Computational methods in relativistic atomic physics

Andrey Surzhykov

Technische Universität Braunschweig
Physikalisch-Technische Bundesanstalt (PTB)

Together with:

Anton Artemyev (Uni Kassel), Stephan Fritzsche (HI-Jena), Sean McConnell (QIT Brisbane)

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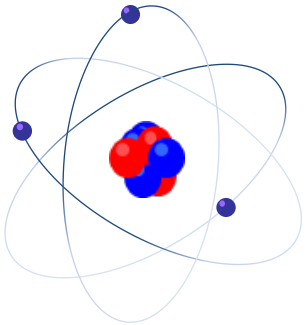
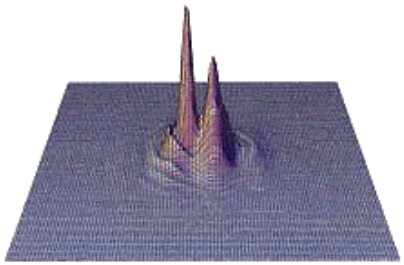
Computational atomic physics

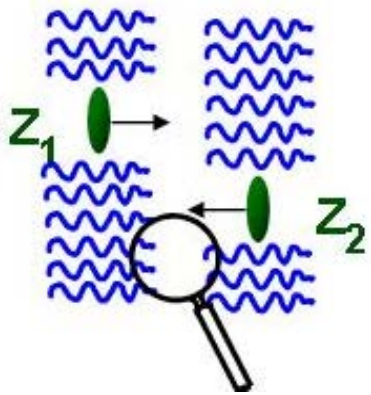
Theoretical studies in relativistic atomic physics and physics of strong electromagnetic fields are quite often very computational demanding:

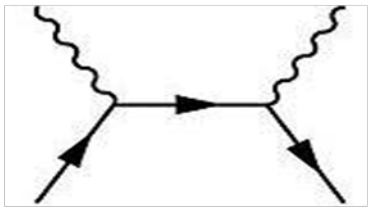
- Large-scale atomic structure calculations
- Electron-atom collisions
- Non-linear light-matter interactions
- Non-perturbative treatment of ion collisions
- Structure of heavy quasi-molecules
- Critical phenomena in strong EM fields



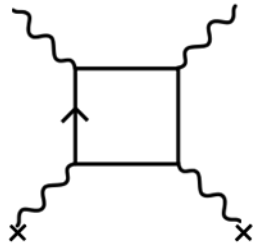
$$\Psi(PJM) = \sum_r c_r \Phi(\gamma_r PJM)$$







Rayleigh scattering



Delbrück scattering

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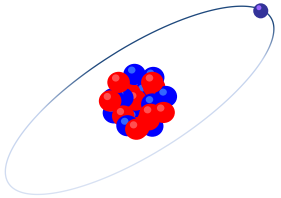
Critical electromagnetic fields

Dirac energy of a *single* hydrogen-like ion (for the point-like nucleus):

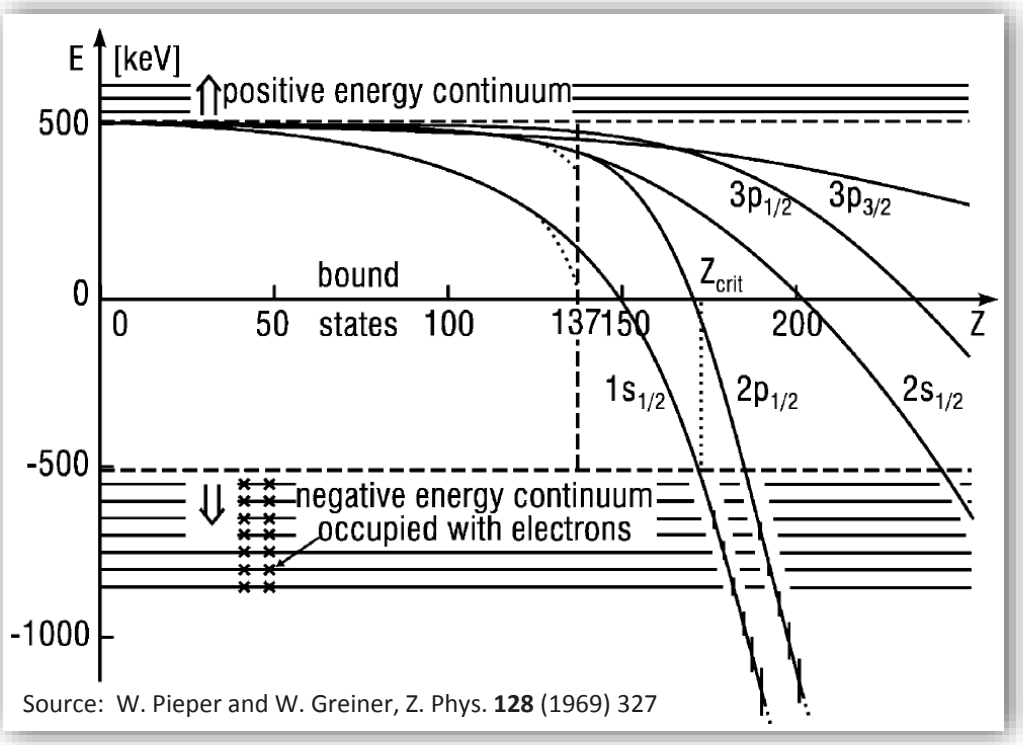
$$E_{nj} = mc^2 \Big/ \sqrt{1+\left(\frac{Z\alpha}{n-|\,j+1/2\,|+\sqrt{(j+1/2)^2-(Z\alpha)^2}}\right)^2}$$



What happens if we increase the nuclear charge Z?

If nuclear charge of the ion is greater than Z_{crit} the ionic levels can "dive" into Dirac's negative continuum.

Physical vacuum becomes unstable: creation of pairs may take place!



Source: W. Pieper and W. Greiner, Z. Phys. **128** (1969) 327

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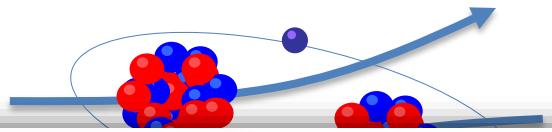
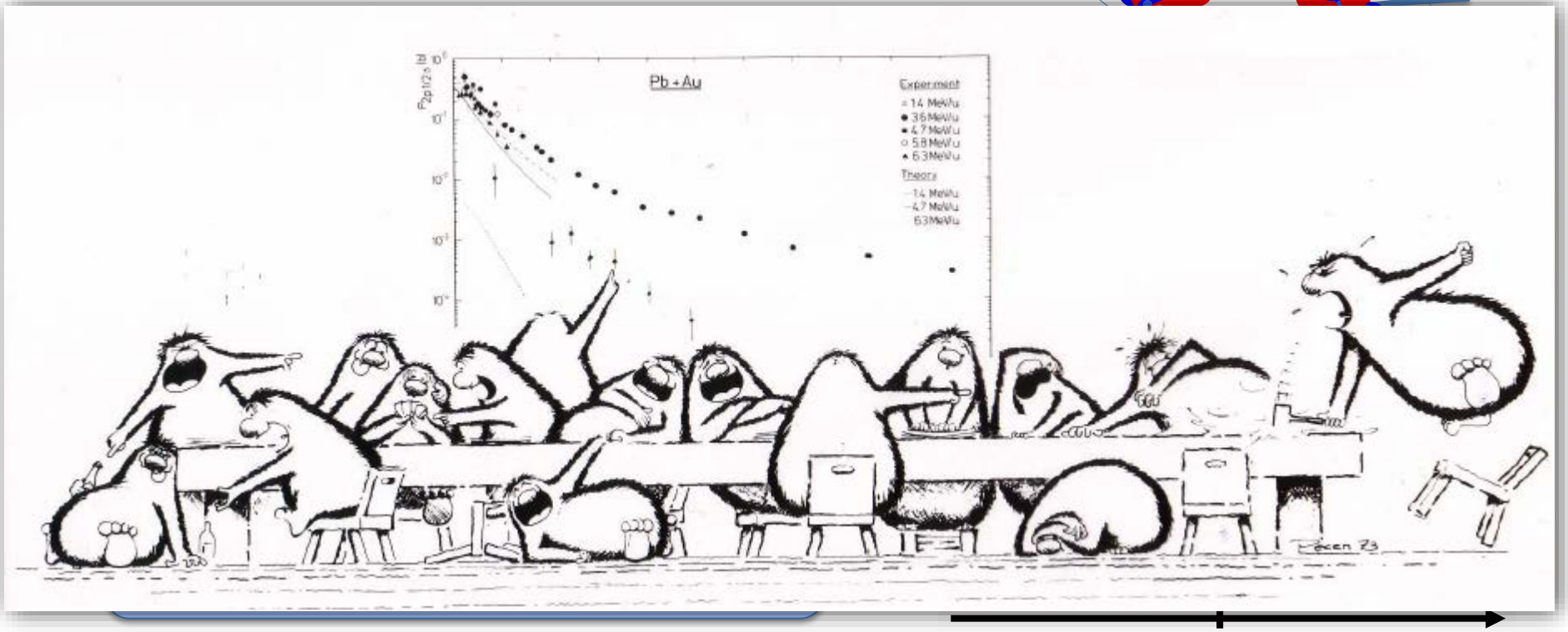
Superheavy quasi-molecules

Alternatively, we may form strong electromagnetic fields in (rather) slow collisions of two heavy ions.





In 70-80's, efforts have been done to observe the 'break' of the vacuum in ion-ion collision.

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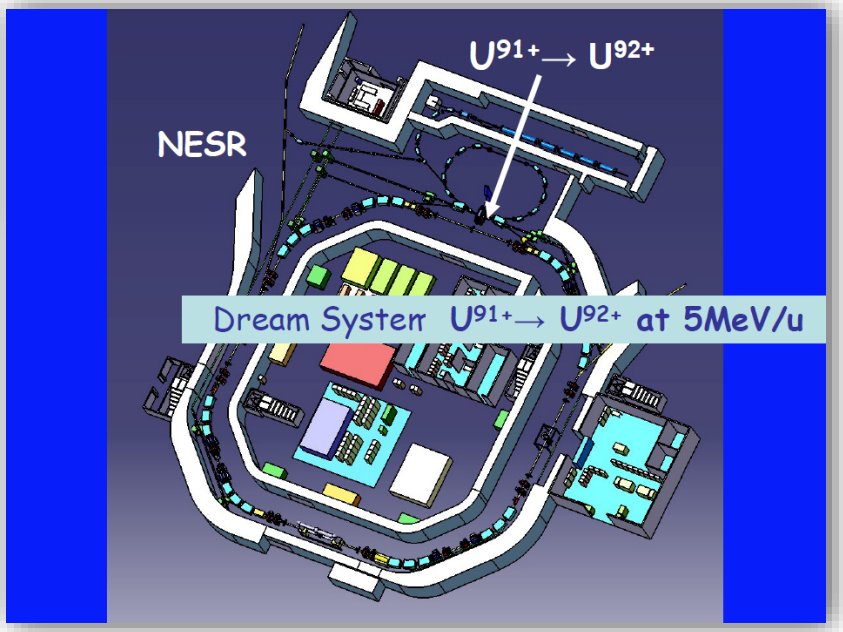
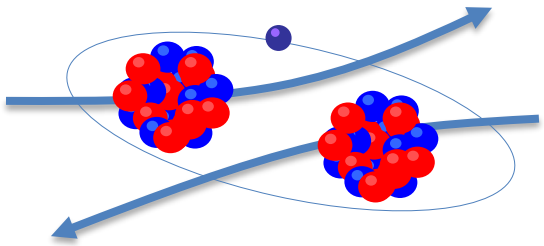
Superheavy quasi-molecules

New generation of “positron experiments” is likely to be performed at the FAIR facility in Darmstadt, HIAF (Shanghai), NICA (Dubna).



There is need for novel theoretical techniques to deal with time-dependent two-center Dirac problem.



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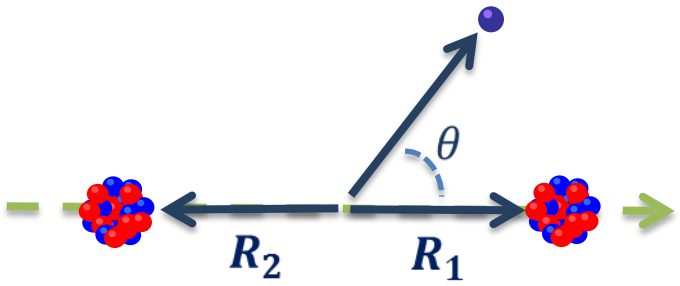
Non-perturbative treatment of ion collisions

We aim to solve the two-center Dirac equation:

$$\hat{H} = \hat{\boldsymbol{\alpha}} \cdot \hat{\boldsymbol{p}} + \beta - \frac{\alpha Z_1}{|\boldsymbol{r} - \boldsymbol{R}_1|} - \frac{\alpha Z_2}{|\boldsymbol{r} - \boldsymbol{R}_2|}$$



We need to develop a method for fast and efficient generation of a *complete* spectrum of such a system, including positive- and negative-energy solutions.

Up to now there were two main approaches to the two-center Dirac problem:

- **LCAO** (linear combination of atomic orbitals): well established approach, deals well with bound states, **but** exhibits problems to include continuum properly
- **Monopole approximation**: provides complete Dirac spectrum for the spherically-symmetric potential, **but** fails to describe "large" distances

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Solutions in the monopole approximation

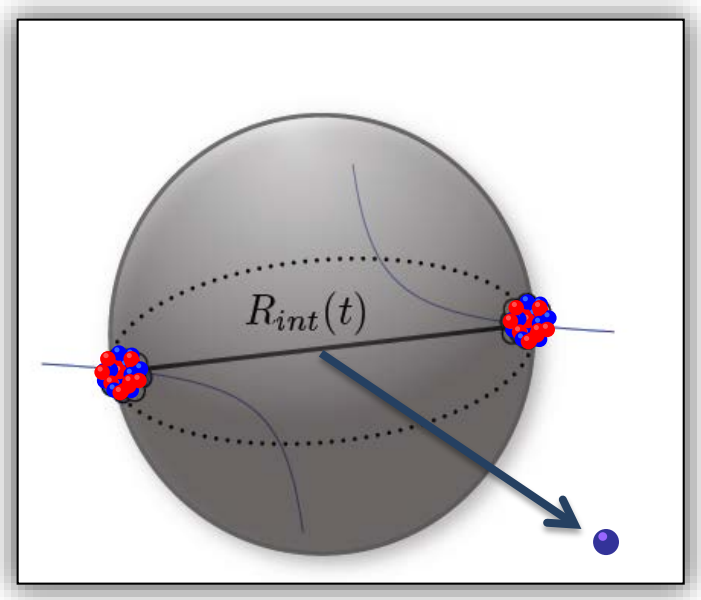
$$\hat{H} = \hat{\boldsymbol{\alpha}} \cdot \hat{\boldsymbol{p}} + \beta - \frac{\alpha Z_1}{|\boldsymbol{r} - \boldsymbol{R}_1|} - \frac{\alpha Z_2}{|\boldsymbol{r} - \boldsymbol{R}_2|}$$

We can perform multipole expansion of the (two-center) interaction operator:

$$V_{TC}(\boldsymbol{r}) = \sum_{L=0}^{\infty} V_L(r, R)\, P_L(\cos\theta)$$

If we restrict expansion to the first (L=0) term only, we obtain the *monopole approximation* whose solutions read as:

$$\phi^{(0)}_{n\kappa\mu}(\boldsymbol{r}) = \begin{pmatrix} G_{n\kappa}(r)\chi_{\kappa\mu}(\theta,\varphi) \\ iF_{n\kappa}(r)\chi_{-\kappa\mu}(\theta,\varphi) \end{pmatrix}$$



Where the radial components are found from:

$$\begin{bmatrix} V_0(r,R) + 1 & -\frac{d}{dr} + \frac{\kappa}{r} \\ \frac{d}{dr} + \frac{\kappa}{r} & V_0(r,R) - 1 \end{bmatrix} \begin{pmatrix} G_{n\kappa}(r) \\ F_{n\kappa}(r) \end{pmatrix} = \epsilon_{n\kappa} \begin{pmatrix} G_{n\kappa}(r) \\ F_{n\kappa}(r) \end{pmatrix}$$

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Finite basis set approach

Radial components of the Dirac's wavefunction can be written as finite expansion over some basis functions (B-splines, for example):

$$\phi^{(0)}_{n\kappa\mu}(\boldsymbol{r}) = \begin{pmatrix} G_{n\kappa}(r)\chi_{\kappa\mu}(\theta,\varphi) \\ iF_{n\kappa}(r)\chi_{-\kappa\mu}(\theta,\varphi) \end{pmatrix}$$

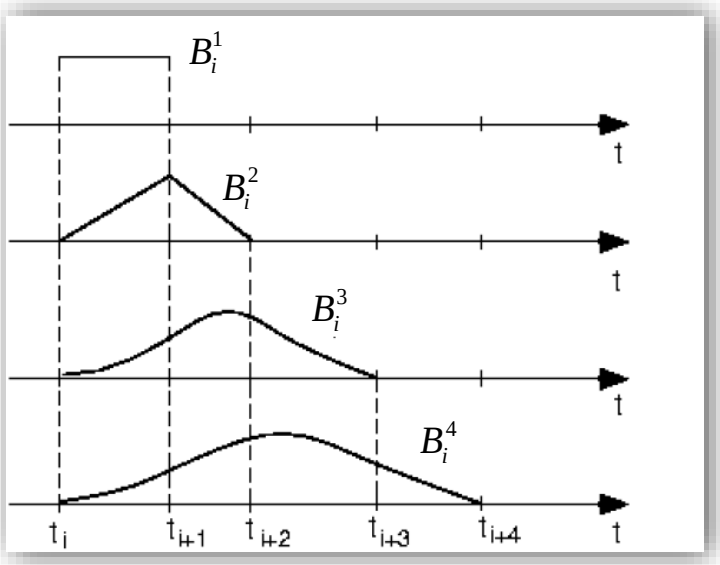
$$G_{n\kappa}(r) = \sum_{i=1}^{N} p_i \, B_i(r)$$

$$F_{n\kappa}(r) = \sum_{i=1}^{N} q_i \, B_i(r)$$

$$B_i^k(x) = \frac{x - t_i}{t_{i+k-1} - t_i} B_i^{k-1}(x) + \frac{t_{i+k} - x}{t_{i+k} - t_{i+1}} B_{i+1}^{k-1}(x)$$

$$B_i^1(x) = \begin{cases} 1, & t_i \leqslant x < t_{i+1} \\ 0, & \text{otherwise} \end{cases}$$

$t_0 \leq t_1 \leq t_2 \leq \ldots \leq t_m$ - knots



Basic properties of B-splines:

- Piecewise polynomials of order k-1
- Are continuous together with their derivatives up to (k-2) order
- At any point there exist only k non-zero B-splines

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In order to find expansion coefficients we shall turn to principle of least action:

$$\delta S_{n\kappa} = 0 \quad \text{where} \quad S_{n\kappa} = \left\langle \phi^{(0)}_{n\kappa\mu} \middle| \hat{H} - \varepsilon \middle| \phi^{(0)}_{n\kappa\mu} \right\rangle$$

By evaluating the variation with respect to change of expansion coefficients we obtain the matrix equation:

$$\boldsymbol{A}v = \epsilon \boldsymbol{B}v \quad \text{where}$$

$$v = (p_1, p_2, \ldots, p_N, q_1, q_2, \ldots, q_N)$$

$$A = \begin{bmatrix} (V) & (D) - \left(\frac{\kappa}{r}\right) \\ -\left[(D) + \left(\frac{\kappa}{r}\right)\right] & -2(C) + (V) \end{bmatrix} + A^{\mathrm{b}}$$

Boundary conditions

$$B = \begin{bmatrix} (C) & 0 \\ 0 & (C) \end{bmatrix}$$

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Where the matrices are given by:

$$(C)_{ij} = \int B_i(r) B_j(r) dr,$$

$$(D)_{ij} = \int B_i(r) \frac{d}{dr} B_j(r) dr,$$

$$\left(\frac{\kappa}{r}\right)_{ij} = \int B_i(r) \frac{\kappa}{r} B_j(r) dr.$$

$$(V)_{ij} = \int B_i(r) V(r) B_j(r) dr$$

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Solutions in the monopole approximation

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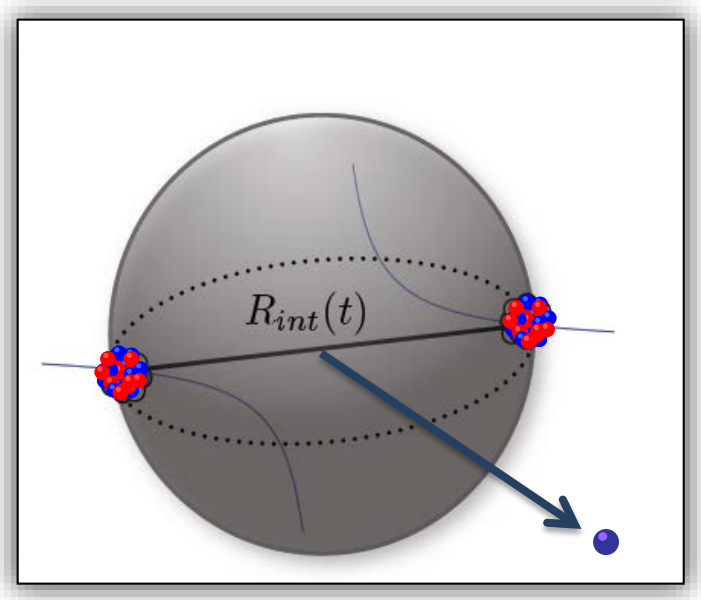

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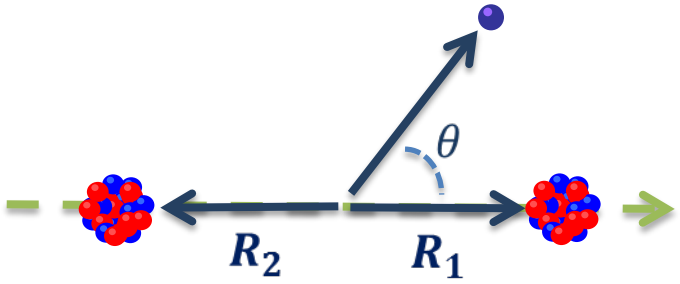
Two-center problem: Exact solutions

- We aim to solve the two-center Dirac equation:

$$\hat{H} = \hat{\boldsymbol{\alpha}} \cdot \hat{\boldsymbol{p}} + \beta - \frac{\alpha Z_1}{|\boldsymbol{r} - \boldsymbol{R}_1|} - \frac{\alpha Z_2}{|\boldsymbol{r} - \boldsymbol{R}_2|}$$



- We propose to present solutions of such an exact eigenproblem in terms of the monopole functions:

$$\phi_{k\mu}(\boldsymbol{r}) = \sum_{n\kappa} C_{kn\kappa\mu}\, \phi^{(0)}_{n\kappa\mu}(\boldsymbol{r})$$

Monopole solutions

Expansion coefficients (found from the generalized eigenvalue problem)

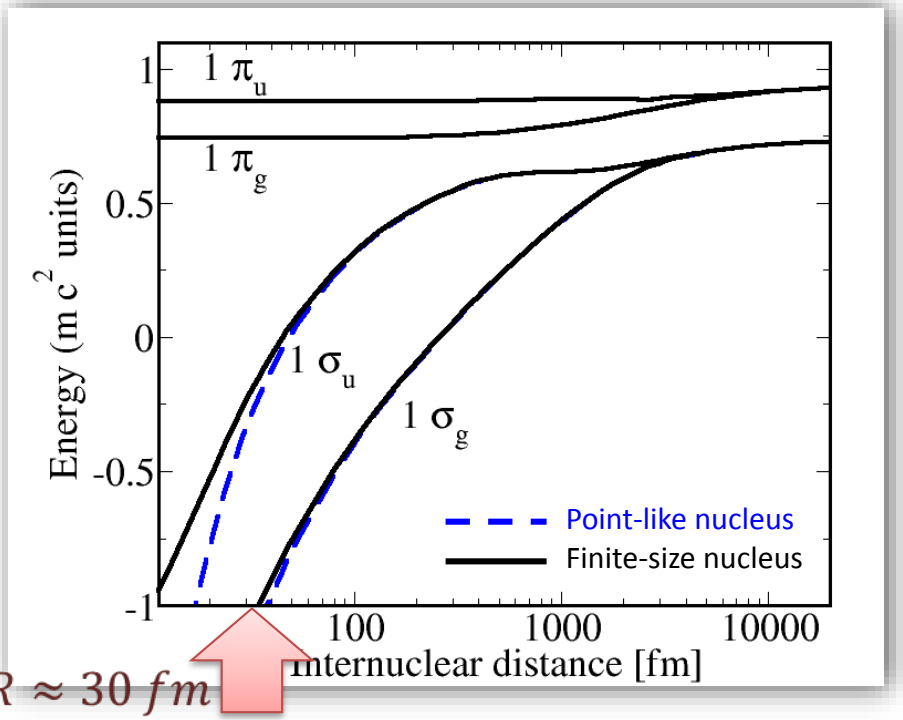
Advantages of the proposed method:

- We generate a complete spectrum of a two-center system (”all included”)
- Solutions are still in spherical coordinates (we can use angular algebra)
- By controlling the number of monopole (basis) functions, we may perform calculations very fast and efficient

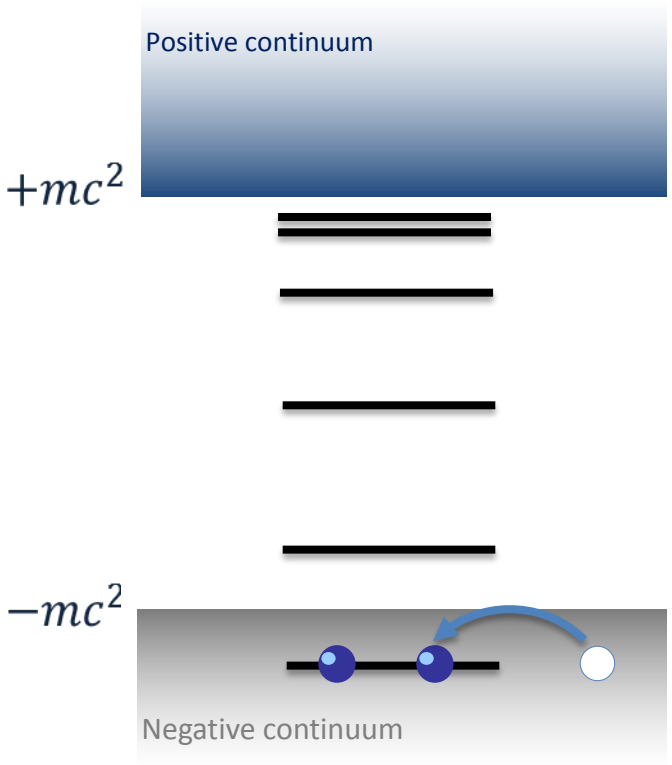
Quasi-molecules: Energy spectrum

Application of the finite-basis set approach can help to investigate the structure properties of heavy quasi-molecules.

Energy spectrum of U^{92+} - U^{91+} quasi-molecule



The finite-nuclear size effect becomes most pronounced when nuclei are close to each other.



Can we observe the "decay" of quantum vacuum into electron-positron pairs?

A. Artemyev, A. S., P. Indelicato, G. Plunien, and Th. Stöhlker, J. Phys. B **43**, 235201 (2010)

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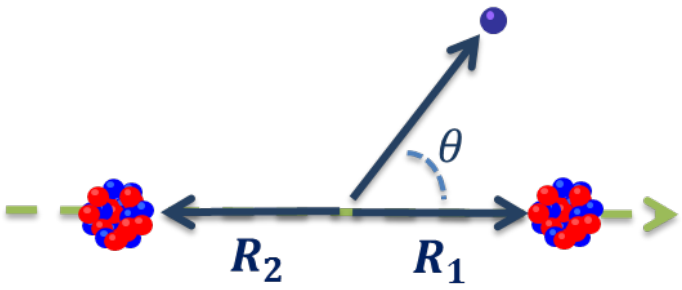
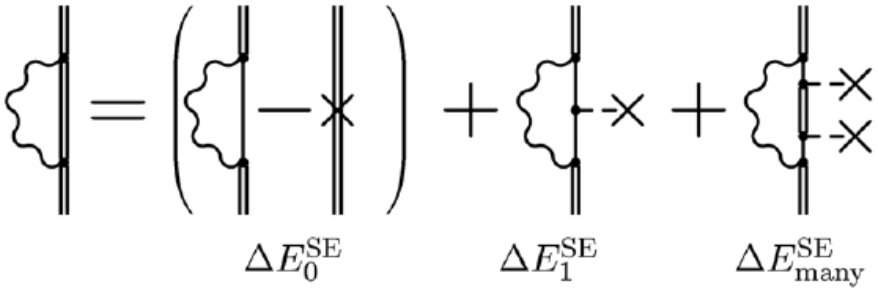
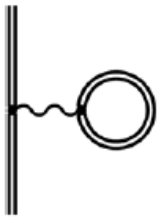
Quasi-molecules: QED corrections



We elaborated an ab initio approach for the evaluation of the one-loop QED corrections to energy levels of diatomic quasimolecules. The approach accounts for the interaction between an electron and two nuclei in all orders in Zα.

To evaluate the self-energy correction, the electron propagator is expanded in powers of the interaction with the effective potential.





The vacuum polarization corrections contains the dominant Uehling and the much weaker Wichmann-Kroll components.

A. Artemyev and A. S., Phys. Rev. Lett. **114** 243004 (2015)

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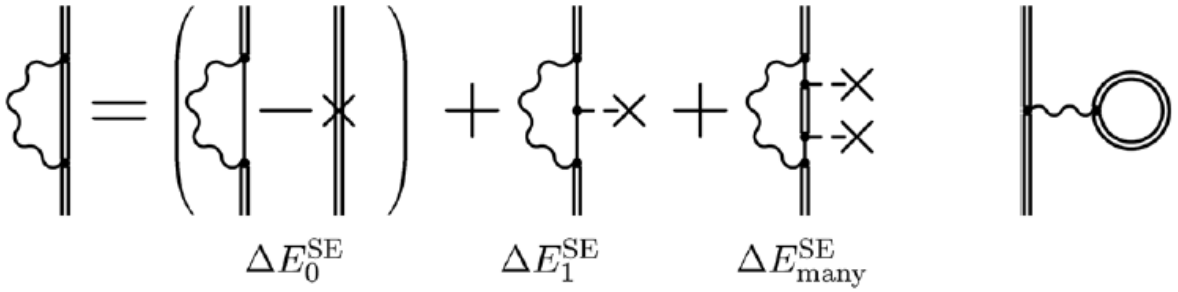
Quasi-molecules: QED corrections



Zeroth-order energy E_0, self-energy ΔE_{SE}, vacuum-polarization ΔE_{VP}, and total ΔE_{QED} QED corrections (in eV) for the $1\sigma_g$ ground state of U_2^{183+} at different internuclear distances (in fm).

Distance	Monopole				Exact			
[fm]	E_0	ΔE_{SE}	ΔE_{VP}	ΔE_{QED}	E_0	ΔE_{SE}	ΔE_{VP}	ΔE_{QED}
40	−437 306	6462.6	−4226.5	2236(11)	−461 436	6851.8	−4807.7	2044(10)
50	−363 273	5392.9	−3144.1	2248(14)	−387 797	5788.4	−3676.7	2111(13)
80	−230 071	3645.5	−1662.5	1983(21)	−253 879	3998.2	−2065.5	1932(21)
100	−175178	3011.9	−1224.1	1787(25)	−198 486	3342.0	−1570.5	1771(25)
200	−26 731	1581.9	−452.6	1129(33)	−48 415	1821.8	−655.3	1166(33)
250	16 151	1260.1	−322.2	938(35)	−5610	1479.9	−494.6	985(35)
500	140 105	561.8	−101.0	461(36)	116 754	736.1	−203.4	533(40)
700	195 746	351.9	−53.4	298(32)	170 247	516.5	−138.6	377(40)
1000	250 848	200.7	−25.4	175(26)	222 742	358.0	−90.8	267(40)

A. Artemyev and A. S., Phys. Rev. Lett. **114** 243004 (2015)

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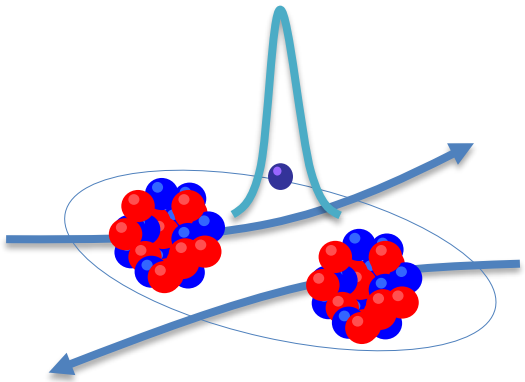
Electron dynamics accompanying ion collisions

- Of special interest is the study of fundamental processes accompanying slow ion collisions.
- Such an analysis requires solution of the time-dependent (two-center) Dirac equation.

$$\Phi(\boldsymbol{r},t) = \sum_k a_k(t)\phi_k(\boldsymbol{r},\boldsymbol{R}(t))e^{-i\epsilon_k t}$$



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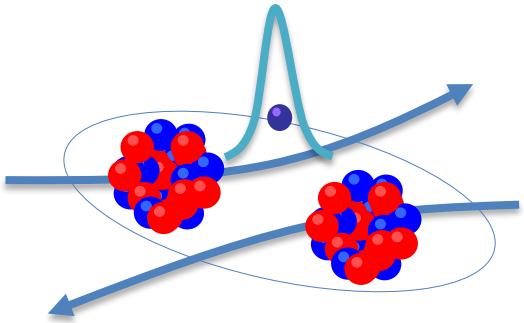
Coupled channel calculations

By substituting basis-set expansion into Hamiltonian:

$$\Phi(\boldsymbol{r},t) = \sum_k a_k(t)\, e^{-i\epsilon_k t}\phi_k(\boldsymbol{r},t) \qquad i\frac{\partial\Phi}{\partial t} = \hat{H}\Phi$$



We find a system of coupled equations for the parameters a_k:

$$i\,\dot{a}_k(t) = \epsilon_k(t)\cdot a_k(t) - i\sum_{n\neq k} a_n(t)\frac{\langle\phi_k|\partial\hat{H}/\partial t|\phi_n\rangle}{\epsilon_k(t)-\epsilon_n(t)}$$

Re-writing this system of equation in the matrix form: $i\frac{\partial}{\partial t}\boldsymbol{a}(t) = M(t)\,\boldsymbol{a}(t)$

$$\boldsymbol{a}(t) = \begin{pmatrix} a_1(t) \\ a_2(t) \\ \vdots \end{pmatrix}, \qquad M = \begin{pmatrix} E_1 & -i\frac{\langle 1|\dot{H}|2\rangle}{E_2-E_1} & -i\frac{\langle 1|\dot{H}|3\rangle}{E_3-E_1} & \cdots \\ -i\frac{\langle 2|\dot{H}|1\rangle}{E_1-E_2} & E_2 & -i\frac{\langle 2|\dot{H}|3\rangle}{E_3-E_2} & \cdots \\ \vdots & & \ddots & \end{pmatrix}$$

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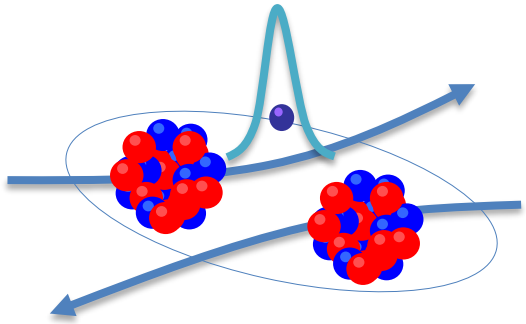

We find a system of coupled equations in matrix form:

$$i\frac{\partial}{\partial t}\boldsymbol{a}(t) = M(t)\,\boldsymbol{a}(t), \qquad \boldsymbol{a}(t) = \begin{pmatrix} a_1(t) \\ a_2(t) \\ \vdots \end{pmatrix}, \qquad M = \begin{pmatrix} E_1 & -i\frac{\langle 1|\dot{H}|2\rangle}{E_2-E_1} & -i\frac{\langle 1|\dot{H}|3\rangle}{E_3-E_1} & \cdots \\ -i\frac{\langle 2|\dot{H}|1\rangle}{E_1-E_2} & E_2 & -i\frac{\langle 2|\dot{H}|3\rangle}{E_3-E_2} & \cdots \\ \vdots & & \ddots & \end{pmatrix}$$

Which we can solve on the grid as:

$$\boldsymbol{a}(t+\Delta t) = e^{-i\bar{M}(t)\Delta t}\boldsymbol{a}(t) + O(\Delta t^3) \quad \text{with} \quad \bar{M}(t) = M(t+\frac{\Delta t}{2})$$

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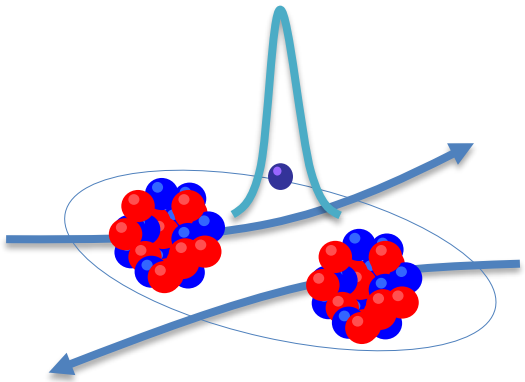
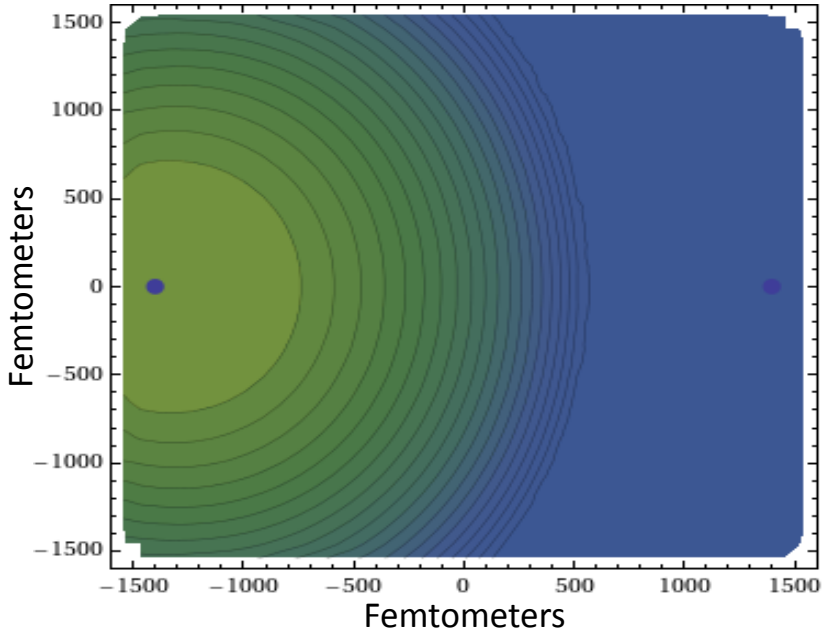


$$\Phi(\boldsymbol{r},t)=\sum_k a_k(t)\phi_k(\boldsymbol{r},\boldsymbol{R}(t))e^{-i\epsilon_k t}$$



- Developed approach allows fast and efficient treatment of charge-transfer, excitation, ionization and even pair production processes!

Calculations: Pb^{81+} + Pb^{82+} collision at energy of 3 MeV/u and *zero* impact parameter.

S. McConnell, A. Artemyev, and A. S., Phys. Rev. A 86 (2012) 052705

Electron dynamics accompanying ion collisions

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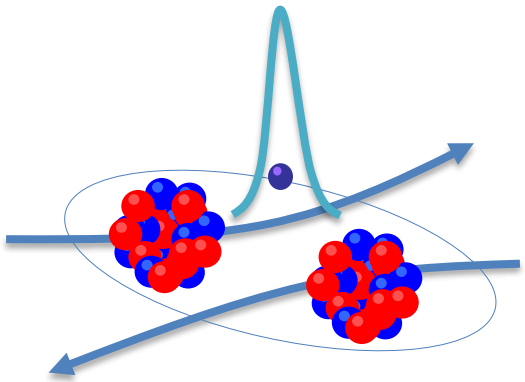

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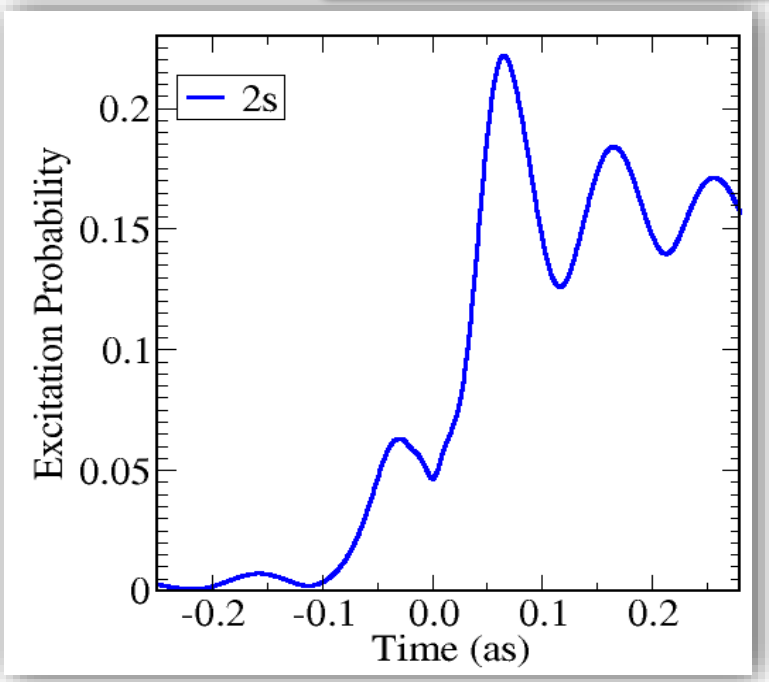

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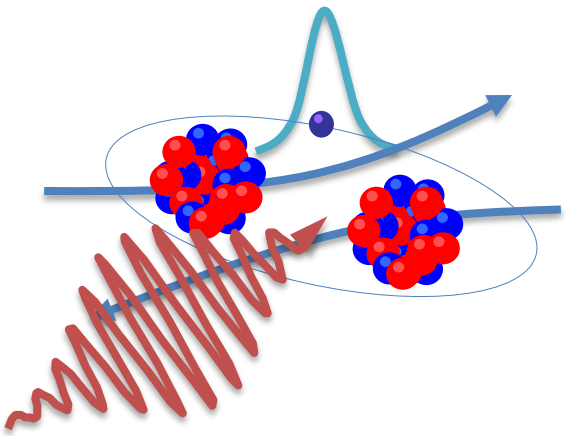
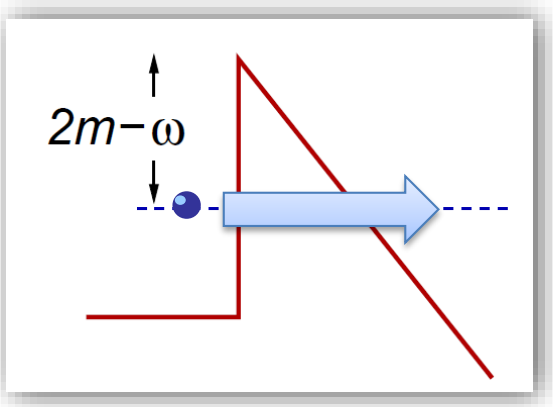
Outlook: Laser-assisted collisions

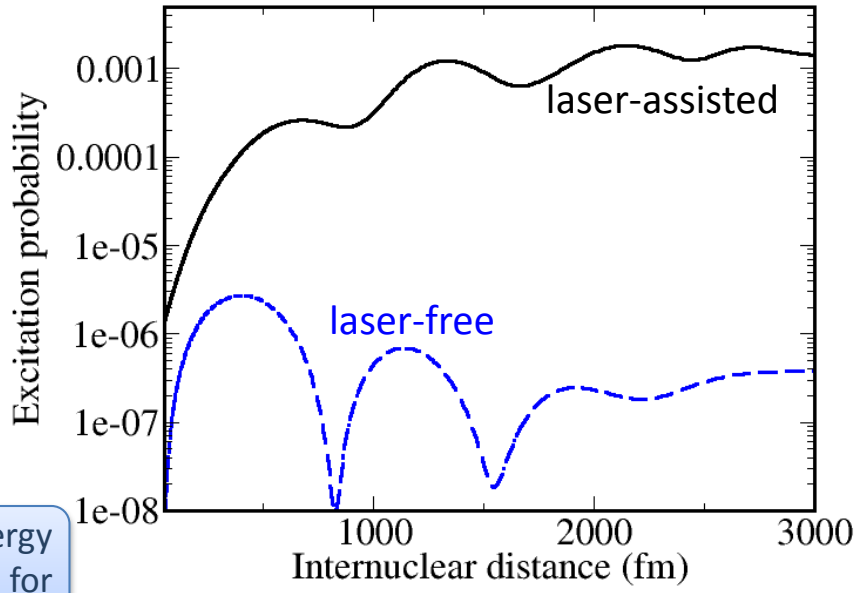
Of special interest is the study of fundamental processes accompanying laser-assisted ion collisions.

Can one catalyze lepton pair production by applying intense laser?

Dynamically assisted Schwinger mechanism attracts now attention in strong laser field physics!







Excitation probability in laser-assisted U^{92+} - U^{91+} collision at energy 3 MeV/u and zero impact parameter. Calculations are perfumed for laser intensity $I = 10^{16} \frac{W}{cm^2}$ and energy $\hbar\omega$=50 eV.

Preliminary results!