)|^2$$

Position of resonances and pair production: $g = 0.8$ (Uranium), $F = 0.2 \times 10^{18}$ V/m $\rightarrow I = 2.5 \times 10^{27}$ W/cm 2



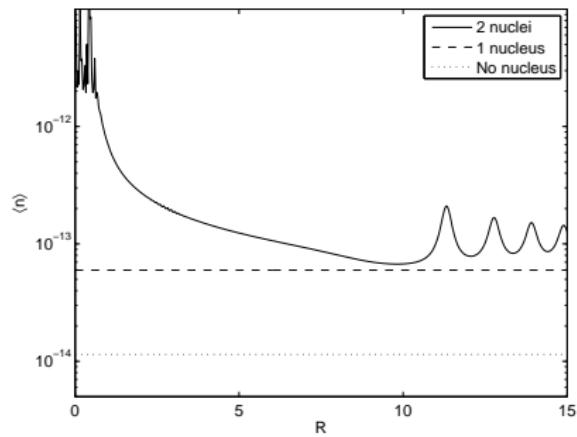
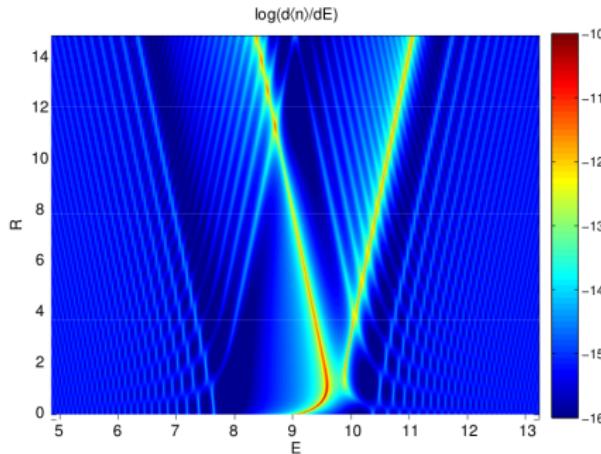
- ① Channel 1: ground state crosses with negative energy resonances
- ② Channel 2: excited state goes through avoided crossing with positive energy resonances
- ③ Channel 3: negative energy states cross with positive energy states

Total rate: $d\langle n \rangle / dt$

For $g = 0.8$ (Uranium),

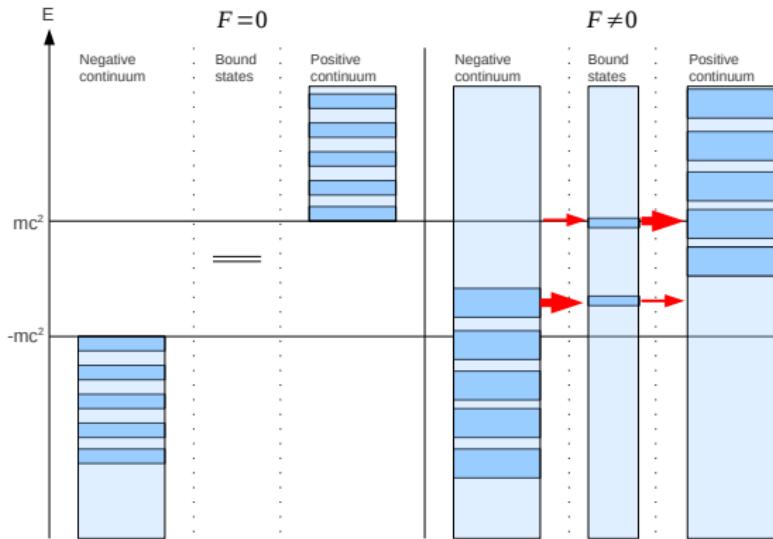
$$F = 0.09 \times 10^{18} \text{ V/m} \rightarrow I = 8.1 \times 10^{26} \text{ W/cm}^2,$$

$$L = 100.0 \times 0.38 \text{ pm}$$



- REPP at large R , dominated by the ground state crossings
- ECEPP at small R

REPP: at LARGE interatomic distance

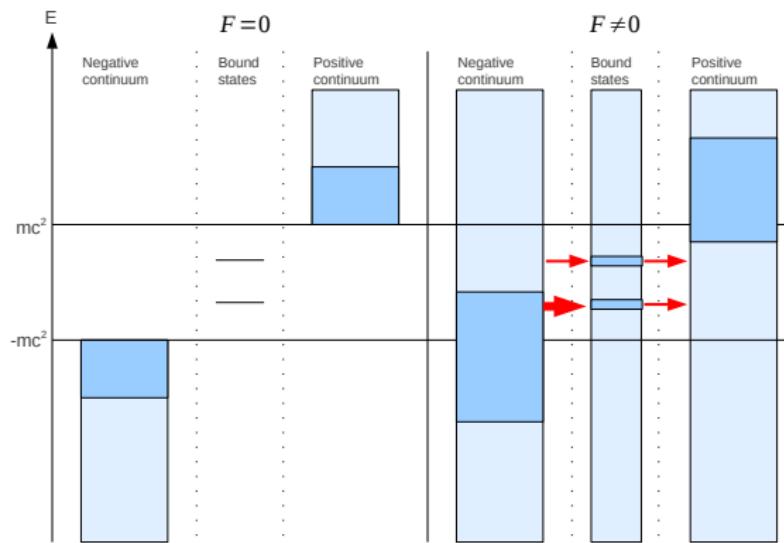
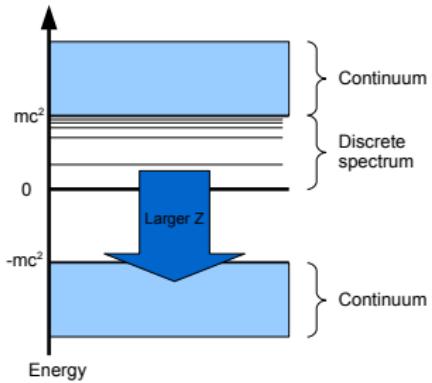


F. Fillion-Gourdeau *et al*, Phys. Rev. Lett. 110, 013002 (2013)

Mechanism: CREI

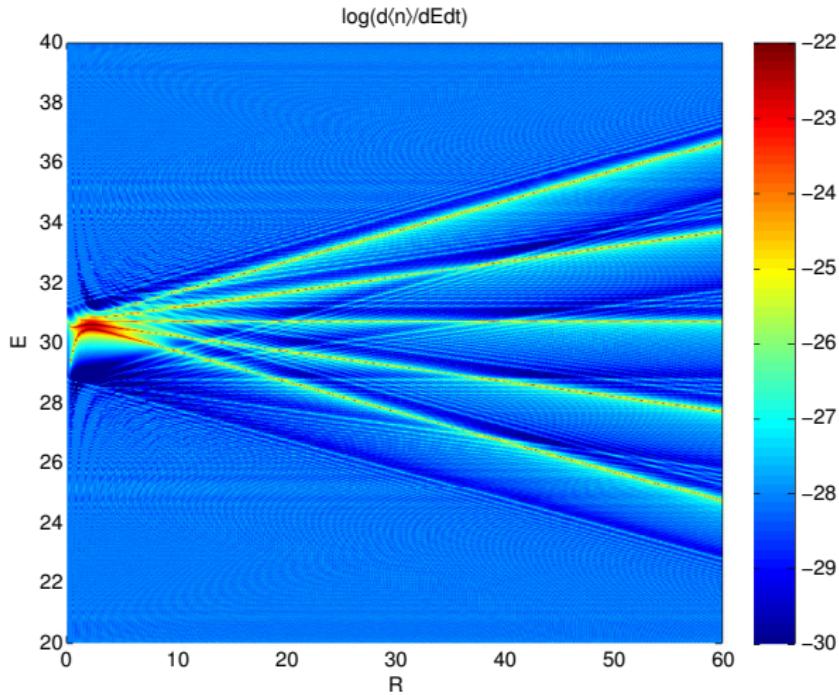
T Seideman, MY Ivanov, PB Corkum , Phys. Rev. Lett. 75, 2819 (1995)
T. Zuo and A. D. Bandrauk , Phys. Rev. A. 52, R2511 (1995)

ECEPP: at SMALL interatomic distance

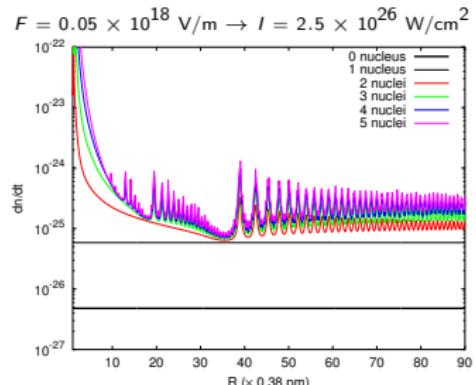
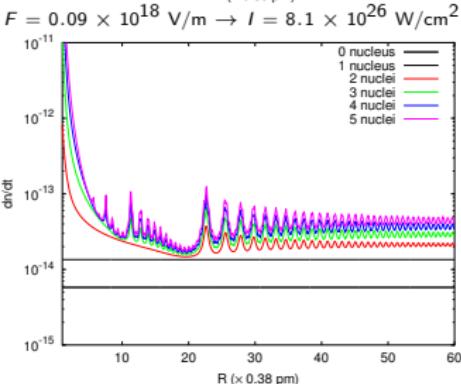
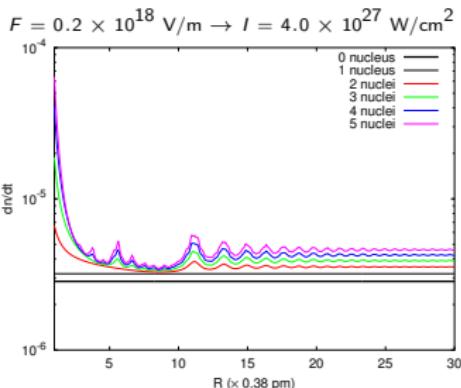


Many-center case: 5 nuclei

$$F = 0.05 \times 10^{18} \text{ V/m} \rightarrow I = 2.5 \times 10^{26} \text{ W/cm}^2$$



Total rate: variation with electric field strength ($g = 0.8$)



- Relative enhancement increases
- REPP occurs at larger R
- Exponential suppression of the rate

Numerical solution of the Dirac equation

Dirac Equation

- Time-dependent:

$$i\partial_t \Psi(x) = [-ic\boldsymbol{\alpha} \cdot \nabla - e\boldsymbol{\alpha} \cdot \mathbf{A}(x) + \beta mc^2 + V(x)] \Psi(x)$$

where $\Psi(x) \in L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$

- Time-independent:

$$E\psi(\mathbf{x}) = [-ic\boldsymbol{\alpha} \cdot \nabla + \beta mc^2 + V(\mathbf{x})] \psi(\mathbf{x})$$

Large and small components are related:

$$\chi(\mathbf{x}) = \frac{-ic\boldsymbol{\sigma} \cdot \nabla}{E + mc^2 - V_c(\mathbf{x})} \phi(\mathbf{x})$$

- \mathbf{A}, V are the potentials of the external field (minimal coupling prescription)

Numerical challenge

① Computation time:

- Time step is small: $\delta t < 1/mc^2$
- Typical time scale of macroscopic field is large
- Many initial and final states to consider (for pair production calculations)

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Basis set expansion (Galerkin method or Rayleigh-Ritz method)

$$E \leq \frac{\langle \psi_0 | H | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle}$$

Numerical challenge

① Computation time:

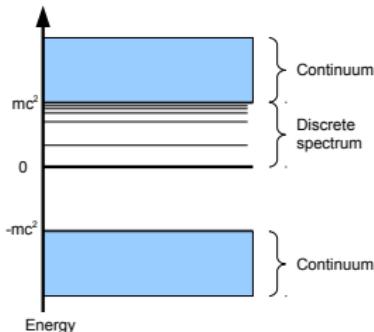
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Multiscale problem

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Basis set expansion (Galerkin method or Rayleigh-Ritz method)

② Spectrum is NOT bounded from below



$$E \leq \frac{\langle \psi_0 | H | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle}$$

Variational collapse

Balance principles for time-independent Dirac

- Basis set expansion with balance principle (W Kutzelnigg, 1984):

$$\begin{aligned}\phi_s(\mathbf{x}) &= \sum_{n=1}^N a_n^{(s)} B_n^{(s)}(\mathbf{x}) \\ \chi_s(\mathbf{x}) &= (\hat{\mathcal{L}}_b)_{ss'} \sum_{n=1}^N c_n^{(s')} B_n^{(s')}(\mathbf{x})\end{aligned}$$

- Possible choices:
 - Kinematic balance:
- Usual variational method:

$$\hat{\mathcal{L}}_{KB} = \frac{1}{2mc^2} \boldsymbol{\alpha} \cdot \mathbf{p}$$

- Atomic balance:

$$\hat{\mathcal{L}}_{AB} = \frac{1}{2mc^2 - V_c} \boldsymbol{\alpha} \cdot \mathbf{p}$$

$$\begin{aligned}\mathcal{E}[\psi] &= \langle \phi | (V_c + mc^2) \phi \rangle_{L^2} + \langle R_0 \phi | \chi \rangle_{L^2} \\ &\quad + \langle \chi | R_0 \phi \rangle_{L^2} + \langle \chi | (V_c - mc^2) \chi \rangle_{L^2} \\ &\quad - E [\langle \phi | \phi \rangle_{L^2} - \langle \chi | \chi \rangle_{L^2}],\end{aligned}$$

Balance principles and spectral pollution

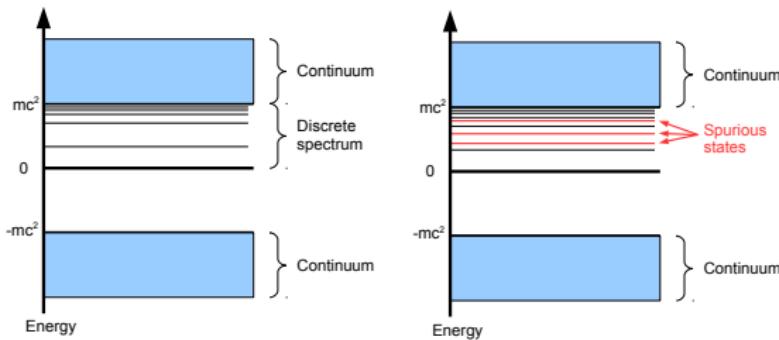
Theorem (Lewin et al, 2010)

Assuming that V_c is such that $V_c(x) \geq -\kappa|x|^{-1}$ for $\kappa \in (0, 3/2)$ with $\sup(V_c) < 2$, $(2 - V_c)^{-2} \nabla V_c \in L^\infty(\mathbb{R}^3)$ and $\max(V_c, 0) \in L^p(\mathbb{R}^3)$ with $p > 3$ and $V_c(x) \rightarrow_\infty 0$, then

$$\overline{\text{Sp}_{\text{u}}(H_0 + V_c, P, L_{AB})} = [-1, -1 + \sup(V_c)]$$

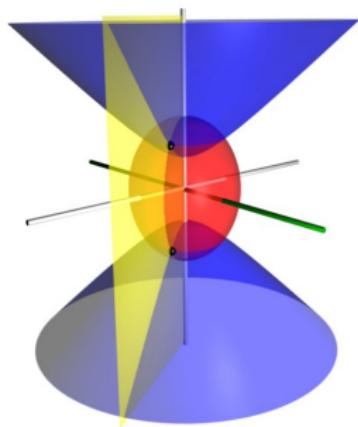
For mere mortals:

For Coulomb potentials, the spurious spectrum is always empty.



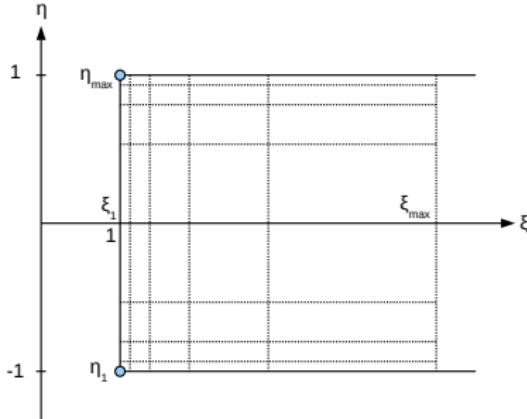
Implementation details

- Prolate spheroidal coordinates



- B-spline basis functions:

$$B_n^{(1,2)}(\xi, \eta) = G^{(1,2)}(\xi, \eta) b_i^{k_\xi}(\xi) b_j^{k_\eta}(\eta)$$



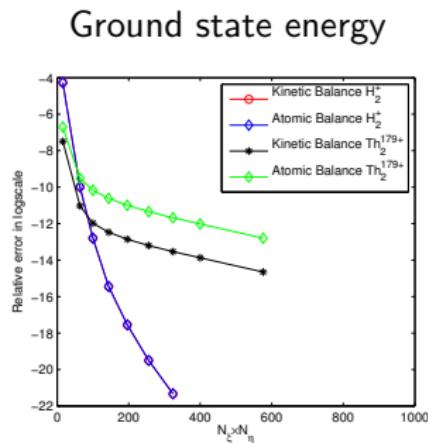
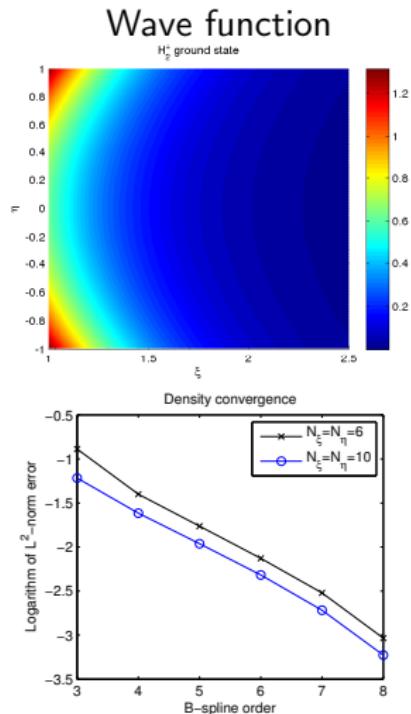
$$\mathbf{Ca} = E\mathbf{Sa}$$

Numerical results: time-independent

Eigenenergies of Th_2^{179+}

| States | Naive RR | Kinetic Balance | Atomic Balance |
|----------|---------------|-----------------|----------------|
| 1 | -9504.7243225 | -9504.7475523 | -9504.6416456 |
| 2 | -6815.4657298 | -6815.5599111 | -6815.3865298 |
| 3 | -4127.8877478 | -4128.1451137 | -4127.8457787 |
| 4 | -3374.5117016 | -3374.5143753 | -3374.4767336 |
| 5 | -2564.1559253 | -2564.1719708 | -2564.0918230 |
| 6 | -2455.9537953 | -2455.9600280 | -2455.9016668 |
| 7 | -2010.6535604 | -2010.4321103 | -2010.4261981 |
| 8 | -1918.4056980 | -1915.7178408 | -1915.6853488 |
| 9 | -1649.2929148 | -1643.9543595 | -1643.9395109 |
| 10 | -1344.0855870 | -1313.8071916 | -1313.7699129 |
| 11 | -1333.5368147 | -1303.6850950 | -1303.6660492 |
| spurious | -1204.6990945 | | |
| 12 | -1159.1761393 | -1089.6415827 | -1089.6370783 |
| 13 | -1131.0151665 | -1084.3699127 | -1084.3522895 |
| 14 | -1045.4764538 | -1028.1920826 | -1028.1920249 |
| 15 | -984.5252901 | -969.6816867 | -969.6482618 |

Wave function and convergence



Generalization to time-dependent: Galerkin method

- For the same (almost...) price: time-dependent Galerkin method

$$a_n, c_n \rightarrow a_n(t), c_n(t)$$

Project on Basis functions (Galerkin method)

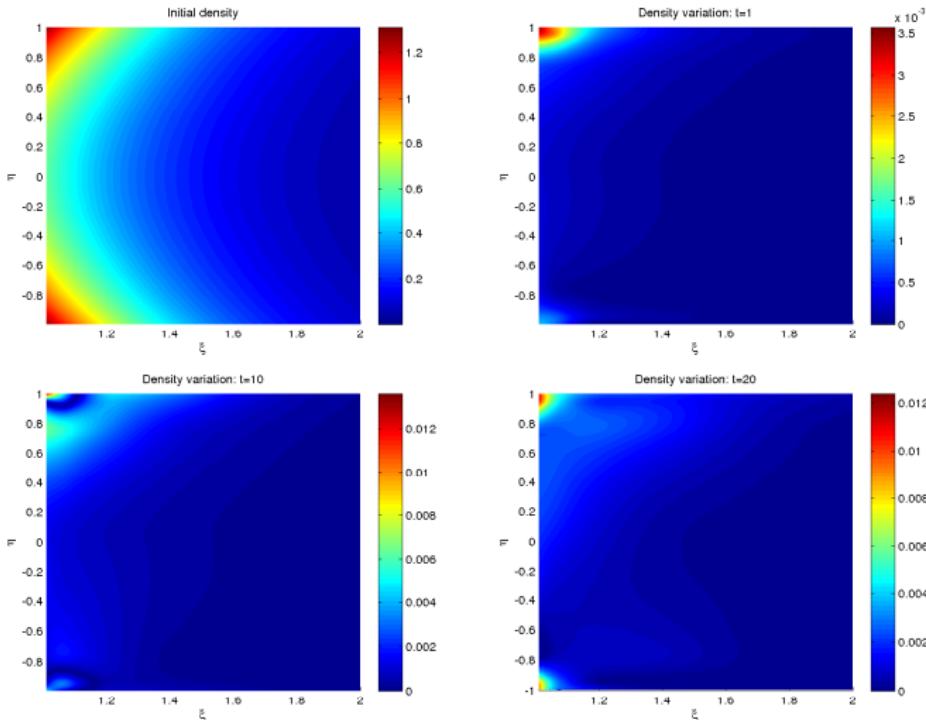
$$\langle \mathcal{B}_j | i\partial_t \psi \rangle_{L^2(\mathbb{R}^3, \mathbb{C}^4)} = \langle \mathcal{B}_j | H \psi \rangle_{L^2(\mathbb{R}^3, \mathbb{C}^4)}, \text{ for } j \in \{1, \dots, N\}$$

$$i\mathbf{S}\dot{\mathbf{a}}(t) = (\mathbf{C} + \mathbf{D}(t))\mathbf{a}(t)$$

- Time discretization: Unitary Crank-Nicolson

$$\mathbf{S}\mathbf{a}^{n+1} = \mathbf{S}\mathbf{a}^n - i\frac{\Delta t_n}{2}(\mathbf{C} + \mathbf{D}^n)\mathbf{a}^n - i\frac{\Delta t_n}{2}(\mathbf{C} + \mathbf{D}^{n+1})\mathbf{a}^{n+1}$$

Numerical results: H_2^+ in a laser field



Conclusion

Conclusion

- **Schwinger pair production in a multi-center system**
 - Position of resonances
 - F. Fillion-Gourdeau *et al.*, 2012 J. Phys. A: Math. Theor. 45 215304
 - Two mechanisms that enhance pair production rate:
 - ① At large R: REPP
 - ② At small R: ECEPP
 - F. Fillion-Gourdeau *et al.*, Phys. Rev. Lett. 110, 013002 (2013)
 - F. Fillion-Gourdeau *et al.*, 2013 J. Phys. B: At. Mol. Opt. Phys. 46 175002
- **Galerkin methods for the Dirac equation**
 - Initial state computed with RR + balance principle + B-splines
 - F. Fillion-Gourdeau *et al.*, Phys. Rev. A 85 (2), 022506
 - Extended to time-dependent case
 - F. Fillion-Gourdeau *et al.*, submitted to J. Comp. Phys.
- **Schwinger pair production in a realistic scenario**
- **In the future...**
 - Numerical work (dispersion error, absorbing boundary conditions, higher order for time discretization)
 - Complex scaling method

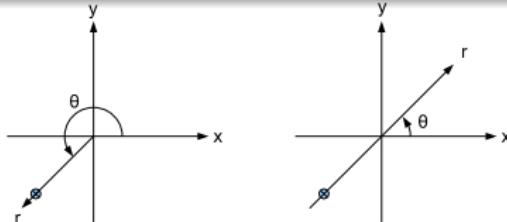
Dirac equation in Cylindrical coordinates

- Cylindrical coordinates

$$x = r \cos \theta$$

$$y = r \sin \theta$$

- Azimuthal symmetry: $A^\mu(r, z)$



Separation of variables:

$$\Psi(\mathbf{x}, t) = \begin{bmatrix} \psi_1(t, r, z) e^{i\mu_1 \theta} \\ \psi_2(t, r, z) e^{i\mu_2 \theta} \\ \psi_3(t, r, z) e^{i\mu_1 \theta} \\ \psi_4(t, r, z) e^{i\mu_2 \theta} \end{bmatrix}$$

Angular momentum

$$\mu_{1,2} := j_z \mp 1/2$$

$$j_z = \dots, -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \dots$$

Boundary condition

($r = 0$):

$$\psi_1(r) = (-1)^{|\mu_1|} \psi_1(-r),$$

$$\psi_2(r) = (-1)^{|\mu_2|} \psi_2(-r),$$

$$\psi_3(r) = (-1)^{|\mu_1|} \psi_3(-r),$$

$$\psi_4(r) = (-1)^{|\mu_2|} \psi_4(-r).$$

$$i\partial_t \psi(t, r, z) = \left\{ \alpha_x \left[-ic\partial_r - ic\frac{1}{2r} - eA_r(t, r, z) \right] + \alpha_y \left[c\frac{j_z}{r} - eA_\theta(t, r, z) \right] \right. \\ \left. + \alpha_z \left[-ic\partial_z - eA_z(t, r, z) \right] + \beta mc^2 + eV(t, r, z) \right\} \psi(t, r, z)$$