Quantum design in study of pycnonuclear reactions in compact stars:

Nuclear fusion, quasibound states, spectroscopy

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Outline :

1) Potential of nuclear interactions, scattering ^{12}C-^{12}C in lattice,
2) Method of Multiple Internal Reflections,
3) New quasibound states in pycnonuclear reactions,
4) Energies of zero-point vibrations of nuclei (Zel'dovich approach).

Pycnonuclear reactions in compact stars

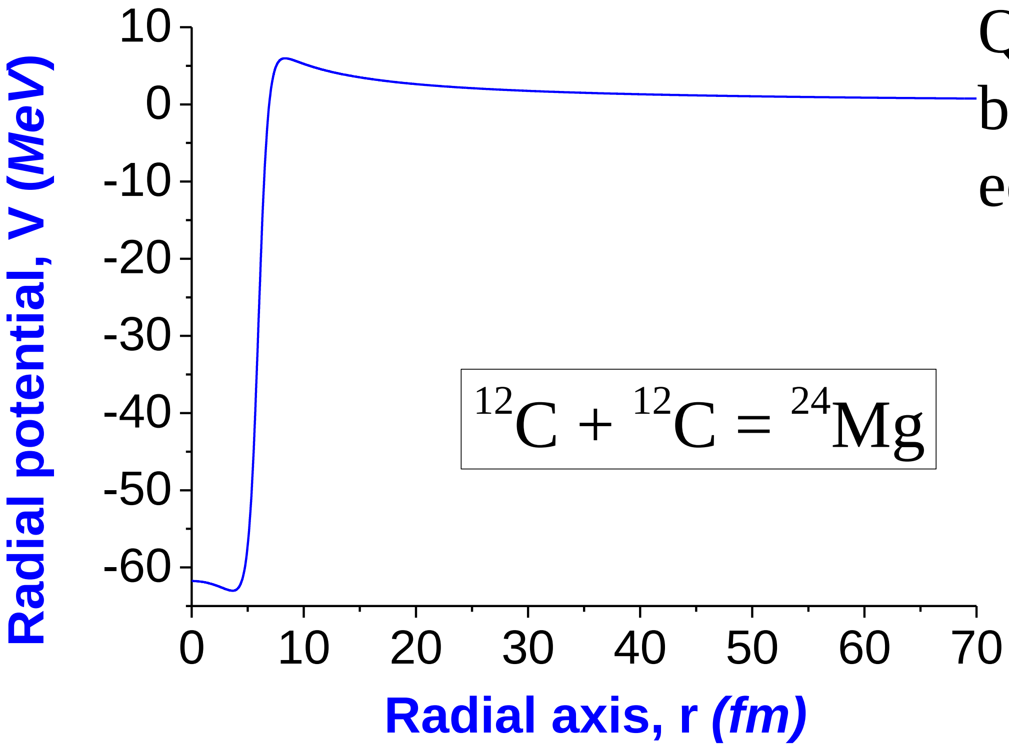
In stars, thermal energy of reacting nuclei overcomes the Coulomb repulsion between them so that a reaction can proceed. At sufficiently high densities, even at zero temperature, energy of nuclei in lattice lead to an appreciable rate of reactions. This phenomenon is known as ***pycnonuclear reaction*** (from “pyknos” as “dense” in Greek) [1].

Pycnonuclear burning occurs in ***dense and cold cores of white dwarfs*** [2] and in ***crusts of accreting neutron stars*** [3].

Astrophysical S-factors are estimated for 946 thermonuclear reactions for isitopes C, O, Ne and Mg for energies 2 - 30 MeV [4]. Large database of *S*-factors [5] is formed for isotopes Be, B, C, N, O, F, Ne, Na, Mg, Si (5000 non-resonant thermo-reactions).

[1] A.G.W.Cameron, *Pycnonuclear reactions and nova explosions*, Astr. J. **130**, 916 (1959).
[2] E.E.Salpeter, H.M.VanHorn, Nuclear reaction rates at high densities, Astr. J. **155**, 183 (1969).
[3] P. Haensel/ et al., Astron. Astr. **229**, 117 (1990); **404**, L33 (2003).
[4] M.Beard, A.V.Afanasjev, et al., At. Dat. Nucl. Dat. Tabl. **96**, 541-566 (2010).
[5] A.V.Afanasjev, M.Beard, et al., Phys. Rev. **C 85**, 054615 (2012).

Potential of interactions



Quantum mechanical study on the basis of solution of Schrodinger equation with potential:

$$V(r) = V_C(r) + V_N(r) + V_{l=0}(r),$$

$$V_N(r) = -\frac{V_R}{1+\exp\left(\frac{r-R_R}{a_R}\right)},$$

$$R_R = r_R(A_1^{1/3} + A_2^{1/3}),$$

$$r_R = 1.30\,fm, \quad a_R = 0.44\,fm.$$

$$V = -75 MeV.$$

$$\rho_0 = \frac{m_A}{V_A} = \frac{Am_u}{4/3\pi R_0^3},$$

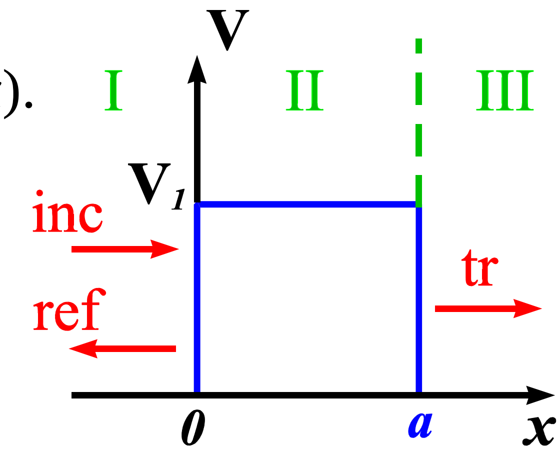
$$R_0 = \left(\frac{Am_u}{4/3\pi\rho_0}\right)^{1/3}. \qquad n_A = \frac{\rho_0}{Am_u}.$$

$$\rho_0 = 6\cdot 10^9\,\frac{g}{cm^3},$$
$$R_0 = 92.5\,fm,$$
$$n_A = 3.014189\cdot 10^{-7}\ fm^{-3}.$$

Method: 1D tunneling (1)

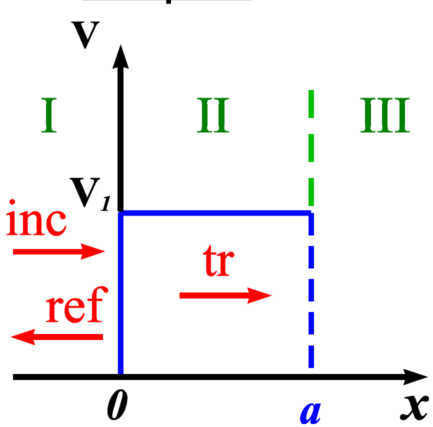
One can understand idea of method the most clearly in the simplest case – analyzing wave, propagating above rectangular barrier.

- Schrodinger equation: $$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi(x)+V(x)\varphi(x)=E\,\varphi(x).$$



- Wave function (WF): $$\varphi(x)=\begin{cases} e^{ikx}+A_R e^{-ikx}, & x\le 0,\\ \alpha e^{-ik_2x}+\beta e^{ik_2x}, & 0\le x\le a,\\ A_T e^{ikx}, & x\ge a\end{cases}$$

- Approach on step-by-step:
- Step 1:



$$\varphi_{inc}^{(1)}=e^{ikx},\qquad x\le 0,$$
$$\varphi_{tr}^{(2)}=\beta^{(0)}e^{ik_2x},\qquad 0\le x\le a,$$
$$\varphi_{ref}^{(1)}=A_R^{(0)}e^{-ikx},\qquad x\le 0.$$

- Continuity condition at $x=0$:

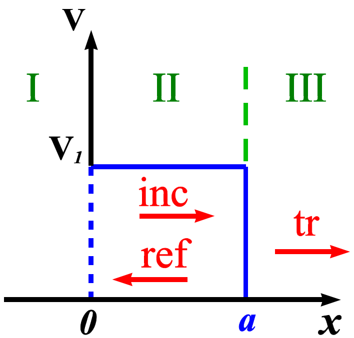
$$\beta^{(0)}=\frac{2k}{k+k_2},\qquad A_R^{(0)}=\frac{k-k_2}{k+k_2}.$$

- Transition to under-barrier tunneling:

$$k_2\Rightarrow i\xi,\qquad k_2=\frac{1}{\hbar}\sqrt{2m(E-V_1)}$$

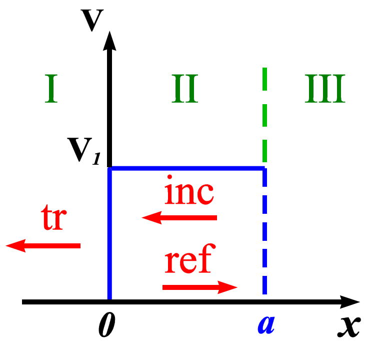
Method: 1D tunneling (2)

- Step 2:



$$\varphi_{inc}^{(2)} = \varphi_{tr}^{(1)} = \beta^{(0)} e^{ik_2 x},$$
$$\varphi_{tr}^{(2)} = A_T^{(0)} e^{ikx},$$
$$\varphi_{ref}^{(2)} = \alpha^{(0)} e^{-ik_2 x}.$$

- Step 3:



$$\varphi_{inc}^{(3)} = \varphi_{ref}^{(2)},$$
$$\varphi_{tr}^{(3)} = A_R^{(1)} e^{-ikx},$$
$$\varphi_{ref}^{(3)} = \beta^{(1)} e^{ik_2 x}.$$

- Continuity WF at $x = 0, a$: $\boxed{\alpha^{(n)}, \beta^{(n)}, A_T^{(n)}, A_R^{(n)}}$

- Amplitudes of transmission, reflection:

$$A_T = T_2^+ T_1^- \left(1 + \sum_{m=1}^{+\infty} (R_2^+ R_1^-)^m \right) = \frac{i4k\xi e^{-\xi a - ika}}{F_{sub}},$$
$$A_R = R_1^+ + T_1^+ R_2^+ T_1^- \left(1 + \sum_{m=1}^{+\infty} (R_2^+ R_1^-)^m \right) = \frac{k_0^2 D_-}{F_{sub}}$$

$$F_{sub} = (k^2 - \xi^2) D_- + 2ik\xi D_+, \quad D_\pm = 1 \pm e^{-2\xi a}$$
$$k_0^2 = k^2 + \xi^2 = \frac{2mV_1}{\hbar^2}$$

- Coefficients:

$$T_1^+ = \beta^{(0)}, \qquad R_1^+ = A_R^{(0)},$$
$$T_2^+ = \frac{A_T^{(n)}}{\beta^{(n)}}, \qquad R_2^+ = \frac{\alpha^{(n)}}{\beta^{(n)}},$$
$$T_1^- = \frac{A_R^{(n+1)}}{\alpha^{(n)}}, \qquad R_1^- = \frac{\beta^{(n+1)}}{\alpha^{(n)}}$$

- Test: $\boxed{|A_T|^2 + |A_R|^2 = 1}$

Method: Arbitrary number of barriers

Calculation of penetrability for arbitrary number of barriers is essentially more complicated, it has been solved.

- Wave function:

$$\varphi(x)=\begin{cases} e^{ikx}+A_R e^{-ikx}, & x\le x_1; \\ \alpha_2 e^{ik_2x}+\beta_2 e^{-ik_2x}, & x_1\le x\le x_2; \\ \ldots & \ldots \\ \alpha_{N-1}e^{ik_{N-1}x}+\beta_{N-1}e^{-ik_{N-1}x}, & x_{N-2}\le x\le x_{N-1}; \\ A_T e^{ikx}, & x_{N-1}\le x \end{cases}$$

- Calculation of coefficients:

$$T_j^+ = \frac{2k_j}{k_j+k_{j+1}} e^{i(k_j-k_{j+1})x_j}, \qquad T_j^- = \frac{2k_{j+1}}{k_j+k_{j+1}} e^{i(k_j-k_{j+1})x_j},$$

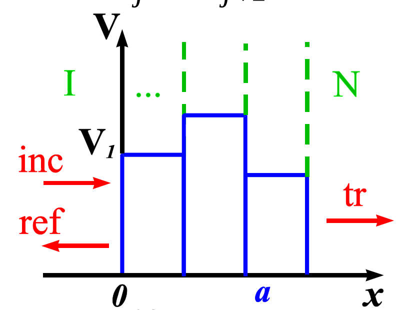
$$R_j^+ = \frac{k_j-k_{j+1}}{k_j+k_{j+1}} e^{2ik_jx_j}, \qquad R_j^- = \frac{k_{j+1}-k_j}{k_j+k_{j+1}} e^{-2ik_{j+1}x_j}.$$

- Recurrent relations:

$$\tilde{R}_{j-1}^+ = R_{j-1}^+ + T_{j-1}^+\tilde{R}_j^+T_{j-1}^-\left(1+\sum_{m=1}^{+\infty}(\tilde{R}_j^+R_{j-1}^-)^m\right) = R_{j-1}^+ + \frac{T_{j-1}^+\tilde{R}_j^+T_{j-1}^-}{1-\tilde{R}_j^+R_{j-1}^-},$$

$$\tilde{R}_{j+1}^- = R_{j+1}^- + T_{j+1}^-\tilde{R}_j^-T_{j+1}^+\left(1+\sum_{m=1}^{+\infty}(R_{j+1}^+\tilde{R}_j^-)^m\right) = R_{j+1}^- + \frac{T_{j+1}^-\tilde{R}_j^+T_{j-1}^-}{1-\tilde{R}_j^-R_{j+1}^+},$$

$$\tilde{T}_{j+1}^+ = \tilde{T}_j^+T_{j+1}^+\left(1+\sum_{m=1}^{+\infty}(R_{j+1}^+\tilde{R}_j^-)^m\right) = \frac{\tilde{T}_j^+T_{j+1}^+}{1-\tilde{R}_j^-R_{j+1}^+}.$$



$$\tilde{R}_{N-1}^+ = R_{N-1}^+,\quad \tilde{R}_1^- = R_1^-,\quad \tilde{T}_1^+ = T_1^+$$

- Amplitudes: $\boxed{A_T = \tilde{T}_{N-1}^+, \quad A_R = \tilde{R}_1^+.}$

- Penetrability, reflection: $\boxed{T = \frac{k_N}{k_1}|A_T|^2, \quad R = |A_R|^2.}$

Cross-section of capture

- Cross-section of capture:

$$\boxed{\sigma_{\text{capture}}(E) = \frac{\pi\hbar^2}{2mE}\sum_{l=0}^{+\infty}(2l+1)T_l P_l.}$$

- Penetrability in WKB-approximation:

$$T_{WKB} = \exp\left\{-2\int_{R_{\text{tp},2}}^{R_{\text{tp},3}}\sqrt{\frac{2m}{\hbar^2}\left(Q_p - V(r)\right)}dr\right\}$$

Here, E is kinetic energy of relative motion of two nuclei in lab. frame, E_1 is kinetic energy of relative motion of two nuclei in the center-of-mass frame (we use $E = E_1$), m is reduced mass of two nuclei, P_l is probability of fusion of two nuclei, T_l is penetrability of barrier.

- Penetrability and reflection for method MR:

$$\boxed{T_{MIR} = \frac{k_1}{k_N}\left|A_T\right|^2, \quad R_{MIR} = \left|A_R\right|^2.}$$

- Test for method MR
- (it is absent in WKB-calc.):

$$T_{MIR} + R_{MIR} + M_{MIR} = 1.$$

- Connection with *S*-factor in astrophysics:

$$\sigma(E) = \frac{S(E)}{E}\times T_{full}.$$

Cross-section of α-capture: method MIR & WKB

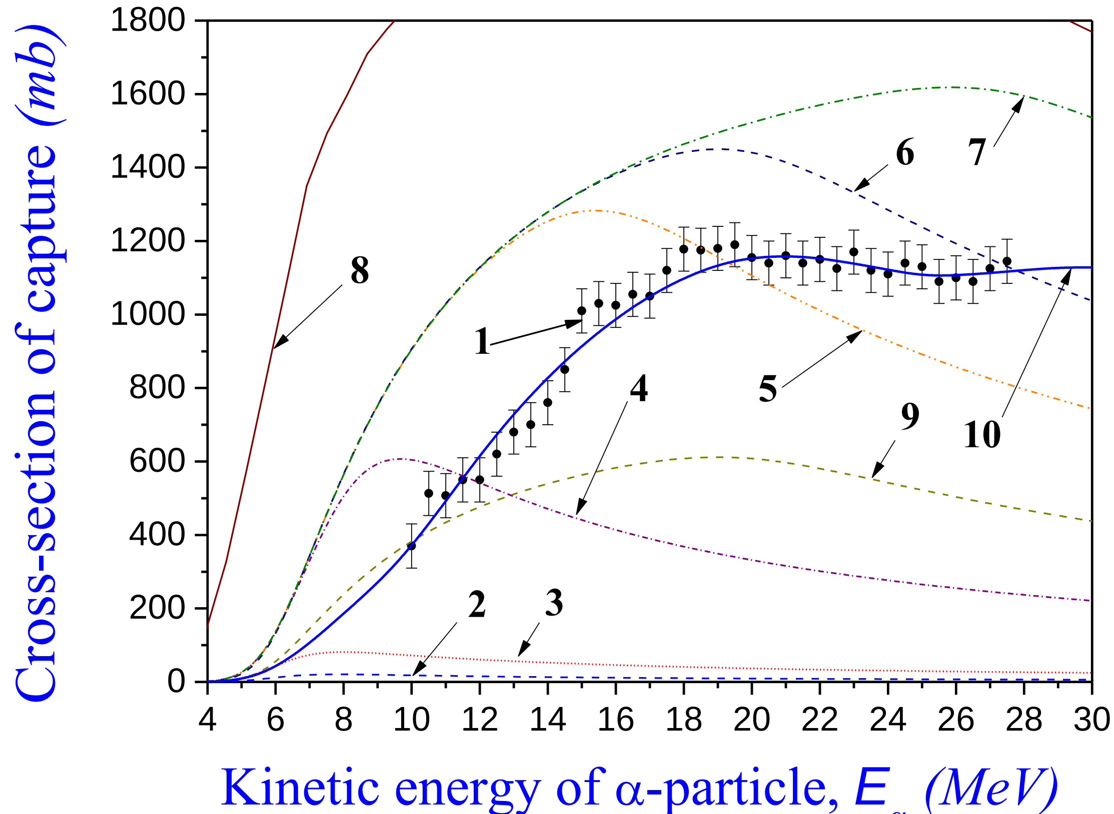


Fig.2. Capture cross-sections of α-particle by nucleus ^{44}Ca, obtained by method MIR (lines 2-7, 9-10) and WKB-approach (line 8). *Line 10 is obtained at inclusion of probabilities of fusion, lines 2-9 are without fusion prob.* [1].

Conclusion: ***Method MIR with included probabilities of fusion (line 10) is in higher agreement with experimental data, than WKB-approach without fusion (line 8).***

Black circles 1 is experimental data, dashed blue line 2 is cross-section at l_{max}=0, short dashed red line 3 is cross-section at l_{max}=1, short dash-dotted purple line 4 is cross-section at l_{max}=5, dash-double dotted orange line 5 is cross-section at l_{max}=10, dashed dark blue line 6 is cross-section at l_{max}=12, dash-dotted green line 7 is cross-section at l_{max}=15, solid brown line 8 is cross-section at l_{max}=20, dashed dark yellow line 9 is renormalized cross-section at l_{max}=17, solid blue line 10 is cross-section at l_{max}=17.

- Cross-section of capture:

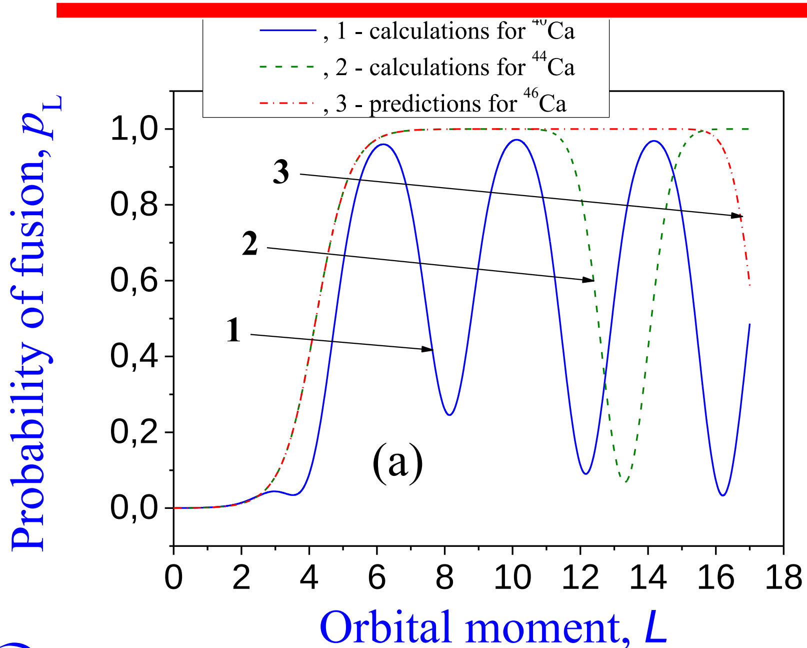
$$\sigma_{\mathrm{capture}}(E) = \frac{\pi \hbar^2}{2mE} \sum_{l=0}^{l_{\max}} (2l+1) T_l P_l .$$

Here, E is kinetic energy of α-particle in lab. frame, E_1 is kinetic energy of relative motion of α-particle and nucleus, m is reduced mass of α-particle and nucleus, P_l is probability of fusion of α-particle and nucleus, T_l is penetrability of barrier.

- Test of method: $T_{MIR} + R_{MIR} = 1.$

[1] Maydanyuk S. P., Zhang P.-M., et al. Nucl. Phys. **A940,** 89-118 (2015).

Formula for probability of fusion



Using fitting procedure, we found probabilities of fusion and described them as

$$\sigma_{capture}(E) = \frac{\pi \hbar^2}{2mE} \sum_{l=0}^{+\infty} (2l+1) T_l P_l .$$

$$p_{full}(L) = 1 - p_1(L) - p_2(L),$$

$$p_1(L) = \frac{c_1}{1 + \exp\left[\dfrac{(L - c_2)}{c_3}\right]}, \quad p_2(L) = f_2(L) \cdot \sum_{n=1} \exp\left\{ - \frac{(L - n \cdot \Delta)^2}{c_{4n}} \right\},$$

$$f_2(L) = 1 - \exp\{-c_5 \cdot (L - c_6)\}, \ \Delta = a \cdot (N - N_{magic}) + b,$$

$$a = 2.31, \quad b = 4.05, \quad c_1 = 1, \quad c_2 = 4.2, \quad c_3 = 0.5.$$

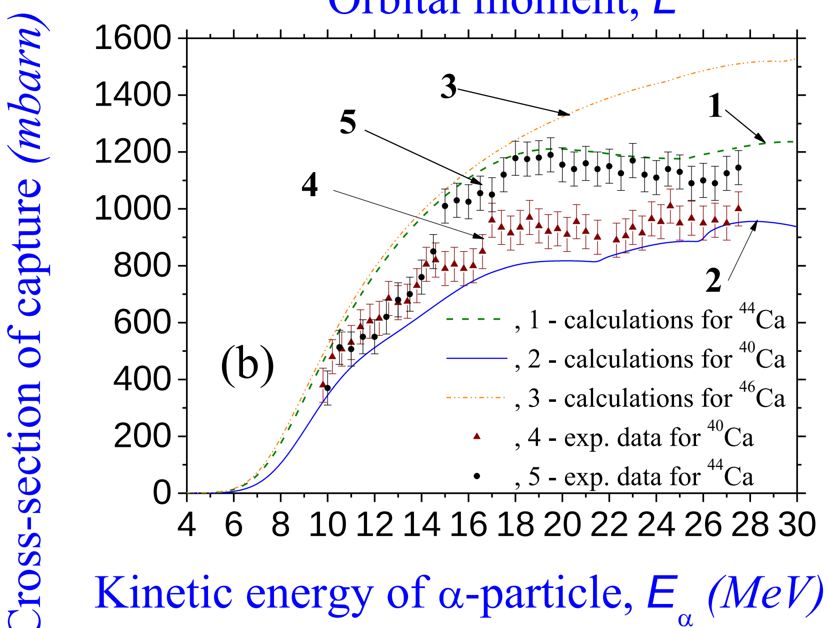


Fig.7. Probabilities of fusion (a) calculated by formulas above and cross-sections (b) for capture of α-particles by ^{40}Ca, ^{44}Ca, ^{46}Ca, obtained by method MIR [1].

[1] Maydanyuk S. P., Zhang P.-M., Belchikov S. V. Nucl. Phys. A. - 2015. - Vol. 940. - P. 89-118.

New quasi-bound states in scattering

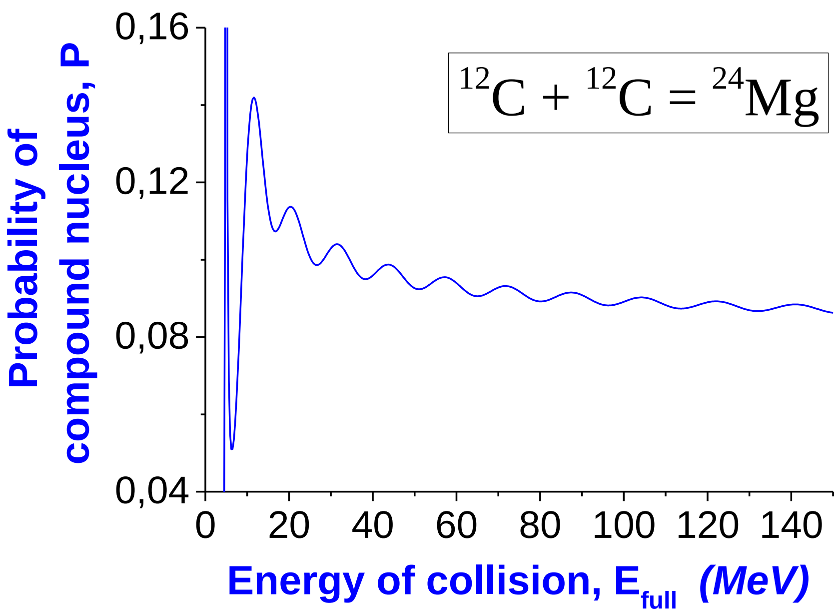
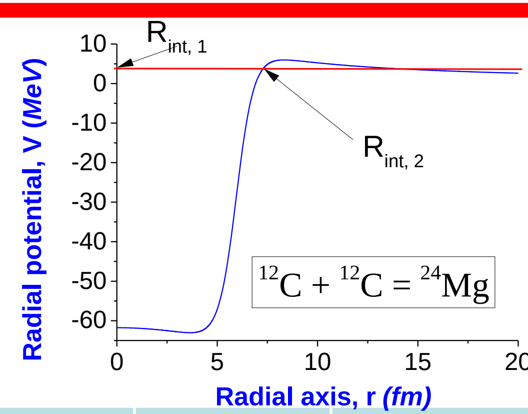


Fig.3. Maximums are clearly visible. These are states of the most probable existence of compound nucleus. We called them as ***quasi-bound states in pycnonuclear reactions***.

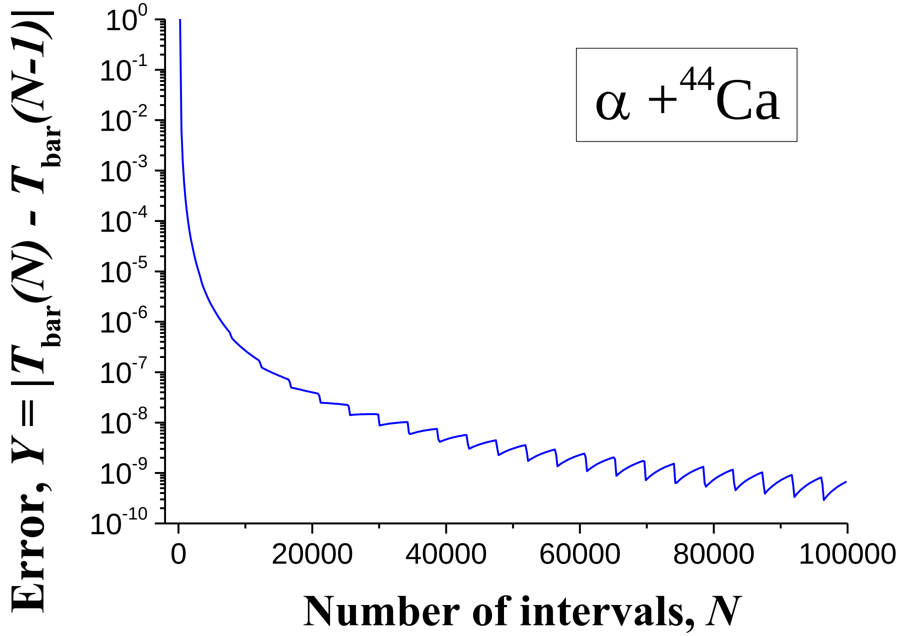


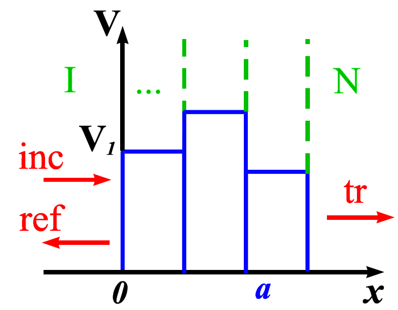
N	E, MeV	P_{cn}	R_{pot}	R_{res}
1	5.0032	0.7805	0.03581	0.6116
2	11.607	0.1419	6.24E-5	0.0038
3	20.313	0.1136	2.07E-6	2.25E-5
4	31.420	0.1040	2.31E-7	1.92E-6
5	43.729	0.0987	4.99E-8	1.71E-8
6	57.238	0.0954	1.57E-8	3.23E-8
7	71.647	0.0931	5.70E-9	3.75E-9

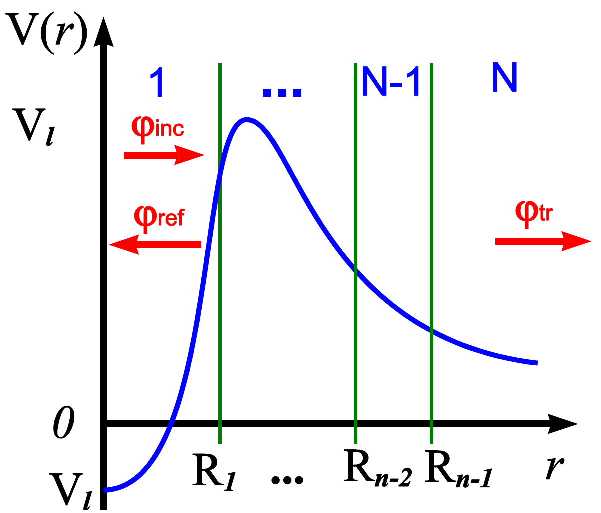
Probability of existence of compound nucleus:

$$P_{\rm cn}(E) = \int\limits_{r_{\rm int,1}}^{r_{\rm int,2}} |\chi(r)|^2 dr = \sum_{j=1}^{n} \left\{ \left(|\alpha_j|^2 + |\beta_j|^2 \right) \Delta r + \frac{\alpha_j \beta_j^*}{2ik_j} e^{2ik_j r} \Big|_{r_{j-1}}^{r_j} + c.c. \right\}.$$

Accuracy of MIR method in capture task







Test of method:

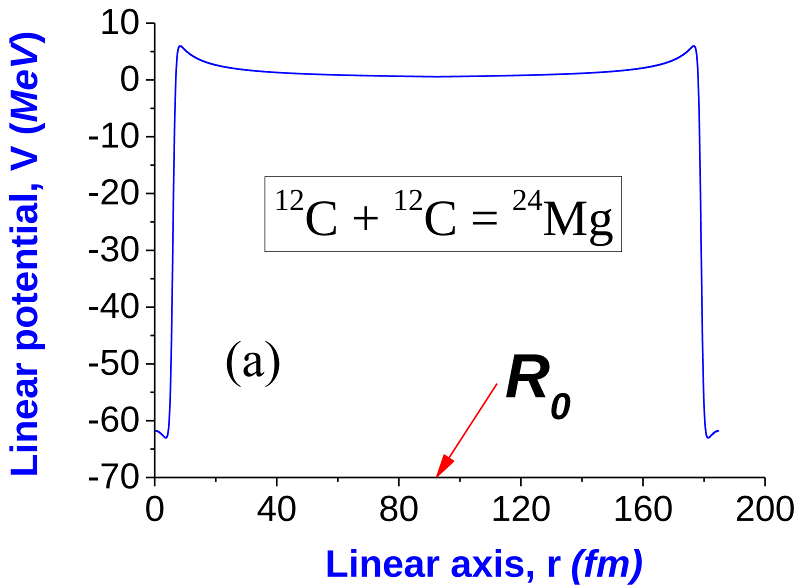
$$T_{\text{bar}} + R_{\text{bar}} = 1.$$

Accuracy of method:

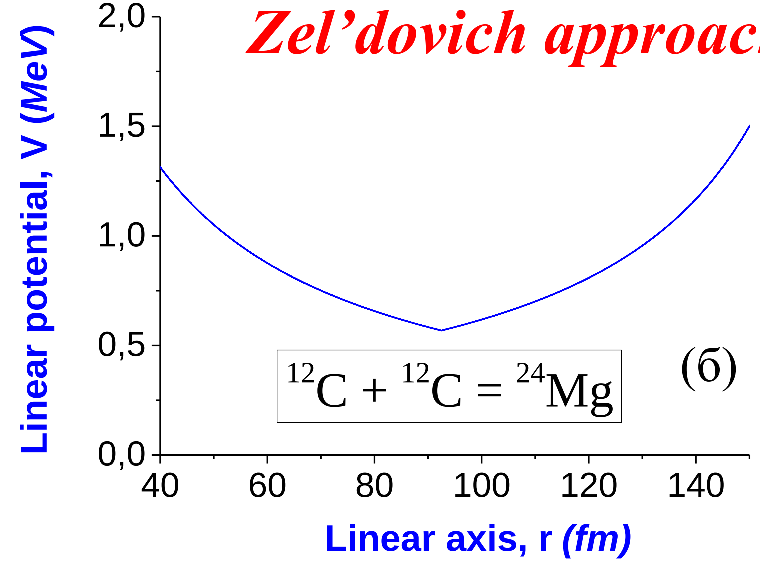
- Our method of Mult. Int. Refl.: 10^{-15} ;
- WKB-method (semiclassical, 1 order): 10^{-3}.

Energy levels of zero-point vibrations (1)

Our method:



Zel'dovich approach:



$$E_0 = \frac{\hbar w}{2} = \frac{\hbar Z e}{\sqrt{m R_0^3}},$$

$$\Delta E = \frac{2Z^2 e^2}{R_0}, \quad E_{full} = E_0 + \Delta E.$$

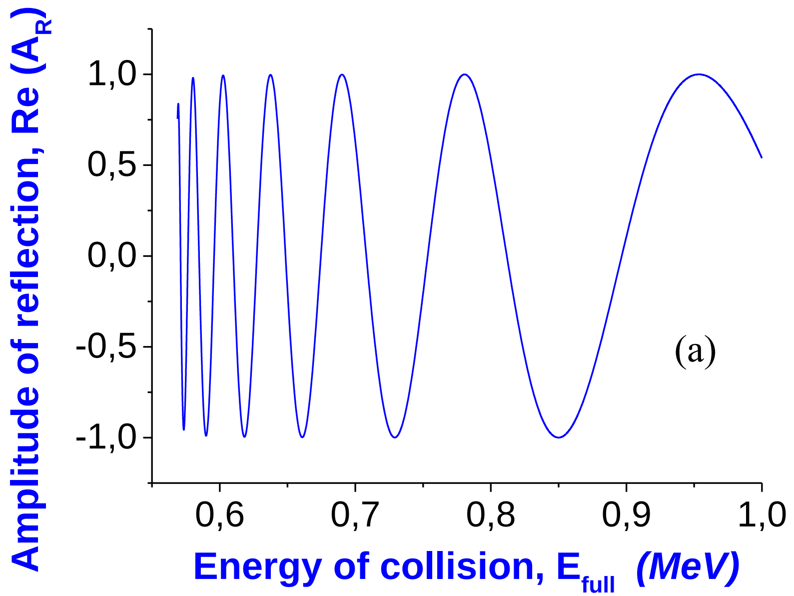
Determination of energy levels:

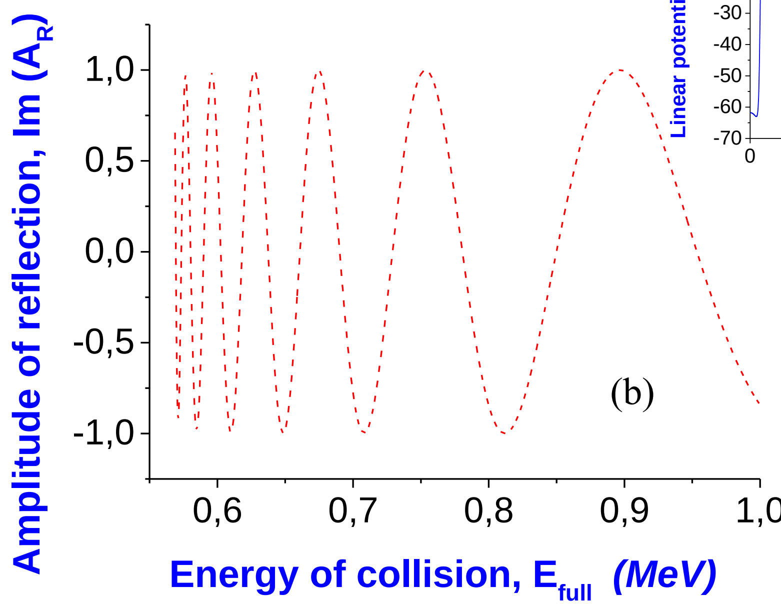
Using method MR, energy levels are calculated, where modulus of WF is minimal or maximal at point R_0 .

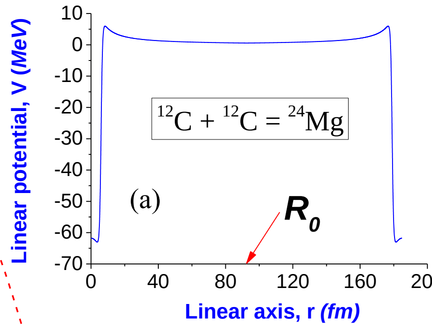
$$R_0 = 92.4\, fm.$$

$$E_0 = 0.021 MeV,$$
$$\Delta E = 0.567 MeV,$$
$$E_{full} = 0.589 MeV.$$

Energy levels of zero-point vibrations (2)







Condition for determination of states:

$$\text{even states:} \quad \chi(R_0) = e^{-ikR_0} + A_R e^{ikR_0} = e^{-ikR_0} + e^{ikR_0}, \quad A_R = +1,$$

$$\text{odd states:} \quad \chi(R_0) = e^{-ikR_0} + A_R e^{ikR_0} = e^{-ikR_0} - e^{ikR_0}, \quad A_R = -1.$$

$$\boxed{\begin{gathered} \mathrm{Re}(A_R) = \pm 1, \\ \mathrm{Im}(A_R) = 0. \end{gathered}}$$

Idea of determination of levels: Using method MR, energy levels are determined, where condition of amplitude A_R at point R_0 is fulfilled.

Energy levels of zero-point vibrations (3)

No.	Energy, MeV	Amplitude AR, Re	Amplitude AR , Im
1	0.569699398797595	0.933197319275621	-0.359364387908423
2	0.574108216432866	-0.929937621506901	0.367717310044127
3	0.580280561122244	0.999976682784241	-0.006828900923611
4	0.589979959919840	-0.999804559327251	0.019769753373290
5	0.603206412825651	0.987566383351778	-0[illegible]
6	0.619078156312625	-0.987872204000573	0.155269148780593
7	0.637595190380762	0.999675512392435	-0.025472925291808
8	0.661402805611222	-0.997827712405446	0.065877586140615
9	0.690501002004008	0.999520247643956	-0.030972157654334
10	0.729298597194389	-0.999921682875423	0.012515115484128
11	0.781322645290581	0.999300653371264	-0.037392568402883
12	0.850100200400802	-0.999977543965837	0.006701609064401
13	0.954148296593186	0.999861191695802	-0.016661252673514

$$E_0^{(Zel'dovich)} = 0.589 MeV.$$

Error in calculation of amplitudes: $\left| |A_T|^2 + |A_R|^2 - 1 \right| < 10^{-14}.$

Conclusions

1) Rates of pycnonuclear reactions are changed essentially after taking into account nuclear forces (i.e., nuclear potential between nuclei).

2) Quantum study reduces rates of reactions up to 1,8 times. This is explained so: the most probable fusion of the nuclei does not happen after leaving nuclear fragment from the tunnel region, but after further propagation to the middle of the internal potential well.

3) Quantum study of the pycnonuclear reaction requires complete analysis of quantum fluxes in the internal region in the nuclear system. This leads to the appearance of new ***quasibound states,*** there formation of compound nuclear system is the most probable.

4) Reaction in quasibound states is essentially more probable, than at energies of zero-point vibrations studied by Zel'dovich and followers. There is a sense to tell about reaction rates for quasi-bound states, rather than for states of zero-point vibrations in lattice sites. This leads to the changes in estimation of the rates of pycnonuclear reactions in stars.

5) Energy spectrum of zero-point vibrations is revised.

Thank you for attention!