

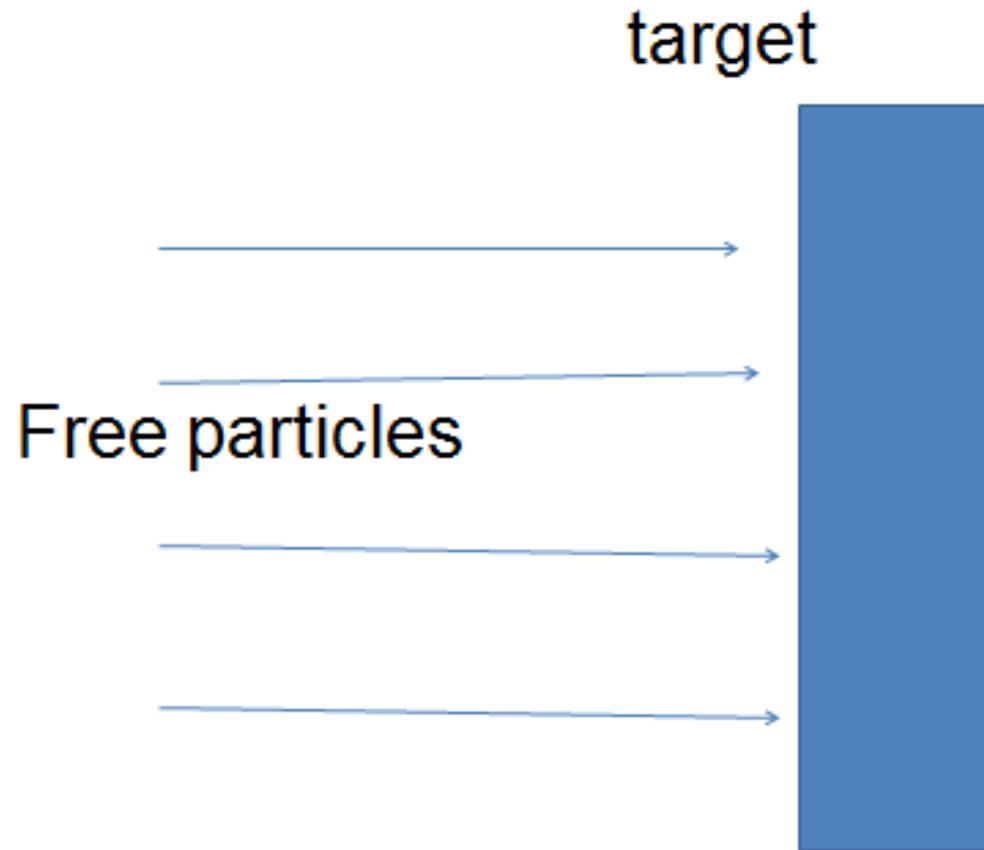
The 7th International Conference
Channeling 2016
Charged & Neutral Particles Channeling Phenomena

Spontaneous Breaking of Symmetry in Problem of Spatial Localization of Particle Moving in a Solid

G.M. Filippov

Chuvash State Pedagogical University, Cheboksary, RF
aLab of bio-nanotechnology, ChSAG Academy, Cheboksary,

RF



Free wave packet wave function

$$|\chi_0\rangle = \sum_{\vec{k}} C_{\vec{k}} |\vec{k}\rangle$$

For a Gauss wave packet

$$\chi_0(\vec{x}, t) = \frac{1}{\left(2\pi(\delta_0^2 + t^2/4m^2\delta_0^2)\right)^{3/4}} \exp\left\{-\frac{(\vec{x} - t\vec{k}_0/m)^2}{4\delta_0^2 + 2it/m} + i(\vec{k}_0\vec{x} - k_0^2 t/2m)\right\}$$

Free wave packet density matrix

Free particle DM (Gauss case)

$$\Gamma_0(\vec{x}_1, \vec{x}_2, t) = \chi_0^*(\vec{x}_1, t) \chi_0(\vec{x}_2, t)$$

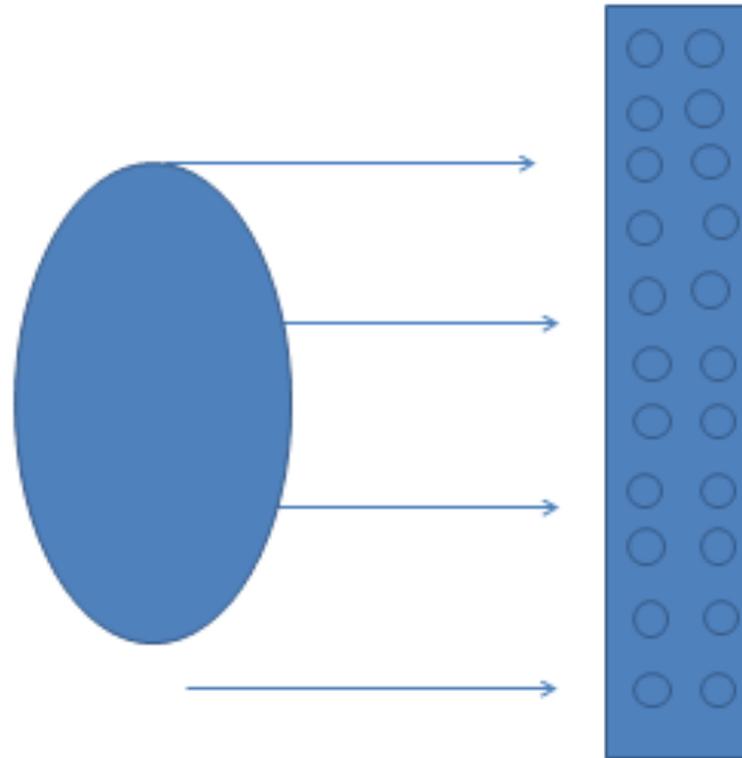
$$\delta(t) = \sqrt{\delta_0^2 + 4t^2 / m^2 \delta_0^2}, \quad t = L/v$$

In our case, as a rule, $\delta_{\min} = \sqrt{L/k} \sim 1 \div 10 \text{ nm}$

The falling of wave packet on film

CHANNELING & ION IMPLANTATION

THEORY: Lindhard, Kagan & Kononetz,



The projectile is moving in a solid

Basic equations

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}} :$$

$$\hat{H}_0 = \int \hat{\psi}^\dagger(\vec{x}) \left(-\frac{\nabla^2}{2M} \right) \hat{\psi}(\vec{x}) dV + \sum_{\alpha, \vec{q}} \omega_\alpha(\vec{q}) \hat{b}_{\alpha\vec{q}}^\dagger \hat{b}_{\alpha\vec{q}} :$$

$$\hat{H}_{\text{int}} = Z \int \hat{\psi}^\dagger(\vec{x}) \hat{\psi}(\vec{x}) \hat{\phi}(\vec{x}) dV ,$$

potential-operator of the electric field, created by quasi-particles

$$\hat{\phi}(\vec{x}) = \sum_{\alpha, \vec{q}} g_{\alpha\vec{q}} \left(\hat{b}_{\alpha\vec{q}} e^{i\vec{q}\vec{x}} + \hat{b}_{\alpha\vec{q}}^\dagger e^{-i\vec{q}\vec{x}} \right)$$

“Individualization” in a mixed state (we haven't a particle's wave function, only DM)

Von Neumann: decomposition for the DM on “pure” states

$$\Gamma(\vec{x}, \vec{x}', t) = \sum_n W_n \psi_n^*(\vec{x}, t) \psi_n(\vec{x}', t) \quad \sum_n W_n = 1$$

Equation for finding the “pure” wave functions in
von Neumann's case: ambiguity in a case of
degenerative eigenvalue problem

$$W_n^{-1} \int \psi_n(x, t) \Gamma(x, y, t) dx = \psi_n(y, t)$$

Wave packet dynamics in homogeneous medium

$$\Gamma_0(\vec{x}_1, \vec{x}_2, t) = \Gamma_0(\vec{x}_1 - \vec{x}_2, t)$$

DM decomposition, different decompositions (degenerative eigenvalues):

1. $\Gamma_0(\vec{x}_1, \vec{x}_2, t) = \Gamma_0(\vec{x}, t) = \int \frac{d^3 k}{(2\pi)^3} \Gamma_0(\vec{k}, t) e^{i\vec{k}(\vec{x}_1 - \vec{x}_2)}$
2. $\Gamma_0(\vec{x}_1 - \vec{x}_2, t) = \int \varphi^*(\vec{x}_1 - \vec{a}, t) \varphi(\vec{x}_2 - \vec{a}, t) d^3 a$

Coherence criterion

function of coherence (Glauber, Klauder, Scully ...)

$$\gamma(\vec{r}_1, \vec{r}_2, t) = \frac{\Gamma(\vec{r}_1, \vec{r}_2, t)}{\sqrt{\Gamma(\vec{r}_1, \vec{r}_1, t) \cdot \Gamma(\vec{r}_2, \vec{r}_2, t)}} \quad \tilde{\gamma}_{cv}(\vec{r}, \vec{r}', t) = \frac{2\Gamma(\vec{r}, \vec{r}', t)}{\Gamma(\vec{r}, \vec{r}, t) + \Gamma(\vec{r}', \vec{r}', t)}$$

Condition: it is to preserve the behavior of function of coherence at definition of ψ .

We should use decompositions of type 2 instead of type 1.

Basic considerations

Parts of the wave field find only in a state of mutual coherence, manifest itself as a single unit in all interactions with the surrounding matter. In the result we can obtain a drastic difference between the initial size of the particle's wave field δ in comparison to the coherence length, $l_c \ll \delta$.

Note, this discrepancy seems similar for quantum mechanical treatment of such famous problem as a reduction of wave function of the particle interacted with the system of displaced detectors. In the each of this cases the Nature elects the one outcome among a number of equivalent outcomes randomly. We could consider that the main cause of this result follows from the existence of quantum fluctuations in the total system particle + environment.

This assumption has the more physically obvious example when we obtain the randomly arisen magnetic moment in the spherically symmetric ferromagnetic at lowering its temperature down the Curie point.

Using the above arguments suppose that after the penetration **in the bulk of a solid target the projectile appears in one of spatially localized states having the short coherence length l_c with the central mean point found in one of infinitely large number of positions predicted by the initial size of the wave packet.**

The projectile having the coherence length which size less than the interatomic distance in the solid can produce the wake potential polarization well of such a size that can capture the projectile in the same quantum-mechanical coupling state.

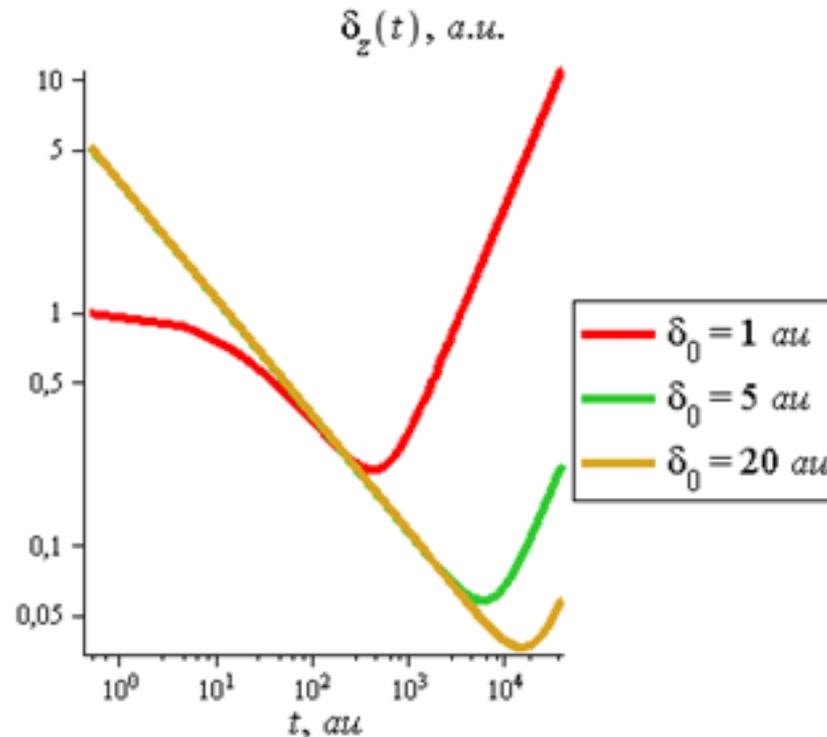
In homogeneous medium broadening of the wave packet simple approximation

$$\Gamma(\bar{x}_1, \bar{x}_2, t) \approx \sum_{\bar{k}_1, \bar{k}_2} C_{\bar{k}_1}^* C_{\bar{k}_2} \exp\left(-i\bar{k}_1 \bar{x}_1 + i\varepsilon_{\bar{k}_1} t + i\bar{k}_2 \bar{x}_2 - i\varepsilon_{\bar{k}_2} t\right) \times \prod_{\beta, \bar{q}} \left(Q_{\beta \bar{q}} \exp\left(i\bar{q}[\bar{x}_1 - \bar{x}_{\bar{k}_1}(t)]\right) \right) \left(Q_{\beta \bar{q}} \exp\left(i\bar{q}[\bar{x}_2 - \bar{x}_{\bar{k}_2}(t)]\right) \right)$$

$$\delta_j(t) = \sqrt{\frac{\delta_0^2 + (1 + 4\Delta^2 k_j \delta_0^2)t^2 / 4\delta_0^2 m^2}{1 + 4\delta_0^2 \Delta^2 k_j}}$$

Among the other peculiarities we see that after exit from a solid the packet width don't follow a free particle behavior. It means the wave packet conserves any information about its previous passage through a solid. We can consider it as a specific memory effect.

Packet width evolution at the quadratic decomposition of the phase



Time evolution of a packet width for proton in Al. Velocity $v=30 \text{ a.u.}$, at different initial widths.

The calculations of density matrix evolution during the passage of the projectile in the bulk of a solid show two different mechanisms which leads to the spatial localization:

- 1) the possibility to forming the sufficiently strong polarization field, and
- 2) the destructing of phase correlations between spatially remote parts of the projectile's wave field. At the beginning of the interaction between the projectile and the solid the second factor seems more important.

A polarization field approximation

$$i \frac{\partial \varphi(\vec{x}, t)}{\partial t} = \left\{ -\frac{\nabla^2}{2M} + Z^2 \sum_{\beta, \vec{q}} g_{\beta \vec{q}}^2 \int d^3 \xi \int_0^\infty d\tau \sin(q(x - \xi)) \varphi^*(\vec{\xi}, t - \tau) \varphi(\vec{\xi}, t - \tau) \right\} \varphi(\vec{x}, t)$$

where the nonlinearity and the retardation
are the feedback effect of the localized projectile
on the environment.

Solutions to this equation show the existent of more

Than one coupling state of the projectile in the own
polarization field (polaron effect)

More correct calculation of the density matrix within the modified PT

$$\Gamma(\vec{x}_1, \vec{x}_2, t) = \frac{1}{\Omega} \left(\frac{m}{2\pi t} \right)^3 \exp \left\{ -i \frac{m}{t} \vec{x} \vec{X} - 2\delta_0^2 \left(\frac{m}{2t} \right)^2 x^2 \right\} \int d^3 y \exp \left\{ -\frac{y^2}{8\delta_0^2} - 2\delta_0^2 \left(\frac{m}{2t} \right)^2 (y^2 - 2\vec{y}\vec{x}) \right\} \times$$

$$\exp \left\{ i \frac{m}{t} \vec{y} \left(\vec{X} - \frac{\vec{k}_0 t}{m} \right) \right\} \exp \left\{ -\sum_{\beta, \vec{q}} |Q_{\beta\vec{q}}(t)|^2 \left(1 - J_0(q_\perp y_\perp) e^{iq_z y_z} \right) \right\}$$

integration over y_z should be estimated with the help of the saddle-point method

$$-\left(\frac{1}{4\delta_0^2} + 4\delta_0^2 \left(\frac{m}{2t} \right)^2 \right) \xi + 4\delta_0^2 \left(\frac{m}{2t} \right)^2 x_z - \sum_{\beta, \vec{q}} |Q_{\beta\vec{q}}(t)|^2 q_z J_0(q_\perp y_\perp) e^{-q_z \xi} \sin(q_z \xi) = 0$$

$$-\left(\frac{1}{4\delta_0^2} + 4\delta_0^2 \left(\frac{m}{2t} \right)^2 \right) \xi + \frac{m}{t} \left(X_z - \frac{k_{0z} t}{m} \right) + \sum_{\beta, \vec{q}} |Q_{\beta\vec{q}}(t)|^2 q_z J_0(q_\perp y_\perp) e^{-q_z \xi} \cos(q_z \xi) = 0$$

Model calculation:

Simple one-mode polarization properties of a medium.

$$\varepsilon = 1 - \frac{\omega_0^2}{\omega^2 + \omega_0^2 - \omega_q^2}; \quad \omega_q = \omega_0 + q^2 / 2$$

$$|Q_{\vec{q}}(\vec{x}, t)|^2 = \frac{2\pi\omega_0^2}{q^2\omega_q\Omega} \left| \int_0^t e^{i\omega_q t' - i\vec{q}\vec{x}_0(t')} dt' \right|^2 \approx \frac{2\pi\omega_0^2}{q^2\omega_q\Omega} t \cdot 2\pi\delta(\omega_q - q_z v)$$

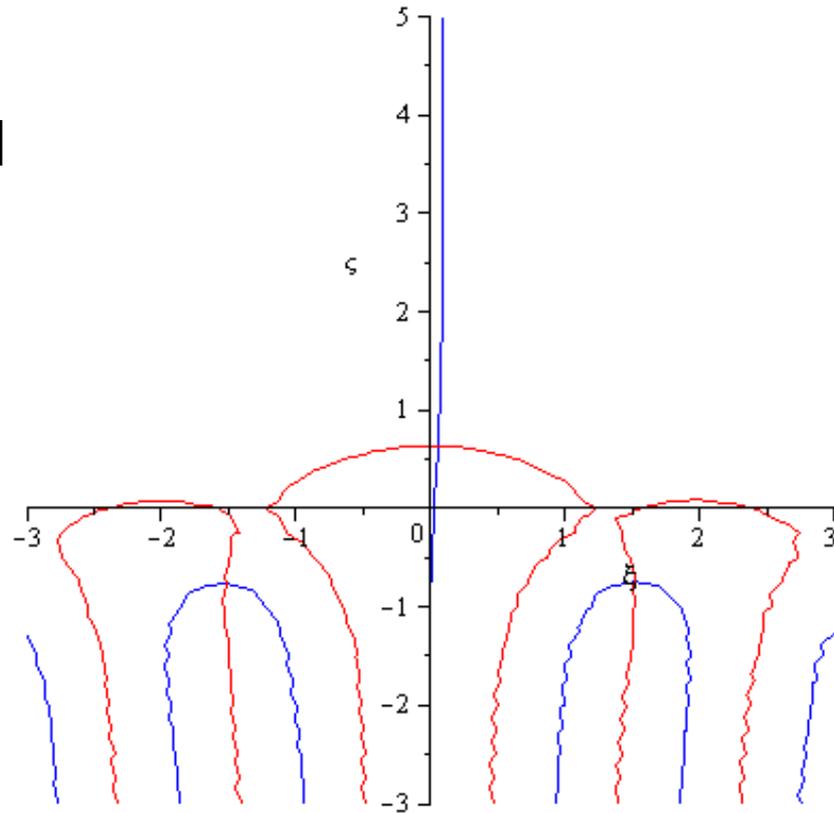
$$v := 2 : rs := 2.075 : w0 := \sqrt{\frac{3}{rs^3}} : wq := w0 + \frac{q^2}{2} : t$$

$$:= 1000 : \delta := 10 : m := 2000 : k0 := m \cdot v : qp := v + \sqrt{v^2 - 2 \cdot w0}$$

$$- 2 \cdot w0) : qm := v - \sqrt{v^2 - 2 \cdot w0} : Xb := v \cdot t : x := 0.1 : y$$

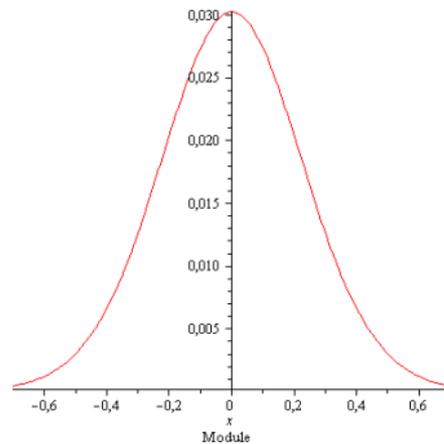
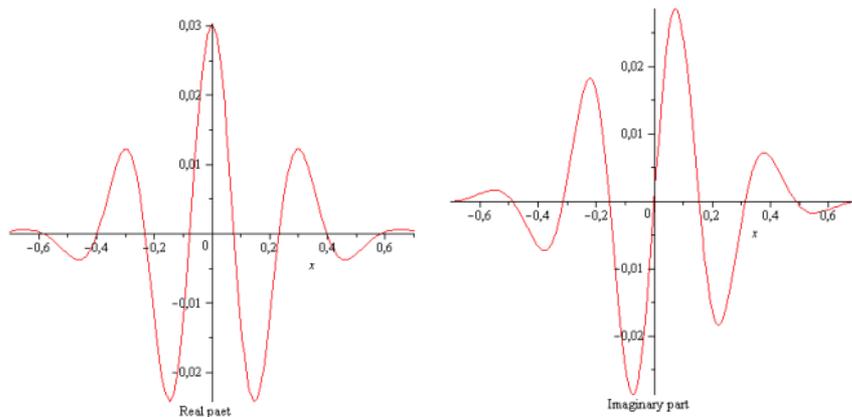
$$:= 0.1 :$$

saddle-point method

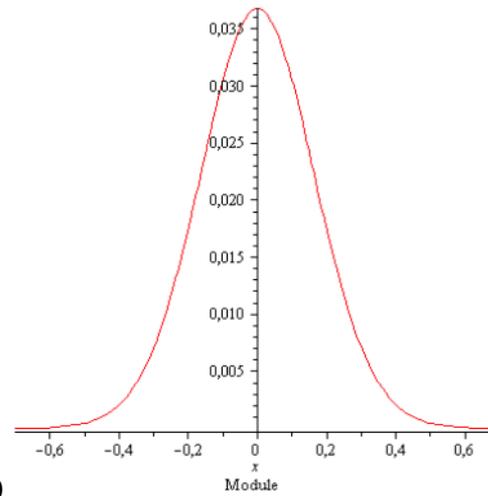
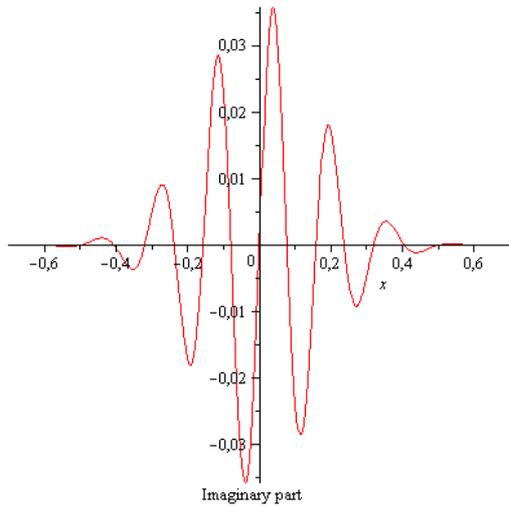


wave packet evolution in the target and beyond

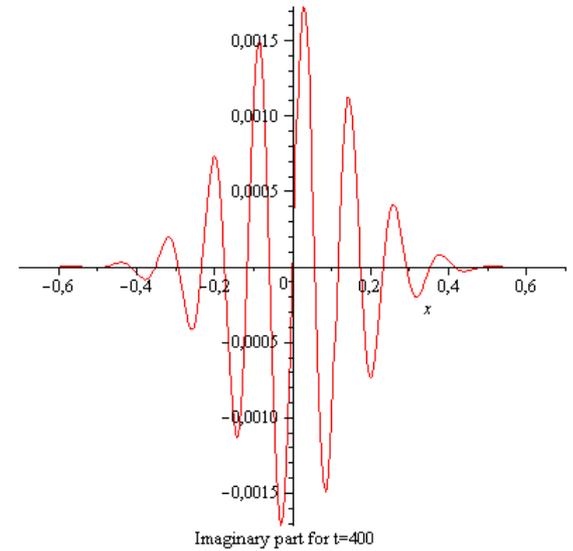
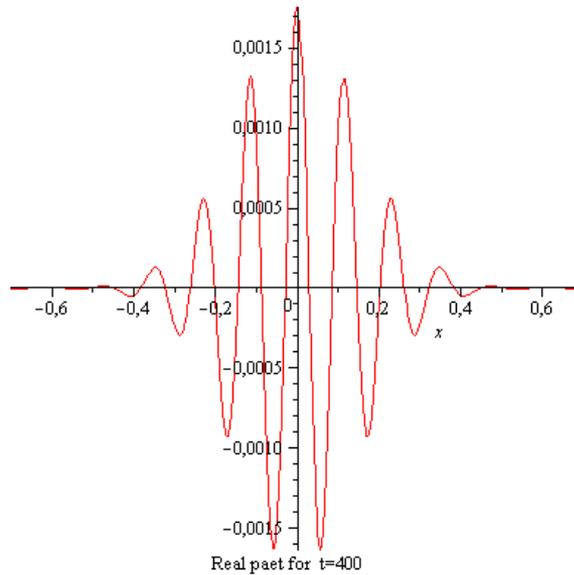
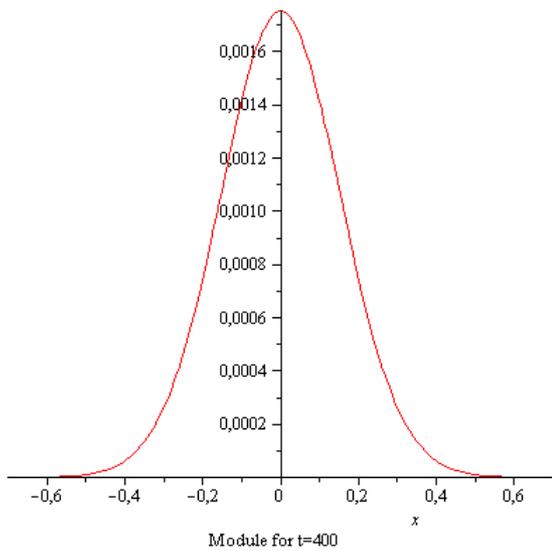
$t_0=300$



The localization phenomenon is seen ($t=100$).



All for $t=200$



CONCLUSION

1. A projectile is impinged from vacuum into a solid film becomes a progressive diminishing of the projectile's coherence length.
2. A special coherence criterion used for to analyse the mixed state of projectile during the interaction with solid film. This approach allows us to get an information about the quantum-mechanical state of the projectile.
3. At performing the individualization procedure we lost a part of information on a system
4. After escaping from a solid film the projectile conserves information about the past interaction with environment

Thank you for the attention