Quantum dynamics of electrons and vacuum decay in low-energy collisions of heavy ions

Vladimir Shabaev

St. Petersburg State University

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Outline of the talk

- Introduction
- The work of the SPbSU group on SHE
- QED at supercritical Coulomb field
- Low-energy heavy-ion collisions
    - Charge transfer
    - Pair creation
- How to observe the vacuum decay
- Conclusion

Electronic structure of superheavy elements

Oganesson $(\mathrm{Og}, Z = 118)$
Ground-state configuration $[\mathrm{Rn}]7s^2 7p^6$ – "noble gas" group.

First element from the noble gases, which can form a weakly-bound negatively charged ion.

E. Eliav *et al.*, Phys. Rev. Lett. 77, 5350 (1996).

Bound-state energy of the additional electron is $0.076(10)$ eV.

M. Y. Kaygorodov *et al.*, Phys. Rev. A 104, 012819 (2021).

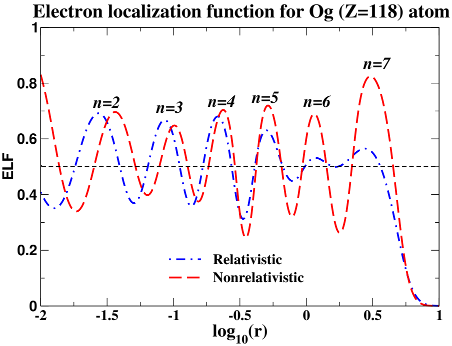
Calculations of the ionization potentials and electron affinities of elements
$\mathrm{Rg}, Z = 111 \quad \mathrm{Cn}, Z = 112$
$\mathrm{Nh}, Z = 113 \quad \mathrm{Fl}, Z = 114.$

M. Y. Kaygorodov *et al.*, Phys. Rev. A 106, 062805 (2022).

Talk at this conference by Ilya Tupitsyn.

Study of the valence electronic density distribution using the electron localization function (ELF)

The value of ELF equal to 0.5 does not mean that the electron density is uniformly distributed.

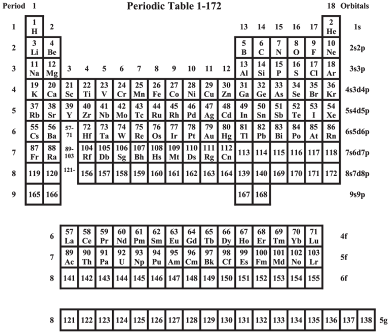


I. I. Tupitsyn *et al.*, Opt. Spectr. 130, 1022 (2022).

Electronic structure of superheavy elements

Possible concepts of the extended Periodic Table, which include relativistic, correlation and QED effects.

Verification of the Periodic law.



Periodic Table 1-172

Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	Orbitals
1	1 H																	2 He	1s
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne	2s2p
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	3s3p
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	4s3d4p
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	5s4d5p
6	55 Cs	56 Ba	57-71	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	6s5d6p
7	87 Fr	88 Ra	89-103	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113	114	115	116	117	118	7s6d7p
8	119	120	121-	156	157	158	159	160	161	162	163	164	139	140	169	170	171	172	8s7d8p
9	165	166											167	168					9s9p

6	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	4f
7	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	5f
8	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	6f

8	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	5g

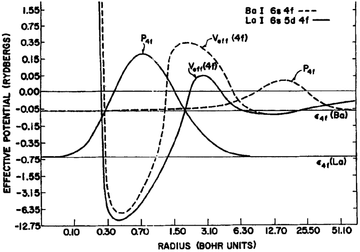
Image taken from P. Pyykkö, Chem. Rev. 112, 371 (2012).

QED effects in supeheavy elements
A. V. Malyshev *et al.*, Phys. Rev. A, in press.

Talk at this conference by Ilya Tupitsyn.

Study of the properties of the $5g$-elements – superactinides

One of the features of the electronic structure of superheavy elements with $5g$-shell $(Z = 125 - 145)$ is that in these elements the so-called orbital collapse can take place, which is analogous to those of the case of rare earth elements.



Example of the orbital collapse for Barium $(\mathrm{Ba}, Z = 56)$.
Image taken from J.-R Connerade and R. C. Kamatak, *Handbook on the Physics and Chemistry of Rare Earths* 28, 1 (2000).

Chemical properties of HgO, CnO, and FlO

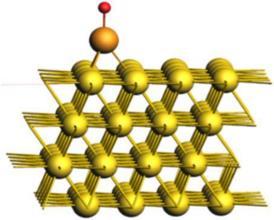
Talk at this conference by Artem Kotov:

Currently investigated:

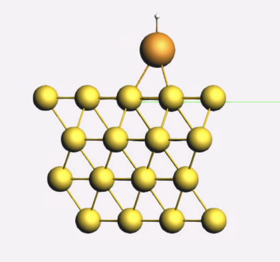
- Formation energy of oxides in the recoil chamber. Most probable ones are:
    - Hg + O = HgO (E = -0.618 eV)
    - Cn + O = CnO (E = -0.733 eV)
    - Fl + O = FlO (E = -1.947 eV)
- Molecular properties evaluated within *ab-initio* coupled-cluster approach with single, double and perturbative triple excitations:
    - Bond length
    - Ionization potential
    - Dipole moment
    - Electric dipole polarizability
- Adsorption on gold and quartz surfaces in the chromatography column

Adsorption of SHEs and their compounds on Au(111) Surface

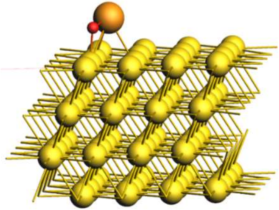
Talks at this conference by Anton Ryzhkov and Artem Kotov:



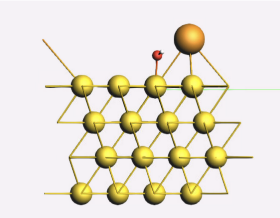
CnO



OgH



FlO

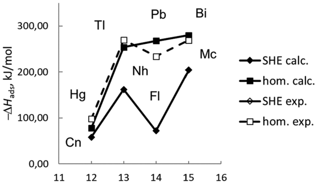


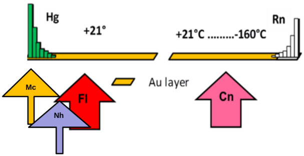
OgOH

Adsorption energy studies of SHEs and their compounds on Au(111) Surface

Talks at this conference by Anton Ryzhkov and Artem Kotov:

Previous study:
Hg/Cn, Tl/Nh, and Bi/Mc

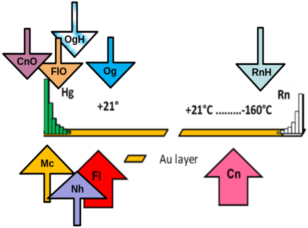




V. Pershina *et al.*, Inorg. Chem. **60**, 9796 (2021)
V. Pershina and M. Iliaś, Dalton Trans. **51**, 7321 (2022)

Present work:

- atoms: Hg/Cn, Tl/Nh, Pb/Fl, Bi/Mc, Po/Lv, At/Ts, and Rn/Og
- hydrids: BiH/McH, PoH/LvH, Ath/TsH, and RnH/OgH
- oxides: HgO/CnO and PbO/FlO
- hydroxides: AtOH/TsOH and RnOH/OgOH



In progress: BiH_3/McH_3 and PoH_2/LvH_2

Calculation of the moscovium ($Z = 115$) ground-state energy by quantum algorithms

Talk at this conference by Vladimir Zaytsev:

Details:

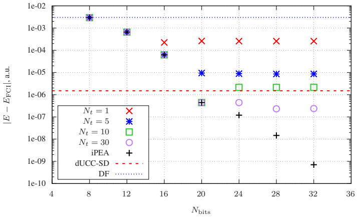
- 15 active electrons
- 26 orbitals
- ~500 000 Sl. dets.

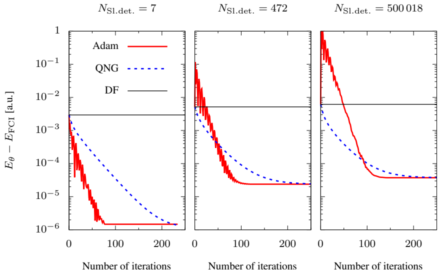
iterative Phase Estimation

- Trotterization
- Number of bits
- Gates reduction strategies

Variational Quantum Eigensolver

- Unitary Coupled Cluster ansatz
- Hardware Efficient ansatz
- Adam vs Quantum Natural Gradients





Tests of QED with atomic systems

Light atoms ($\alpha Z \ll 1$, weak fields):
Tests of QED to lowest orders in α and αZ.

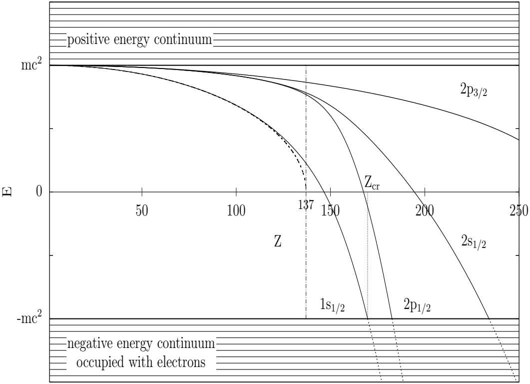
Heavy few-electron ions ($\alpha Z \sim 1$, strong fields):
Tests of QED in nonperturbative in αZ regime.

Low-energy heavy-ion collisions at $Z_1 + Z_2 > 173$ (supercritical fields):
Tests of QED in supercritical regime.

QED at supercritical Coulomb field

Supercritical Coulomb field

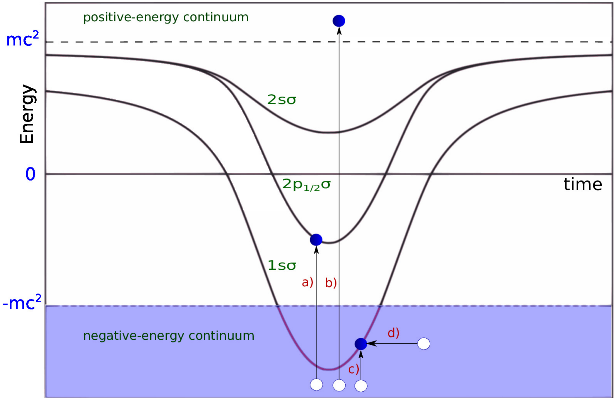
S.S. Gershtein, Ya.B. Zel'dovich, 1969; W. Pieper, W. Greiner, 1969



The $1s$ level dives into the negative-energy continuum at $Z_{\text{crit}} \approx 173$.

Low-energy heavy-ion collisions

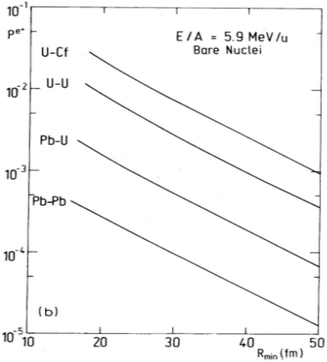
Creation of electron-positron pairs in low-energy heavy-ion collisions, with $Z_1 + Z_2 > 173$



Dynamical mechanism: a),b),c). Spontaneous mechanism (vacuum decay): d). The $1s$ state dives into the negative-energy continuum for about 10^{-21} sec.

Low-energy heavy-ion collisions

Positron production probability in 5.9 MeV/u collisions of bare nuclei as a function of distance of closest approach $R_{\rm min}$
(J. Reinhardt, B. Müller, and W. Greiner, Phys. Rev. A, 1981).



Conclusion by Frankfurt's group (2005):The vacuum decay could only be observed in collisions with nuclear sticking, in which the nuclei are bound to each other for some period of time by nuclear forces.

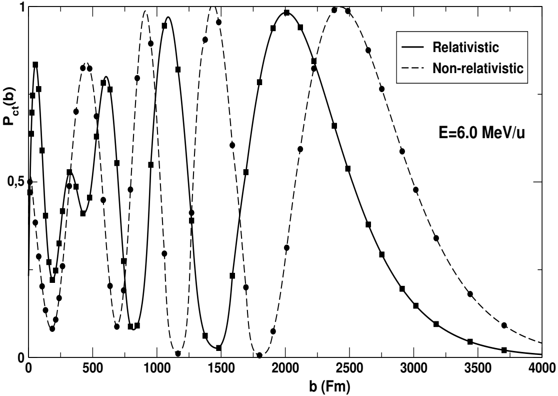
Low-energy heavy-ion collisions

New methods for calculations of quantum dynamics of electron-positron field in low-energy heavy-ion collisions at subcritical and supercritical regimes have been developed:

- *I.I. Tupitsyn, Y.S. Kozhedub, V.M. Shabaev et al., Phys. Rev. A 82, 042701 (2010).*
- *I. I. Tupitsyn, Y. S. Kozhedub, V. M. Shabaev et al., Phys. Rev. A 85, 032712 (2012).*
- *G. B. Deyneka, I. A. Maltsev, I. I. Tupitsyn et al., Russ. J. of Phys. Chem. B 6, 224 (2012).*
- *G. B. Deyneka, I. A. Maltsev, I. I. Tupitsyn et al., Eur. Phys. J. D 67, 258 (2013).*
- *Y.S. Kozhedub, V.M. Shabaev, I.I. Tupitsyn et al., Phys. Rev. A 90, 042709 (2014).*
- *I.A. Maltsev, V.M. Shabaev, I.I. Tupitsyn et al., NIMB, 408, 97 (2017).*
- *R.V. Popov, A.I. Bondarev, Y.S. Kozhedub et al., Eur. Phys. J. D 72, 115 (2018).*
- *I.A. Maltsev, V.M. Shabaev, R.V. Popov et al., Phys. Rev. A 98, 062709 (2018).*

Low-energy heavy-ion collisions

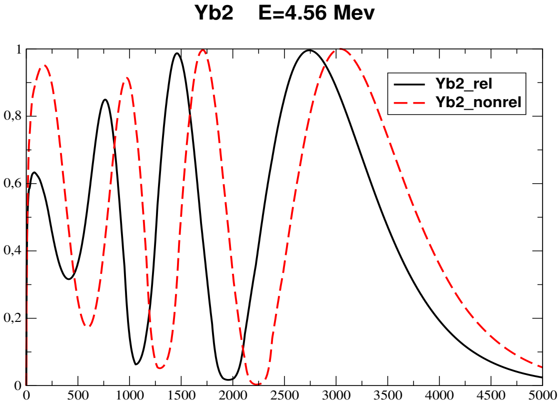
Charge-transfer probability for the $\mathrm{U}^{91+}(1s)-\mathrm{U}^{92+}$ collision



Charge-transfer probability as a function of the impact parameter b for the projectile energy of 6 MeV/u *(I.I. Tupitsyn et al., PRA, 2012)*. The same results are obtained by a different method *(I.A. Maltsev et al., Phys. Scr., 2013)*.

Low-energy heavy-ion collisions

Charge-transfer probability for the $\mathrm{Yb}^{69+}(1s)-\mathrm{Yb}^{70+}$ collision

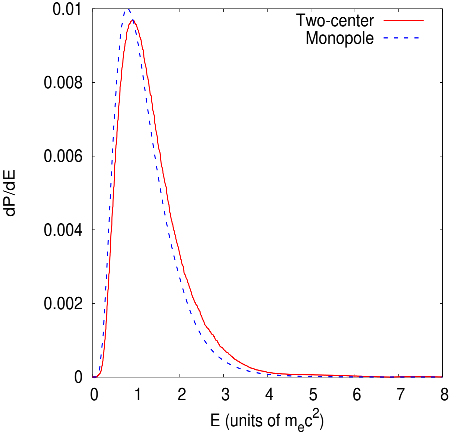


Charge-transfer probability as a function of the impact parameter b for the projectile energy of 4.6 MeV/u.

Low-energy heavy-ion collisions

Pair creation beyond the monopole approximation

Positron energy spectrum for the U−U head-on collision at energy $E_{\rm cm}$ = 740 MeV *(I.A. Maltsev, V.M. Shabaev, R.V. Popov et al., PRA, 2018)*.



Low-energy heavy-ion collisions

Pair creation beyond the monopole approximation

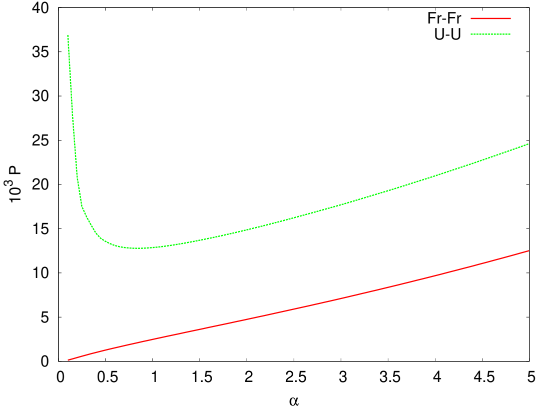
U-U, $E_{\rm cm}$ = 740 MeV

Expected number of created pairs as a function of the impact parameter b *(I.A. Maltsev, V.M. Shabaev, R.V. Popov et al., PRA, 2018)* .

b (fm)	Monopole approximation	Two-center approach
0	1.29×10^{-2}	1.38×10^{-2}
10	7.26×10^{-3}	8.01×10^{-3}
20	2.75×10^{-3}	3.46×10^{-3}
30	1.04×10^{-3}	1.42×10^{-3}
40	4.12×10^{-4}	7.04×10^{-4}

The two-center result for $b = 0$ has been confirmed by a different method *(R.V. Popov, A.I. Bondarev, Y.S. Kozhedub et al., EPJD, 2018)* .

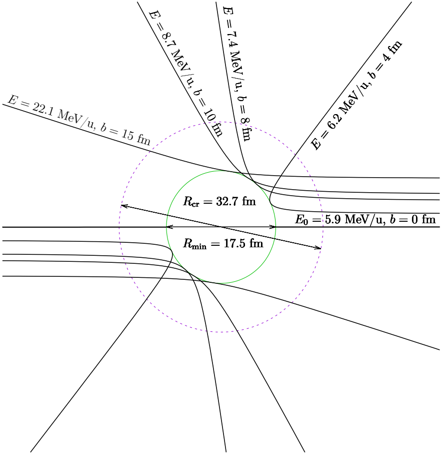
Low-energy heavy-ion collisions



Pair creation with artificial trajectories for the supercritical U−U and subcritical Fr−Fr head-on collisions at $E_{\rm cm} = 674.5$ and $E_{\rm cm} = 740$ MeV, respectively. The trajectory $R_\alpha(t)$ is defined by $\dot{R}_\alpha(t) = \alpha \dot{R}(t)$, where $R(t)$ is the classical Rutherford trajectory *(I.A. Maltsev, V.M. Shabaev, I.I. Tupitsyn et al., PRA, 2015)*.

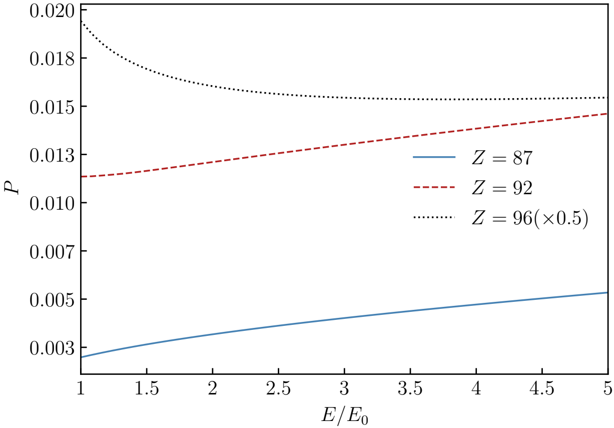
How to observe the vacuum decay

(I.A. Maltsev et al., PRL, 2019; R.V. Popov et al., PRD, 2020)



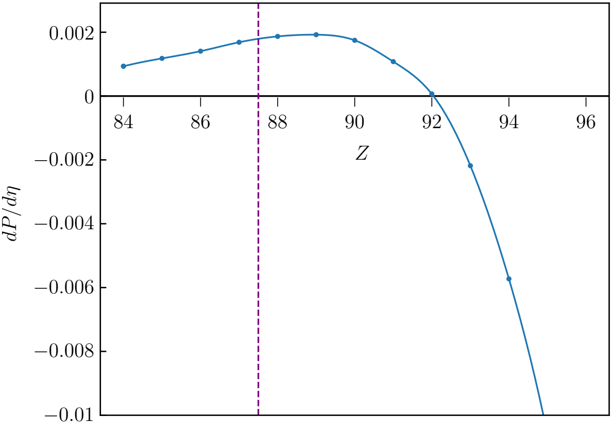
We consider only the trajectories for which the minimal internuclear distance is the same: $R_{\mathrm{min}} = 17.5$ fm. We introduce $\eta = E/E_0 \geq 1$.

How to observe the vacuum decay



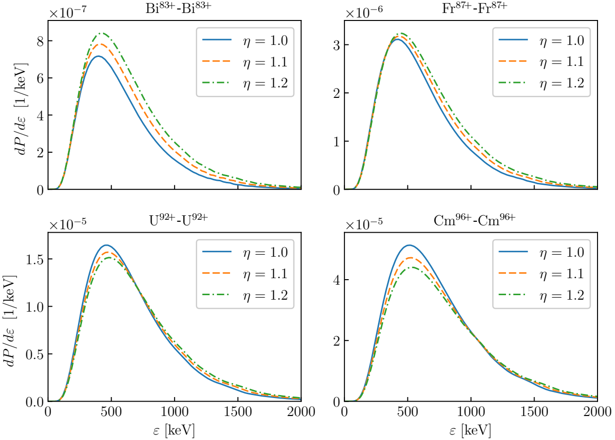
Total pair-production probability for symmetric ($Z = Z_1 = Z_2$) collisions as a function of the collision energy at $R_{\text{min}} = 17.5$ fm.

How to observe the vacuum decay



The derivative of the pair-production probability with respect to the energy $dP/d\eta$, where $\eta = E/E_0$, at the point $\eta = 1$ as a function of the nuclear charge number $Z = Z_1 = Z_2$ at $R_{\min} = 17.5$ fm.

How to observe the vacuum decay



Positron spectra in symmetric ($Z = Z_1 = Z_2$) collisions for different collision energy $\eta = E/E_0$ at $R_{\rm min} = 17.5$ fm.

Conclusion

The experimental study of the proposed scenarios would either prove the vacuum decay in the supercritical Coulomb field or lead to discovery of a new physics, which is beyond the presently used QED formalism.

The same scenarios can be applied to observe the vacuum decay in collisions of bare nuclei with neutral atoms.

For details:

I.A. Maltsev, V.M. Shabaev, R.V. Popov, Y.S. Kozhedub, G. Plunien, X. Ma, Th. Stöhlker, and D.A. Tumakov, Phys. Rev. Lett. 123, 113401 (2019).

R.V. Popov, V.M. Shabaev, D.A. Telnov, I.I. Tupitsyn, I.A. Maltsev, Y.S. Kozhedub, A.I. Bondarev, N.V. Kozin, X. Ma, G. Plunien, T. Stöhlker, D.A. Tumakov, and V.A. Zaytsev, Phys. Rev. D 102, 076005 (2020).

Thank You for Attention