Coupled channel method for heavy ion fusion reactions

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Contents

- Introduction on deep sub-barrier fusion hindrance
- The modified CC theoretical framework
- Results and discussions

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Time independent sub-barrier quantum tunneling



There are generally two ways to get the tunneling probability:

• Semi-classical approaches: WKB et al.

$$P_l^{\text{WKB}}(E) = \exp[-2\int_{r_{\text{min}}}^{r_{\text{max}}} \sqrt{2\mu[V_l(r) - E]/\hbar^2} dr],$$

• Schrödinger equation under certain boundary conditions.

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V_N^{(0)}(r) + \frac{Z_P Z_T e^2}{r} - E\right] \psi(r) = 0$$

Explanations: adiabatic approximation & deep potential



T. Ichikawa, K. Hagino and A. Iwamoto, Phys Rev C 75, 064612 (2007); Phys Rev Lett 103, 202701 (2009); T. Ichikawa, Phys Rev C 92 (6), 064604 (2015).

On top of the conventional CC method, an extra one-dimensional adiabatic potential barrier is assumed after the reacting nuclei contact with each other, considering the formation of the composite system.

 K. Hagino, A. B. Balantekin, N. W. Lwin et al, Phys Rev C 97, 034623 (2018). Two Woods-Saxon potentials with different slopes.

$$\sigma_{fus}(E) = \frac{\pi \hbar^2}{2\mu E} \sum_{L=0} (2L+1)T_L(E)P(L,E)$$

Adiabatic representation KANTBP To obtain an appropriate adiabatic representation known in computational mathematics as the Kantorovich method [L.V. Kantorovich and V.I. Krylov, Approximate methods of higher analysis (Intersci. Publ., NY, 1958)] — reduction of a BVP to a system of ODEs of the second order that explains the above abbreviation for the proposed method KANTBP one needs to make a gauge transformation $\mathcal{U}_{nn'}(r)$ depending on parameter r [S. I. Vinitsky, B. L. Markovski, and A. A. Suz'ko, Sov. J. Nucl. Phys. 55, 371 (1992)]:

$$\psi_{nn_o}(r) = \sum_{n'=1}^{N} \mathcal{U}_{nn'}(r) \mathbf{y}_{n'n_o}(r), \ \mathbf{y}_{n'n_o}(r) = \sum_{n=1}^{N} \mathcal{U}_{n'n}^{-1}(r) \psi_{nn_o}(r), \tag{1}$$

that transforms Eq. (11) to the following system of ODEs

$$\sum_{n'=1}^{N} \left(\left(-\frac{d^2}{dr^2} - (\tilde{E} - \tilde{W}_{nn}(r)) \delta_{nn'} + U_{nn'}(r) \right) y_{n'n_o}(r) = 0.$$
 (2)

Here $\tilde{E} = (2\mu/\hbar^2)E$ and effective potentials $U_{nn'}(r)$ reads as

$$U_{nn'}(r) = H_{nn'}(r) + Q_{nn'}(r)\frac{d}{dr} + \frac{dQ_{nn'}(r)}{dr}$$
(3)

$$H_{nn'}(r) = H_{n'n}(r) = \sum_{n''=1}^{N} \frac{d(\mathcal{U}(r))_{nn''}^{-1}}{dr} \frac{d\mathcal{U}_{n''n'}(r)}{dr},$$
(4)

$$Q_{nn'}(r) = -Q_{n'n}(r) = -\sum_{n''=1}^{N} (\mathcal{U}(r))_{nn''}^{-1} \frac{d\mathcal{U}_{n''n'}(r)}{dr}.$$
(5)

Adiabatic representation KANTBP

In the above formula $\mathcal{U}(r)$ is orthogonal matrix $\mathcal{U}(r)_{nn'}^{-1} = \mathcal{U}(r)_{nn'}^{T}$ composed by eigenvectors of the parametric algebraic eigenvalue problem at each value of parameter $r \in [r_{min}, r_{max}]$:

$$\sum_{n'=1}^{N} (W_{nn'}(r) - \delta_{nn'} \tilde{W}_{n'n'}(r)) \mathcal{U}_{n'n}(r) = 0.$$
(6)

$$\sum_{n''=1}^{N} \mathcal{U}_{nn''}^{\mathsf{T}}(r) \mathcal{U}_{n''n'}(r) = \delta_{nn'}, \ \sum_{n''=1}^{N} \mathcal{U}_{nn''}(r) \mathcal{U}_{n''n'}^{\mathsf{T}}(r) = \delta_{nn'}.$$
(7)

These eigenvectors $\mathcal{U}_{n'n}(\mathbf{r})$ and eigenvalues $\tilde{W}_{n'n'}(\mathbf{r})$ have the bounded and continuous derivatives $\frac{d\mathcal{U}_{nn'}(\mathbf{r})}{d\mathbf{r}}$ and $\frac{d\tilde{W}_{nn'}(\mathbf{r})}{d\mathbf{r}}$ with respect to the parameter \mathbf{r} , that are calculated by solving the nonhomogeneous parametric algebraic problem at each value of parameter $\mathbf{r} \in [\mathbf{r}_{min}, \mathbf{r}_{max}]$:

$$\sum_{n'=1}^{N} (W_{nn'}(r) - \delta_{nn'} \tilde{W}_{n'n'}(r)) \frac{\partial \mathcal{U}_{n'n}(r)}{\partial r}$$
$$= -\sum_{n'=1}^{N} (\frac{\partial W_{nn'}(r)}{\partial r} - \delta_{nn'} \frac{\partial \tilde{W}_{n'n'}(r)}{\partial r}) \mathcal{U}_{n'n}(r).$$
(8)

These problems are solved by means of the adapted symbolic-numerical algorithms and programs [S.I. Vinitsky et al, Progr. Comput. Soft. 33 105 (2007)]. Further application of the adiabatic representation for study of the the BVP under consideration is beyond scope of the present talk and will be done elsewhere.

Explanations: sudden approximation & shallow potential



- Ş. Mişicu and H. Esbensen, Phys Rev Lett 96 (11), 112701 (2006); Phys Rev C 75, 034606 (2007); Hindrance of Heavy-Ion Fusion due to Nuclear Incompressibility. Double-folding potential with M3Y forces supplemented by a repulsive core.
- C. Simenel, A. S. Umar, K. Godbey, et al, Phys Rev C 95, R031601 (2017). Density constrained time dependent Hartree-Fock model. It is concluded that: "...to explain experimental fusion data at deep sub-barrier energies, then cannot be justified by an effect of incompressibility. It is more likely that it simulates other effects such as Pauli repulsion."
- V. V. Sargsyan, G. G. Adamian, N. V. Antonenko et al, Eur Phys J A 56, 19 (2020). Extended quantum diffusion approach + Double folding potential.

Some open questions

About deep sub-barrier fusion hindrance:

• Whether could the CC calculation of the fusion cross section be stable at the deep sub-barrier energy region?

Some works used an extra imaginary potential around the potential minimum to eliminate the fluctuations of the conventional CC calculation. However, one has to add more parameters.

• Is Woods-Saxon potential able to describe the deep sub-barrier fusion hindrance phenomenon well enough?

It is said that it is not able to describe it in many works. And hybrid potential model, other potential models, and reaction mechanisms are widely used now.

• What's the mechanism of the fusion hindrance? The shallow potential or deep potential. Import gradients for solving the coupled-channels equation

There are several parts to construct the coupled-channels approach:

- Nuclear potential: real potential (double folding, proximity, Woods-Saxon potential), complex potential: Extended Optical Model(EOM)
- Coupled potential: full order coupling, linear coupling, or the quadratic coupling
- Boundary condition:

regular boundary condition, incoming wave boundary condition

Numerical method:

finite difference method (Numerov , three-point difference), finite element method (KANTBP), R-matrix method.

O. Chuluunbaatar, A. A. Gusev, et al, CPC. 177, 649 (2007)
 A. A. Gusev, O. Chuluunbaatar, S. I. Vinitsky et al, CPC 185, 3341 (2014)

Extended Optical Model(EOM) [B. Buck et al, Phil. Mag.(1963)]

$$\begin{pmatrix} -\frac{h^2}{2\mu}\frac{d^2}{dr^2} + V_L(r) - E \end{pmatrix} \Psi(r) = 0, \ V_L(r) = V_N(r) - \imath g(E)\frac{dV_N(r)}{dr} + V_C(r) + \frac{h^2}{2\mu}\frac{L(L+1)}{r^2}, \\ {}^{16}O + {}^{144}Sm : A_P = 16, \ A_T = 144.0, \ Z_P = 8, \ Z_T = 62, \ \mu = A_PA_T/(A_P + A_T) \\ V_0 = 105, \ R_{00} = 1.1, \ A_0 := 0.75; \ R_0 = R_{00}(A_P^{1/3} + A_T^{1/3}) \text{ in zero approximation:} \\ V_N(r) = -\frac{V_0}{1 + \exp((r - R_0)/a)}, \ V_C(r) = Z_PZ_T \begin{cases} 1/r \\ (3R_C^2 - r^2)/(2R_C^3) \\ r < R_C \end{cases}, \ R_C = R_0. \end{cases}$$

EOM B. Buck et al, Phil. Mag.(1963)&IWBC Hagino et al CPC (1999)

Boundary conditions IWBC at g(E) = 0

$$IWBC: \Psi_{as}(r_{L}^{\min}) = \frac{\exp(-i\sqrt{E - V_{L}(r_{L}^{\min})})}{\sqrt{k}} T_{L}(E), \ k = \sqrt{E}$$
$$\Psi_{as}(r_{L}^{\max}) = \frac{1}{\sqrt{k}} (\hat{H}_{L}^{-}(kr) - \hat{H}_{L}^{+}(kr)R_{L}(E)), \ |T_{L}(E)|^{2} = 1 - |R_{L}(E)|^{2}$$

Boundary conditions EOM with unknown g(E) > 0

$$EOM: rac{d\Psi_{as}(r_L^{\min})}{dr}|_{r=r_L^{\min}}=0,$$

$$\Psi_{as}(r_L^{\max}) = \frac{1}{\sqrt{k}} (\hat{H}_L^-(kr) - \hat{H}_L^+(kr)S_L(E)), |T_L(g(E))|^2 = 1 - |S_L(g(E))|^2,$$

constraints: g(E)>0: $S_L(g(E))=R_L(E)$, $|S_L(g=0,E)|^2=1$, $|T_L(g=0,E)|^2=0$, for calculating g(E)>0 using known $R_L(E)$ from solving IWBC at g(E)=0

$$\begin{split} \sigma_{el}(E) &= \frac{\pi}{k^2} \sum_{L=0} (2L+1) |(1-S_L(g))|^2, \ \sigma_{fus}(E) &= \frac{\pi}{k^2} \sum_{L=0} (2L+1) (1-|S_L(g)|^2), \\ \sigma_{tot}(E) &= \sigma_{el}(E) + \sigma_{fus}(E) = \frac{2\pi}{k^2} \sum_{L=0} (2L+1) (1-\Re S_L(g)). \end{split}$$

Eigenfunctions of scattering states IWBC in comparison with EOM at g = 0.00429, L = 0 and nonresonance energy E = 61 MeV



Eigenfunctions of scattering states in vicinity of resonance energy $E \approx 57.7330$ MeV at g = 0.001 in vicinity of second peak of g(E) plot and L = 0 (EOM) in comparison with g = 0



Eigenfunctions of the three metastable states $E_{16} = 53.773 - 0.0001i$, $E_{17} = 57.733 - 0.014i$ and $E_{18} = 61.170 - 0.162i$ in vicinity of first, second and third peaks of g(E) plot, below maximum $V^B_{max} = 62$ MeV of potential barrier at g = 0.001 and g = 0.00001, and L = 0(EOM) in comparison with g = 0



The nuclear potential

The Akyüz-Winther (AW) type Woods-Saxon potential as starting point:

$$V_N^{(0)}(r) = -rac{V_0}{1 + \exp((r - R_0)/a_0)}. \ = rac{-16\pi\gamma a_0 ar{R}}{1 + \exp[(r - R_P - R_T)/a_0]},$$

A. Winther, Nucl. Phys. A 594, 203 (1995)

 with

$$\frac{1}{a_0} = 1.17[1 + 0.53(A_P^{-1/3} + A_T^{-1/3})]$$

$$\bar{R} = \frac{R_P R_T}{R_P + R_T} \qquad R_i = 1.2A_i^{1/3} - 0.09, \ i = P, T$$

$$\gamma = 0.95\left(1 - 1.8\frac{(N_P - Z_P)(N_T - Z_T)}{A_P A_T}\right)$$

No free parameters and widely used for fusion reaction.

The coupled potential (full order coupling)

The nuclear coupling Hamiltonian can be generated by changing the potential radius to a dynamical operator $R_0 + \hat{O}$ with $\hat{O} |\alpha\rangle = \lambda_{\alpha} |\alpha\rangle$

$$\hat{O} = \sum_{i=P,T} \frac{\beta_{\lambda}}{\sqrt{4\pi}} r_{\text{coup}} A_i^{1/3} (a_{\lambda 0}^{\dagger} + a_{\lambda 0}) \qquad \begin{array}{c} \text{Bohr, A. and Mottelson, B. R.} \\ \text{Nuclear Structure II, (1969)} \end{array}$$

The nuclear coupling potential is given on top of the potential as

$$V_N'(r, \hat{O}) = -rac{V_0}{1 + \exp((r - R_0 - \hat{O})/a_0)}.$$

It is considered with full order by diagonalizing the matrix \hat{O}

$$O_{nm} = \sum_{i=P,T} \frac{\beta_{\lambda}}{\sqrt{4\pi}} r_{\text{coup}} A_i^{1/3} (\sqrt{m} \delta_{n,m-1} + \sqrt{n} \delta_{n,m+1})$$

The nuclear coupling matrix elements between phonon state $|n\rangle$ and $|m\rangle$ is

$$V_{nm}^{(N)} = \langle n | V_N'(r, \hat{O}) | m \rangle - V_N^{(0)} \delta_{n,m} = \sum_{\alpha} \langle n | \alpha \rangle \langle \alpha | m \rangle V_N'(r, \lambda_{\alpha}) - V_N^{(0)} \delta_{n,m}$$

H. Hagino et al, Comput. Phys. Commun. 123 143 (1999);

The incoming wave boundary condition

The incoming wave boundary conditions (IWBC)

$$\psi_n(r) = \begin{cases} T_n \exp\left(-ik_n(r_{\min})r\right), & r \le r_{\min} \\ H_l^-(k_n r)\delta_{n,0} - R_n H_l^+(k_n r), & r \ge r_{\max} \end{cases}$$

Here $k_n = k_n(r \to +\infty)$, and $k_n(r)$ is the local wave number for *n*-th channel

$$X_n(r) = \sqrt{\frac{2\mu}{\hbar^2}} \left(E - \epsilon_n - \frac{l(l+1)\hbar^2}{2\mu r^2} - V_N^{(0)}(r) - \frac{Z_P Z_T e^2}{r} - V_{nn}(r) \right)^2}$$



There are problems in the previous boundary condition.

- The plane wave boundary condition at the left boundary r_{\min} involves only the diagonal part. This requires that the off-diagonal matrix elements tend to zero.
- However, at r_{\min} , the distance between two nuclei is so short that the off-diagonal matrix elements are usually not zero. There can be sudden noncontinuous changes in the left boundary.
- A linear transformation should be done at the left boundary.

V.V. Samarin, V.I. Zagrebaev, 2004 NPA 734 E9;V.I. Zagrebaev, V.V. Samarin, 2004 Phys. Atom. Nucl. 67 1462;

The new method KANTBP

The coupled-channels Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{l(l+1)\hbar^2}{2\mu r^2} + V_N^{(0)}(r) + \frac{Z_P Z_T e^2}{r} + \epsilon_n - E\right] \psi_{nn_0} + \sum_{n'=1}^N V_{nn'}(r)\psi_{n'n_0}(r) = 0,$$
(9)

with

- n_o is a number of the open entrance channel with a positive relative energy $E_{n_o} = E \epsilon_{n_o} > 0$, $n_o = 1, ..., N_o \le N$.
- $\{\psi_{nn_0}(r)\}_{n=1}^N$ are components of a desirable matrix solution.

Let **W** is the symmetric matrix of dimension $N \times N$

$$W_{nm} = W_{mn} = \frac{2\mu}{\hbar^2} \left[\left(\frac{l(l+1)\hbar^2}{2\mu r^2} + V_N^{(0)}(r) + \frac{Z_P Z_T e^2}{r} + \epsilon_n \right) \delta_{nm} + V_{nm}(r) \right].$$
(10)

Then the equation can be expressed as

$$-\psi_{nm}^{''}(r) + \sum_{m'} W_{nm'} \psi_{m'm}(r) = \frac{2\mu E}{\hbar^2} \psi_{nm}(r), \qquad (11)$$

The new method KANTBP

Diagonalize the matrix at $r = r_{\min}$

$$\mathbf{WA} = \mathbf{A}\tilde{\mathbf{W}}, \quad \{\tilde{\mathbf{W}}\}_{nm} = \delta_{nm}\tilde{W}_{mm}, \quad \tilde{W}_{11} \le \tilde{W}_{22} \dots \le \tilde{W}_{NN}.$$
(12)

The functions $y_m(r)$ are solutions of the uncoupled equations

$$y_m''(r) + K_m^2 y_m(r) = 0, \quad K_m^2 = \frac{2\mu E}{\hbar^2} - \tilde{W}_{mm}.$$
 (13)

In open channels at $K_m^2 > 0$, $m = 1, ..., M_o \le N$ the solutions $y_m(r)$ have the form:

$$y_m(r) = \frac{\exp(-\imath K_m r)}{\sqrt{K_m}}.$$
(14)

In this case $\psi_{nn_0}(r)$ expressed by the linear combinations of the linear independent solutions

$$\psi_{nn_0}(r) = \sum_{m=1}^{M_0} A_{nm} y_m(r) \hat{T}_{mn_0}, \quad r = r_{\min}.$$
 (15)

In this way, the off-diagonal matrix elements have been considered in the calculation.

The new method KANTBP



At fixed orbital momentum I, it is given by summation over all possible intrinsic states:

$$T_{n_0n_0}^{(l)}(E) = \sum_{m=1}^{M_0} \left| \hat{T}_{mn_0} \right|^2, \quad R_{n_0n_0}^{(l)}(E) = \sum_{n=1}^{N_0} \left| \hat{R}_{nn_0} \right|^2, \quad T_{n_0n_0}^{(l)}(E) = 1 - R_{n_0n_0}^{(l)}(E)$$
(18)

The condition $T_{n_0n_0}^{(l)}(E) + R_{n_0n_0}^{(l)}(E) - 1 = 0$ fulfills with ten significant digits by the element method KANTBP.

O. Chuluunbaatar, A. A. Gusev, A.G. Abrashkevich et al, CPC. 177, 649 (2007) A. A. Gusev, O. Chuluunbaatar, S. I. Vinitsky et al, CPC 185, 3341 (2014) A. A. Gusev, O. Chuluunbaatar, S. I. Vinitsky et al, Math. Mod. Geom. 3, 2 22 (2015) V. I. Zagrebaev, Phys. Rev. C 78 047602 (2008)

$^{32}S+^{182}W$: the coupled potential

S. I. Vinitsky, P. W. Wen, A. A. Gusev, O. Chuluunbaatar, R. G. Nazmitdinov, A. K. Nasirov, C. J. Lin, H. M. Jia and A. Góźdź, Acta Phys. Pol. B Proc. Suppl. 13 (3), 549 (2020).



There are many non-diagonal elements of $\hat{O}_{nm}(r)$ at r_{\min} . $\hat{O}|\alpha\rangle = \lambda_{\alpha}|\alpha\rangle$

$$V_{nm}^{(N)} = \langle n | V_N'(r, \hat{O}) | m \rangle - V_N^{(0)} \delta_{n,m}$$

=
$$\sum_{\alpha} \langle n | \alpha \rangle \langle \alpha | m \rangle V_N'(r, \lambda_{\alpha}) - V_N^{(0)} \delta_{n,m}$$

$^{32}\mathrm{S+}^{182}\mathrm{W},\,^{28}\mathrm{Si+}^{178}\mathrm{Hf:}$ Near barrier fusion

S. I. Vinitsky, P. W. Wen, A. A. Gusev, O. Chuluunbaatar, R. G. Nazmitdinov, A. K. Nasirov, C. J. Lin, H. M. Jia and A. Góźdź, Acta Phys. Pol. B Proc. Suppl. 13 (3), 549 (2020).



There are obvious differences in sub-barrier energy region.

 $\rm ^{64}Ni+^{100}Mo:$ Deep sub-barrier fusion





New calculations are more stable and agree with experimental data better

 ${}^{64}\mathrm{Ni}{+}{}^{100}\mathrm{Mo},\,{}^{64}\mathrm{Ni}{+}{}^{64}\mathrm{Ni},\,{}^{28}\mathrm{Si}{+}{}^{64}\mathrm{Ni}$

P. W. Wen, C. J. Lin, R. Nazmitdinov, S. I. Vinitsky, et al. PRC, 103, 054601, 2021.



Woods-Saxon potential and multiphonon coupling are enough.

 $S(E) = E\sigma_{fus} \exp(2\pi(\eta - \eta_0)), \quad \eta_0 = 105.74, 75.23, 71.25 \text{ resp.}$

$^{64}\mathrm{Ni}+^{100}\mathrm{Mo:}$ Potential details

TABLE I. Woods-Saxon potential parameters V_0 (MeV), a_0 (fm), and R_0 (fm) for 64 Ni + 100 Mo, 64 Ni + 64 Ni, and 28 Si + 64 Ni reaction systems. The potential barrier V_B and the minimum of the potential pocket V_P are also listed.

	⁶⁴ Ni + ¹⁰⁰ Mo	⁶⁴ Ni + ⁶⁴ Ni	²⁸ Si + ⁶⁴ Ni
V_0 (MeV)	79.938	65.829	53.529
a_0 (fm)	0.686	0.801	0.944
R_0 (fm)	10.190	9.239	7.790
V _B (MeV)	136.993	96.389	51.946
V _P (MeV)	119.344	85.699	43.298





 $\langle I \rangle$ could be used as a probe to separate these two mechanisms.

Ichikawa, T. (2015). Phys Rev C 92: 064604.

Summary

Potential answers to the previous questions based on sudden approximation:

• Whether could the calculation of the fusion cross section be stable at the deep sub-barrier energy region? The calculations are stable now with the coupled-channels approach adopting

the finite element method KANTBP with the improved boundary condition.

• Is Woods-Saxon potential able to describe the deep sub-barrier fusion hindrance phenomenon well enough?

The deep sub-barrier fusion cross sections, as well as the S facotr, of several typical reactions have been successfully described by using the most simple 3 parameter WS potential and multiphonon couplings.

• What's the mechanism of the fusion hindrance?

 $\langle I\rangle$ could be used to clarify shallow or deep potential.

Perspective

• What's the systematics of the maximum of fusion hindrance and S(E) factor with respect to different reaction systems?

We have fitted several reactions with hindrance feature at deep sub-barrier energy region, and are trying to see the systematics by fitting more reactions. We find that our current results for medium nuclei manifest the hindrance factor for system with $Z_T Z_P \sqrt{M_T M_P / (M_T + M_P)} \ge 2000$. However, for the lightest systems $Z_T Z_P \sqrt{M_T M_P / (M_T + M_P)} \le 200$ the logarithmic slopes of the $S^*(E)$ factor exhibit resistance to increasing tendency with the energy. It is supported by the empirical trends, discussed for hindrance factor in C.L.Jiang, et al. Phys.Rev.C. 73,014613 (2006).

- The impact of the finite elements method on complex potential and regular boundary condition? Further adaptation of KANTBP code is possible.
- Open questions: The role of other mechanisms like transfer and etc. on deep sub-barrier fusion hindrance?

Resume

- We analyzed sub-barrier heavy ion fusion reactions based on the coupled-channels description with the correct incoming wave boundary conditions, implemented by means of the finite element method.
- With the aid of the Woods-Saxon potential the experimental cross sections and the so-called S factors of these reactions are remarkably well reproduced within the sudden approximation approach with the correct incoming wave boundary conditions.
- We found that accounting for the nondiagonal matrix elements of the coupling matrix, traditionally neglected in the conventional coupled-channels approaches in setting the entangled left boundary conditions inside the potential pocket, and its minimal value are crucially important for the interpretation of experimental data.

Thank you for your attention!