A Monte Carlo technique for the Wigner-Boltzmann equation

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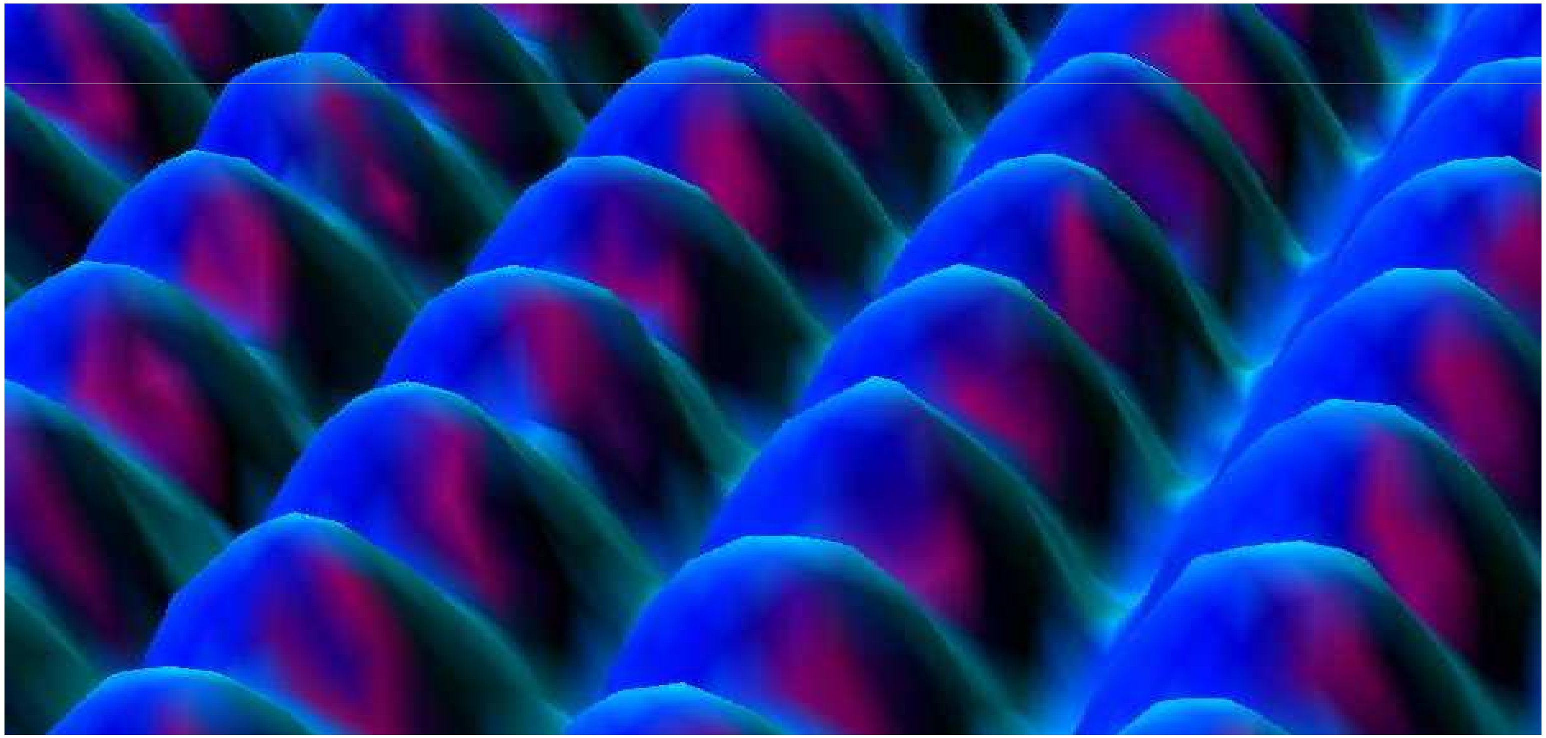
Topics

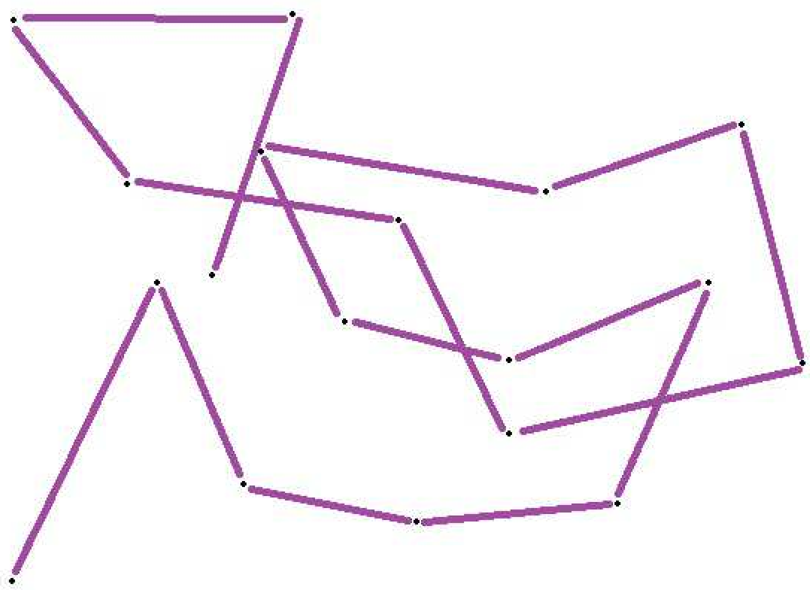
- *What is a semiconductor device? What is the physics involved?*
- *The Wigner-Boltzmann equation*
- *1D Results*
- *2D Preliminary results*

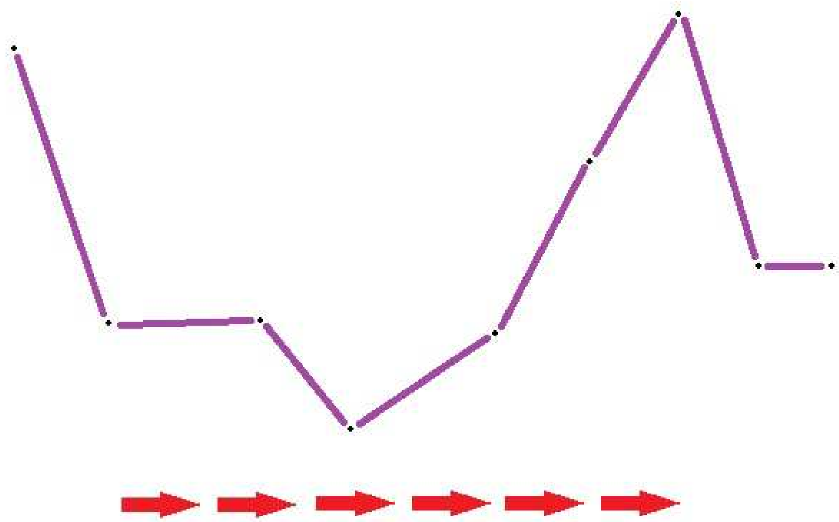
What REALLY is a semiconductor material

- *A semiconductor material, at the atomic level, is simply an highly ordered arrangement of atoms (or molecules) known as lattice.*

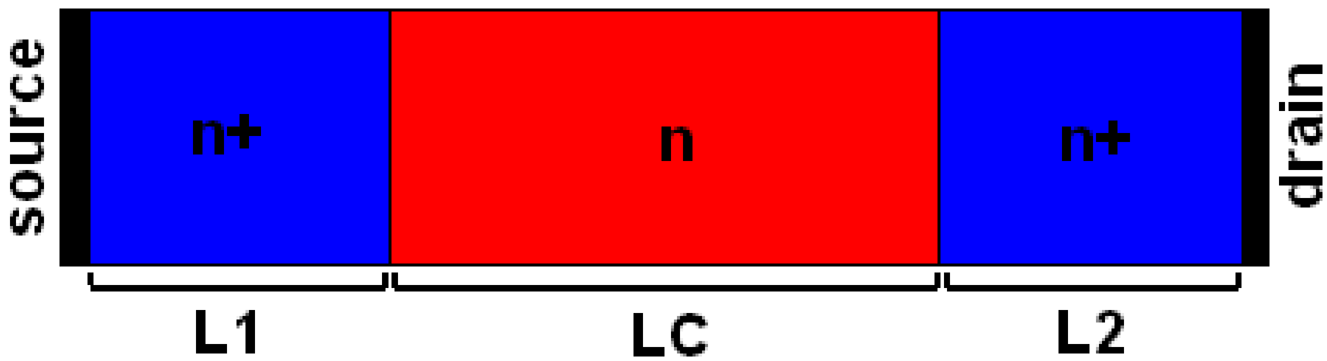


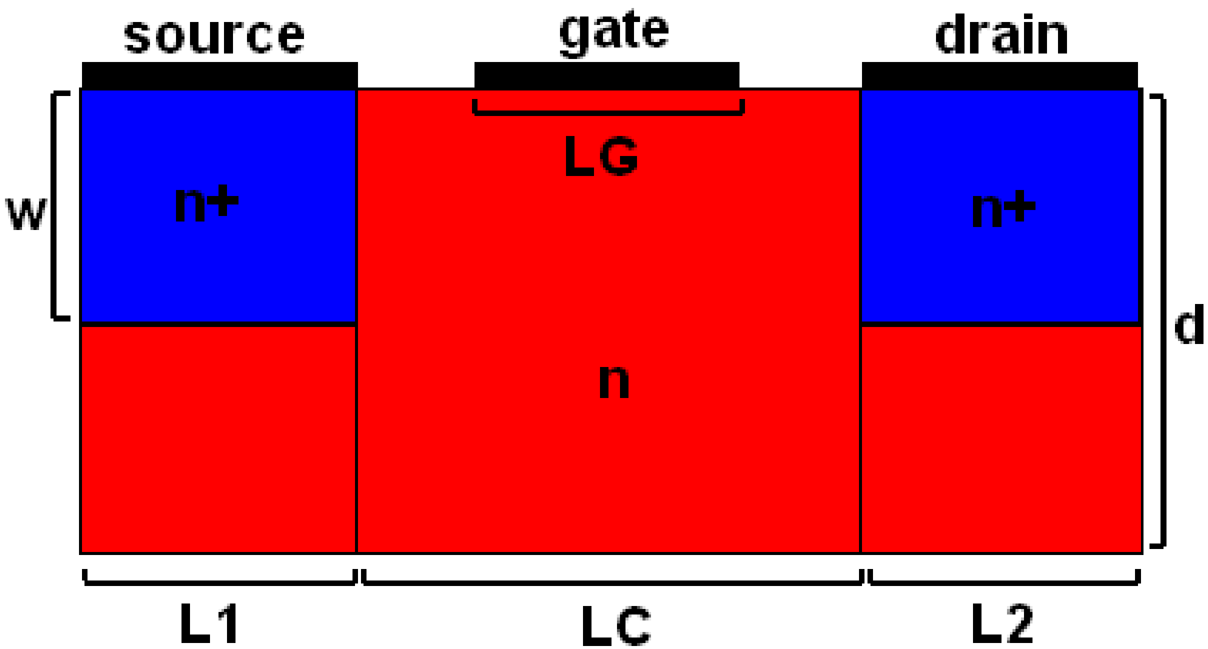
- *An electron moves as a free particle with an effective mass.*
- *An electron scatters with the phonons, the bigger the temperature, the more it scatters.*
- *An electron is subject to an eventually applied electric field.*





Examples of semiconductor devices





The problem of Quantum Effects

- *When device dimensions are reduced, quantum effects start to appear.*

- *Particles can tunnel through barriers, energies are discretized.*

- *The behavior of an electron is more similar to a wave than to a particle.*

The Wigner-Boltzmann equation

- *The equation is recovered by the Wigner equation where the scattering term is the Boltzmann one.*

$$\frac{\partial f_W\left(\vec{r},\vec{k},t\right)}{\partial t}+\frac{1}{\hbar}\nabla_{\vec{k}}\varepsilon\left(\vec{k}\right)\nabla_{\vec{r}}\, f_W\left(\vec{r},\vec{k},t\right)=Qf_W\left(\vec{r},\vec{k},t\right)+\left[\frac{\partial f_W}{\partial t}\right]_{collision}$$

- *where*

$$Qf_W\left(\vec{r},\vec{k}\right)=\int d\vec{k}' V_W\left(\vec{r},\vec{k}-\vec{k}'\right)f_W\left(\vec{r},\vec{k}'\right)$$

$$V_W\left(\vec{r},\vec{k}\right)=\frac{1}{i\hbar(2\pi)^d}\int d\vec{r}'\, e^{-i\vec{k}\cdot\vec{r}'}\left(V\left(\vec{r}+\frac{\vec{r}'}{2}\right)-V\left(\vec{r}-\frac{\vec{r}'}{2}\right)\right)$$

Wigner equation in semi-discrete form

- *Taking into account the fact that a semiconductor device has limited dimensions, it is possible to re-formulate the Wigner equation in a semi-discrete form.*

$$\frac{\partial f_W(\vec{r},M,t)}{\partial t}+\frac{\hbar}{m^*}M\Delta\vec{k}\nabla_{\vec{r}}f_W(\vec{r},M,t)=\sum_{n=-\infty}^{+\infty}V_W(\vec{r},n)f_W(\vec{r},M-n,t)$$

$$V_W(\vec{r},n)=\frac{1}{i\hbar}\frac{1}{L}\int_0^{L/2}d\vec{s}\,e^{-2m\Delta\vec{k}\cdot\vec{s}}\left(V(\vec{r}+\vec{s})-V(\vec{r}-\vec{s})\right)$$

- *The phase space is discretized w.r.t. the pseudo-wave vector coordinates.*

Wigner equation in integral form

- *The semi-discrete Wigner equation can be re-formulated in terms of an integro-differential equation.*

$$f_W(\vec{x},m,t) - e^{-\int_0^t \gamma(\vec{x}(y))dy} f_i(\vec{x}(0),m) =$$

$$\int_0^{\infty} dt' \sum_{m'=-\infty}^{+\infty} f_W(\vec{x}(t'),m',t')\Gamma(\vec{x}',m,m')e^{-\int_{t'}^{t} \gamma(\vec{x}(y))dy}\theta(t-t')\delta(\vec{x}'-\vec{x}(t'))\theta_D(\vec{x}')$$

- *where*

$$\gamma(\vec{x}) = \sum_{m=-\infty}^{+\infty} V_W^+(\vec{x},m) = \sum_{m=-\infty}^{+\infty} V_W^-(\vec{x},m) \qquad \vec{x}(t') = x - \frac{\hbar m \Delta\vec{k}}{m^*}(t-t')$$

$$\Gamma(\vec{x}(t'),m,m') = V_W^+(\vec{x}(t'),m-m') - V_W^+(\vec{x}(t'),m'-m) + \gamma(\vec{x}(t'))\delta_{m,m'}$$

Mean value of a function

- *Finally, using the fact that the adjoint equation of the integro-differential equation is a Fredholm integral equation of second type, one can show that:*

$$\langle A\rangle(\tau)=\int_0^\infty dt\int d\vec{x}\sum_{m=-\infty}^{+\infty} f_W(\vec{x},m,t)A(\vec{x},m)\delta(t-\tau)=\sum_{i=0}^{+\infty}\langle A\rangle_i$$

- *where (for example)*

$$\langle A\rangle_0(\tau)=\int d\vec{x}'\sum_{m'=-\infty}^{+\infty} f_i(\vec{x}_i,m')e^{-\int_0^\tau \gamma(x_i(y))dy}A(x_i(\tau),m')$$

$$\langle A\rangle_1(\tau)=\int_0^\infty dt'\int dx_i\sum_{m'=-\infty}^{+\infty} f_i(\vec{x}_i,m)e^{-\int_0^{t'} \gamma(x_i(y))dy}\theta_D(x_1)\cdot$$

$$\cdot\int_{t'}^\infty dt\sum_{m=-\infty}^{+\infty}\Gamma(x_1,m,m')e^{-\int_{t'}^{t} \gamma(x_1(y))dy}A(x_1(t),m,t)\delta(t-\tau)$$

Physical interpretation of the terms

- *One can give a physical interpretation of the terms <A>$_i$. If one takes the first term of the series:*

$$\langle A\rangle_0(\tau)=\int d\vec{x}'\sum_{m'=-\infty}^{+\infty} f_i(\vec{x}_i,m')e^{-\int_0^\tau \gamma(x_i(y))dy}A(x_i(\tau),m')$$

the interpretation is as follows.

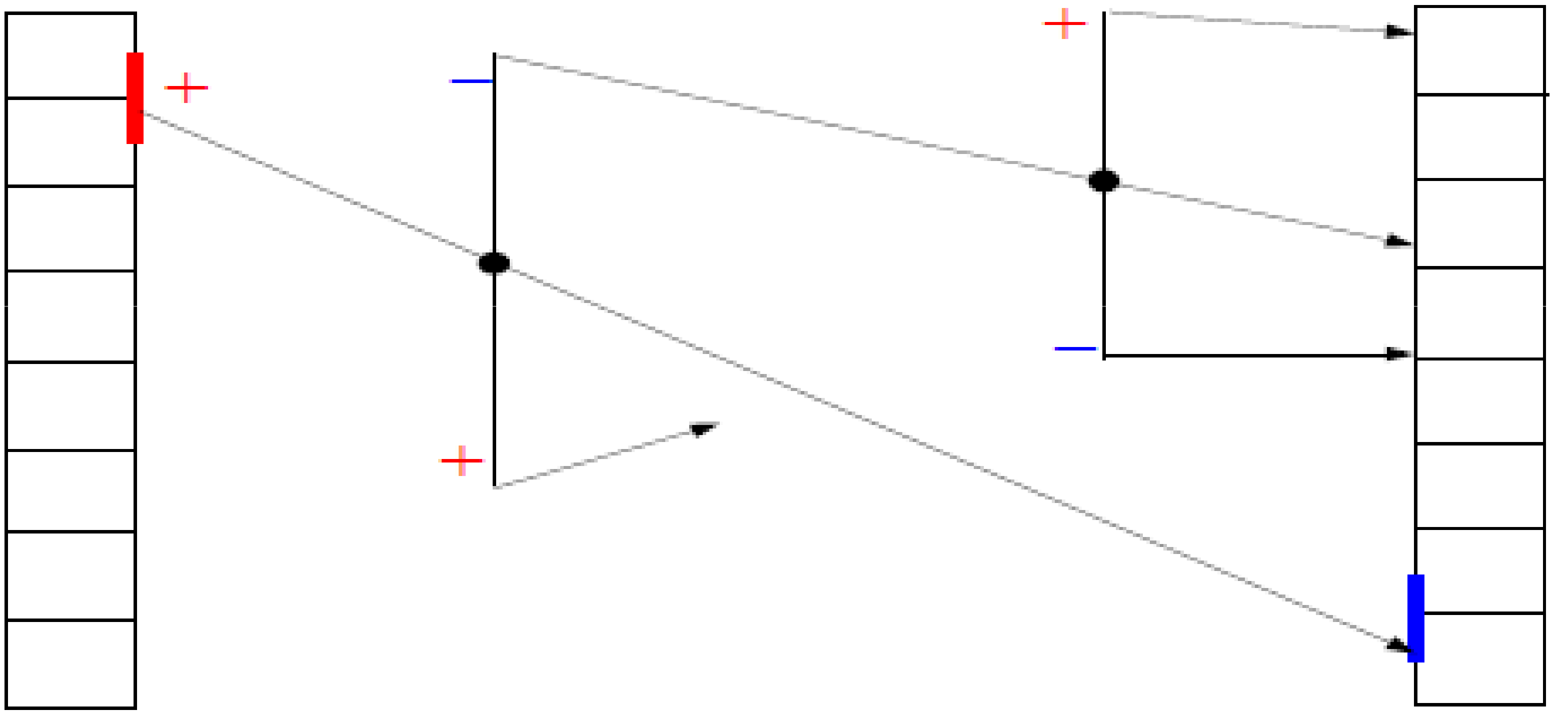
A particle starts at x_i with momentum m'Δk at time 0. The exponent gives the probability that the particle remains on the trajectory, provided that the scattering rate isϒ.

Designing a new Monte Carlo algorithm

- *Consider* $\gamma(\vec{x}) = \sum_{m=-\infty}^{+\infty} V_W^+(\vec{x}, m) = \sum_{m=-\infty}^{+\infty} V_W^-(\vec{x}, m)$ *as a particle generation rate.*

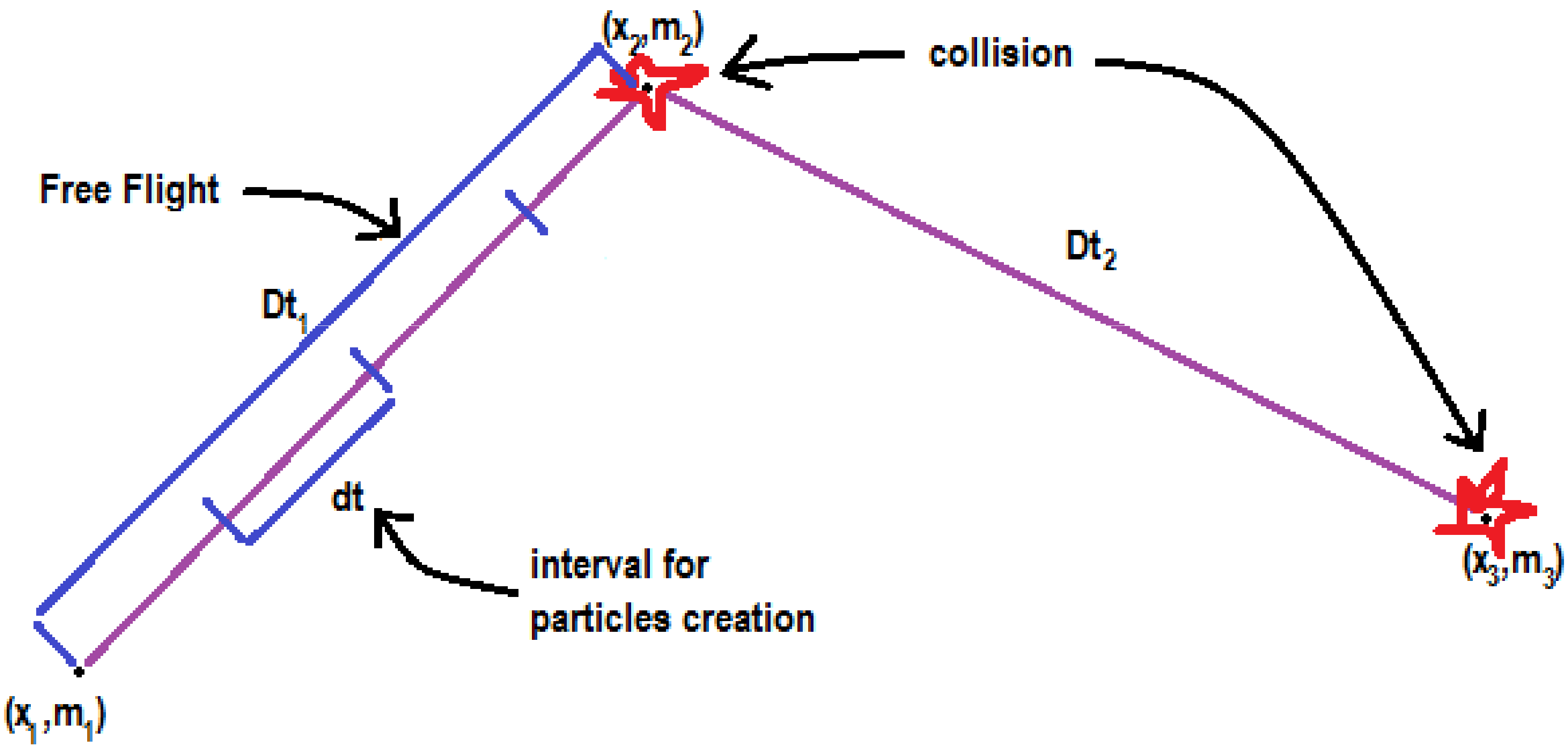
  The Wigner potential gives rise to the creation of two particles, one positive and one negative, and the sign carries the quantum information.

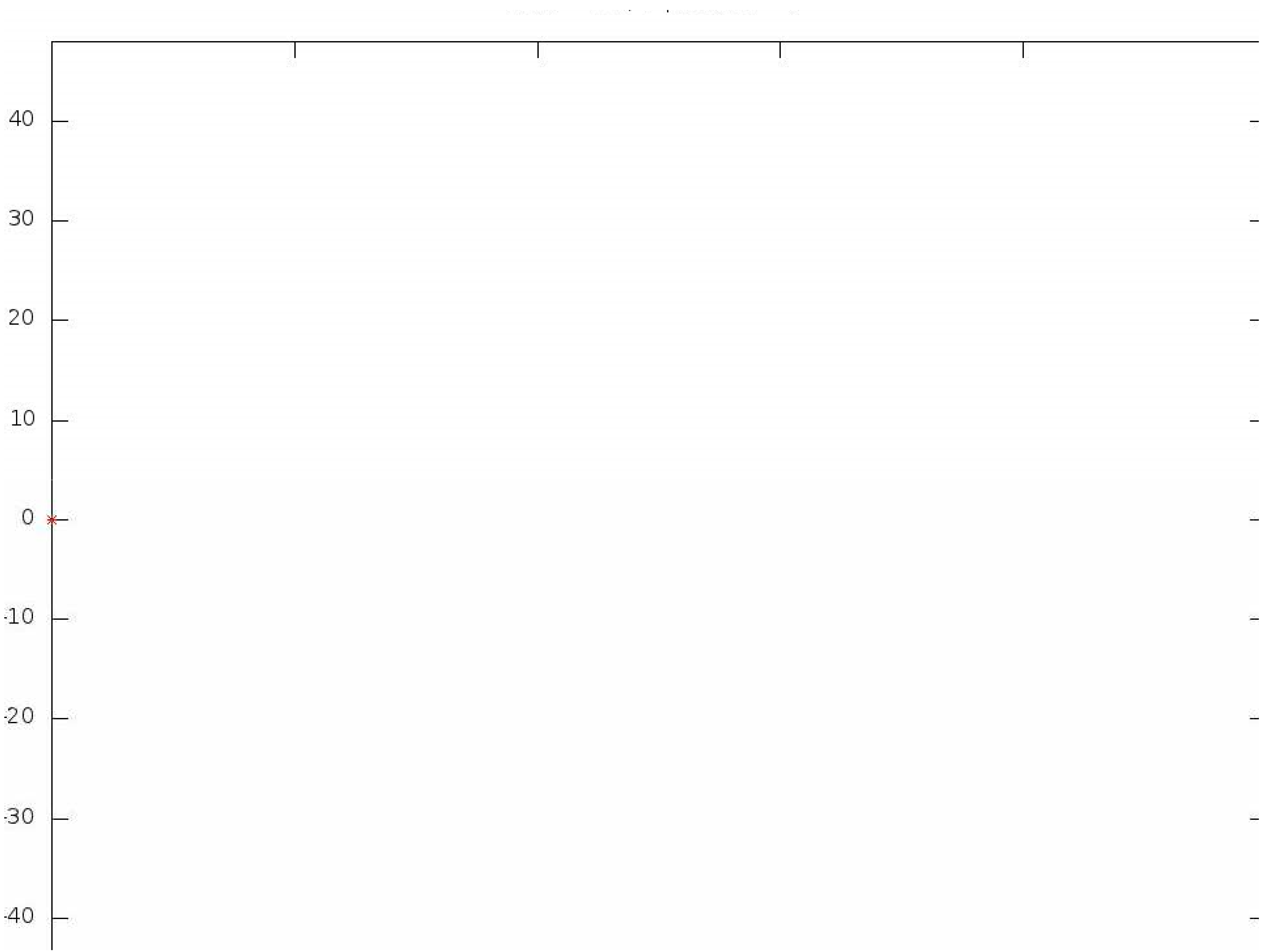
The new algorithm, visually

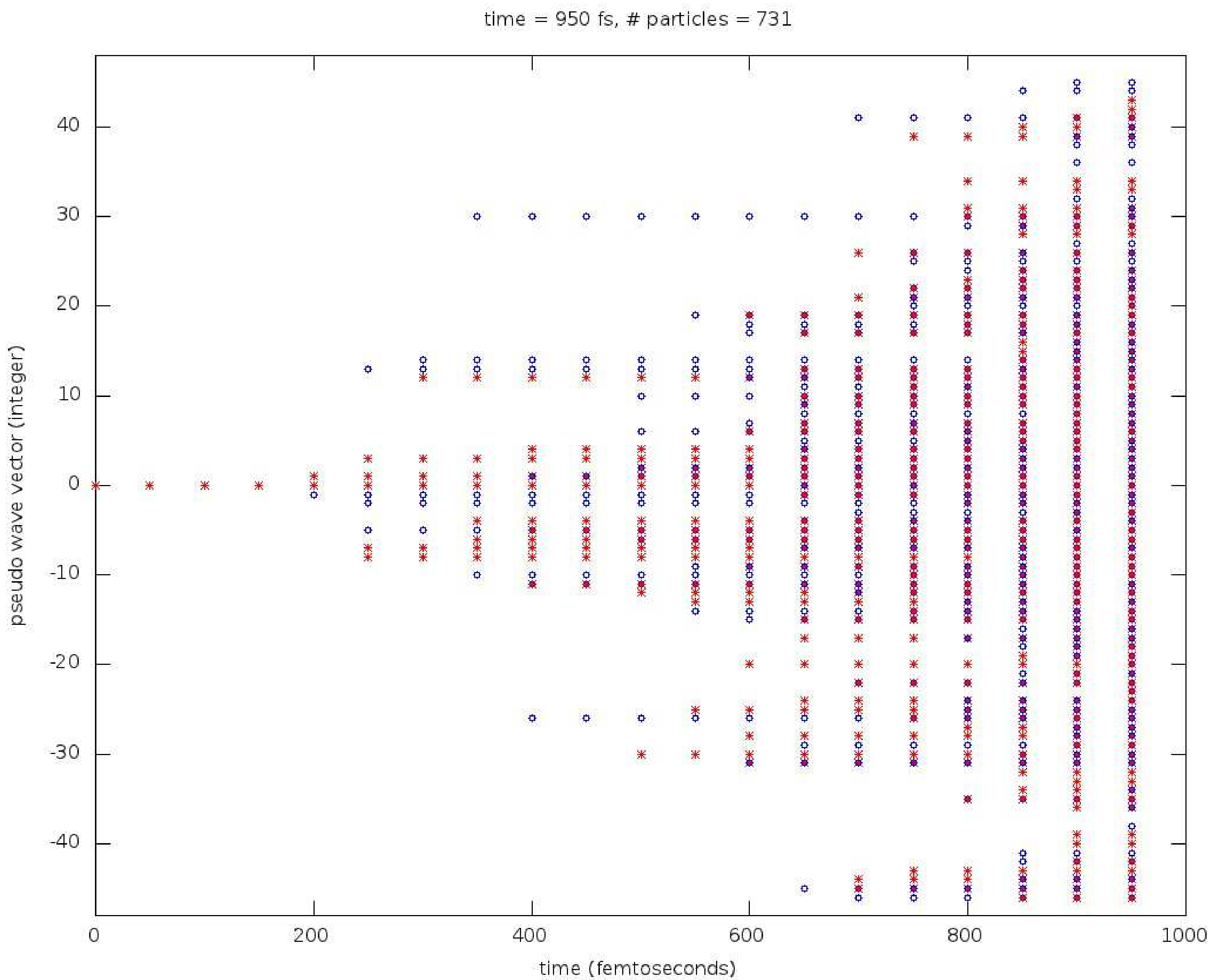


Dt=0.1fs
dt=0.01fs

Wigner, an intuitive picture




40
30
20
10
0
-10
-20
-30
-40

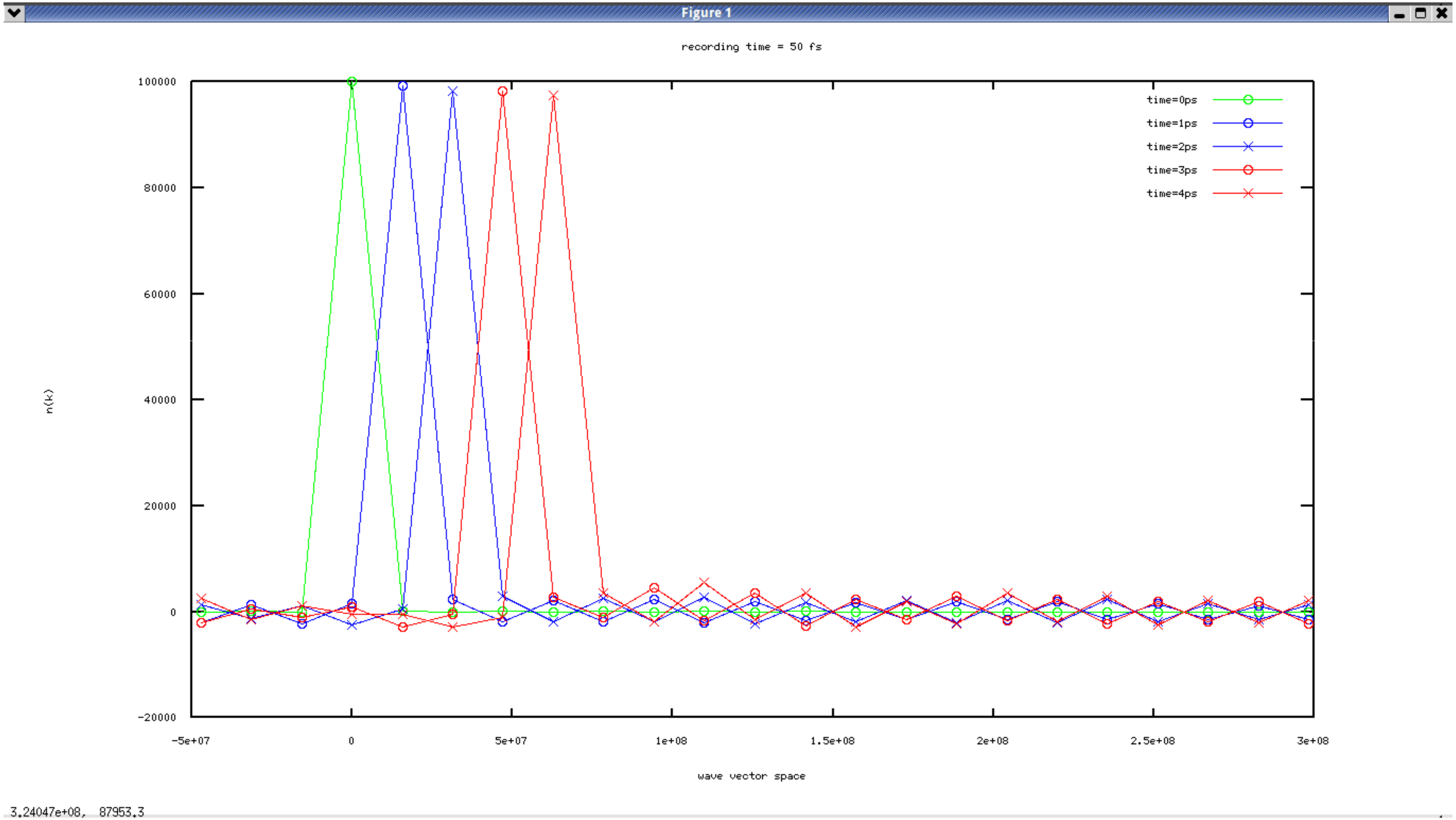


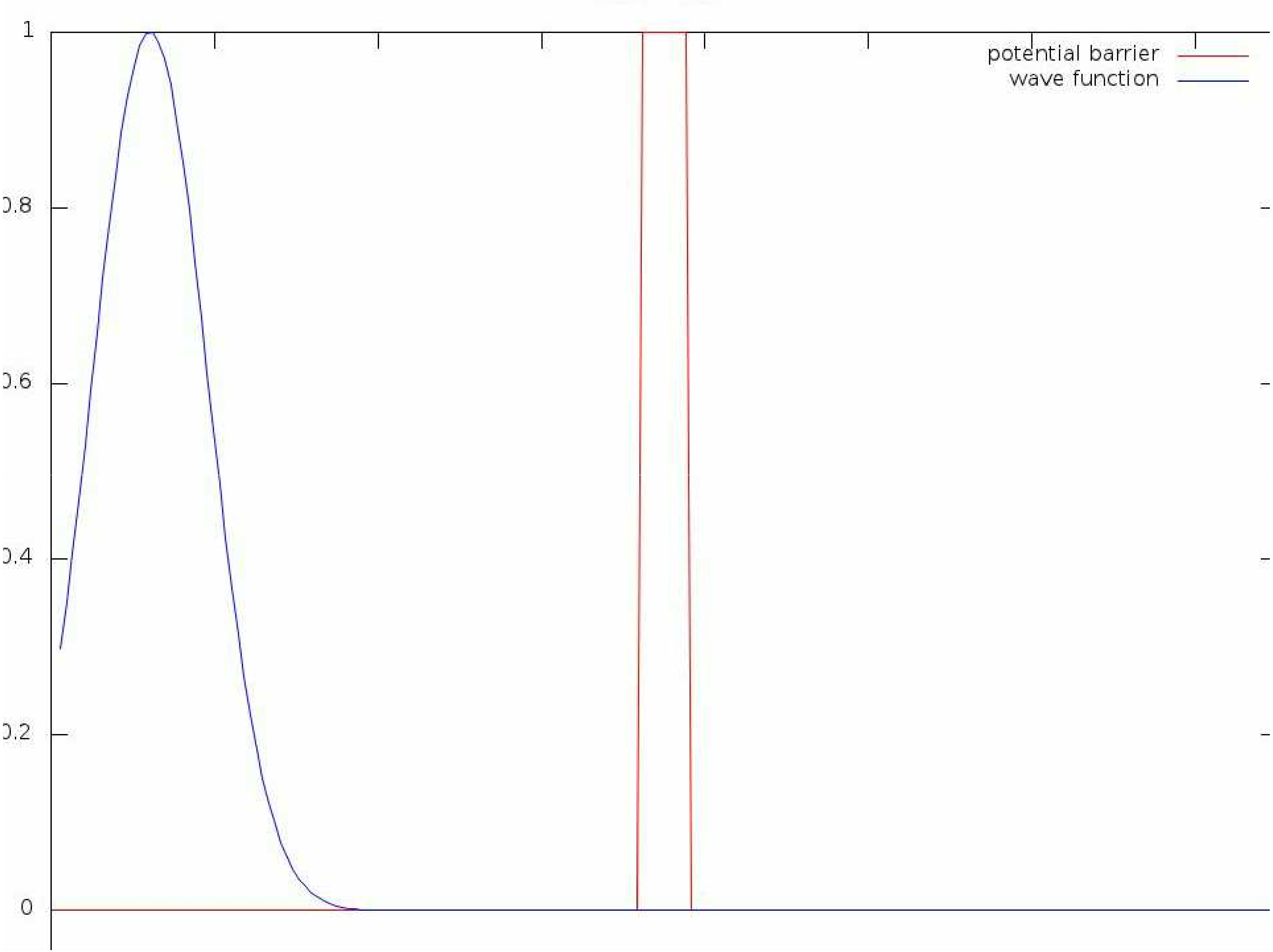
time = 950 fs, # particles = 731
pseudo wave vector (integer)
time (femtoseconds)
40
30
20
10
0
-10
-20
-30
-40
0
200
400
600
800
1000

Results

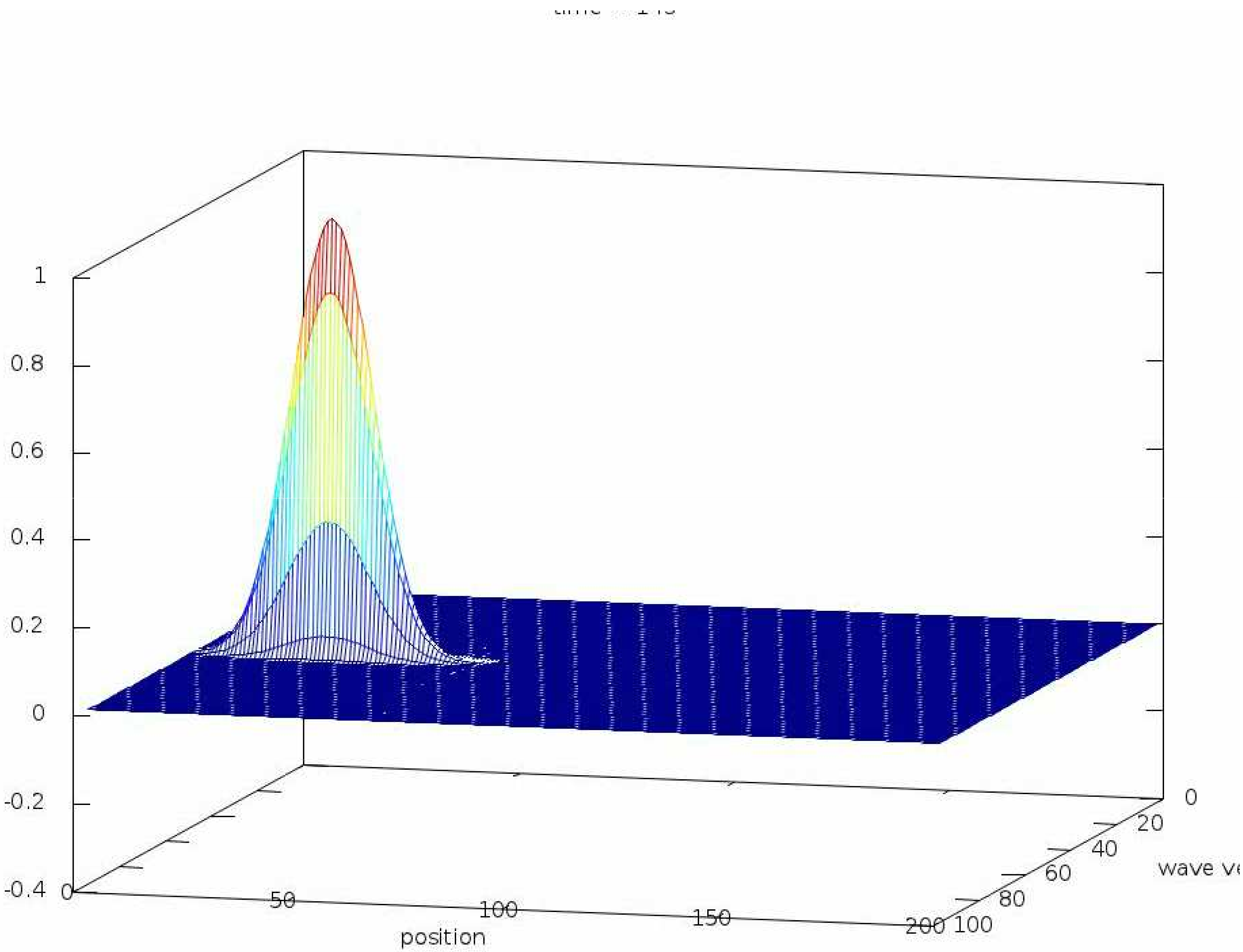
- Benchmark test: particles in constant field
- 1D Wave packet tunneling through a barrier
- Wigner distribution function of a wave packet

Constant field





1
0.8
0.6
0.4
0.2
0
potential barrier
wave function


1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
0
50
100
150
200
position
0
20
40
60
80
100

2D Preliminary results

- 2D delta function in pseudo-wave space

- 2D wav packet against a wall

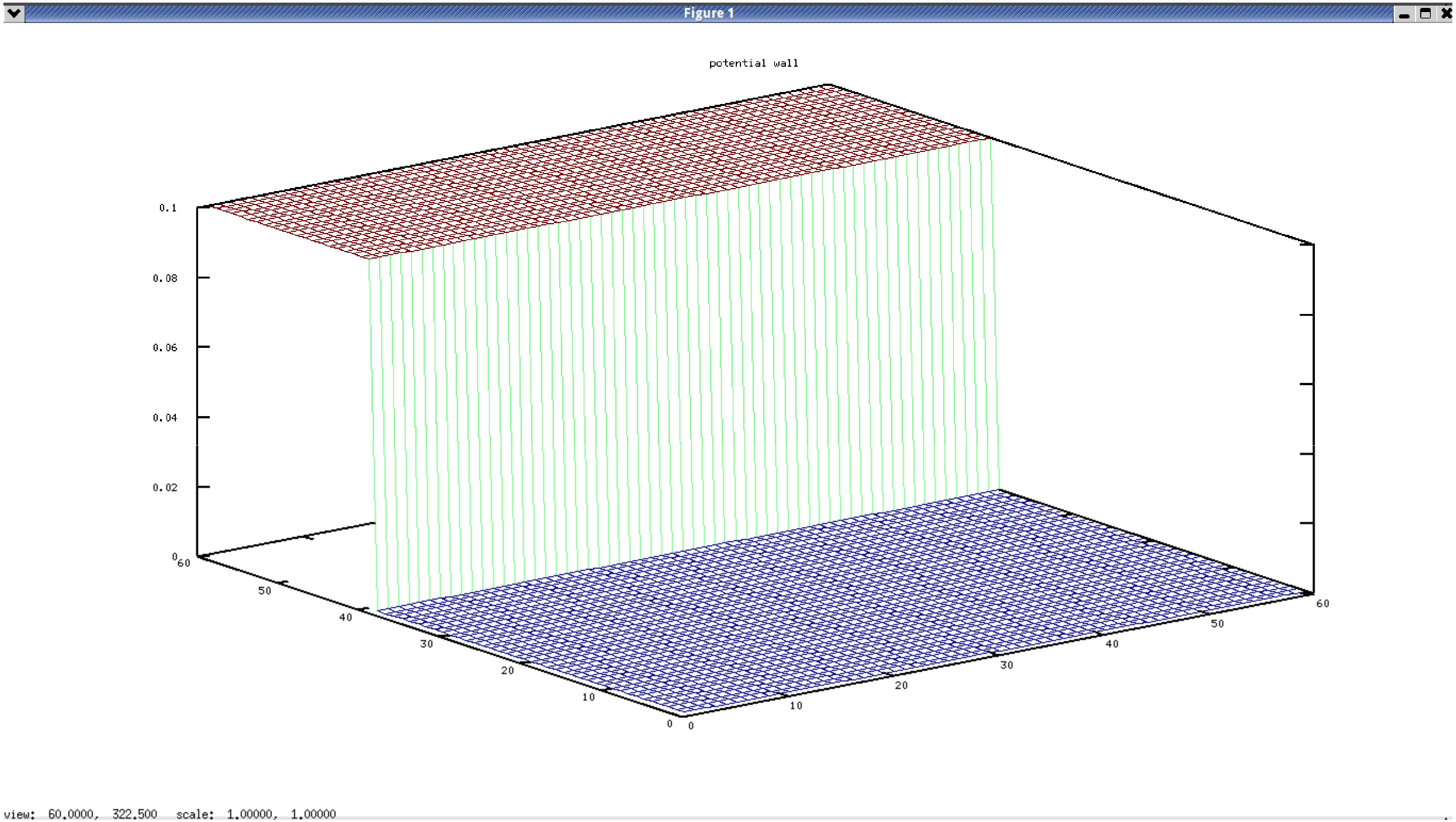
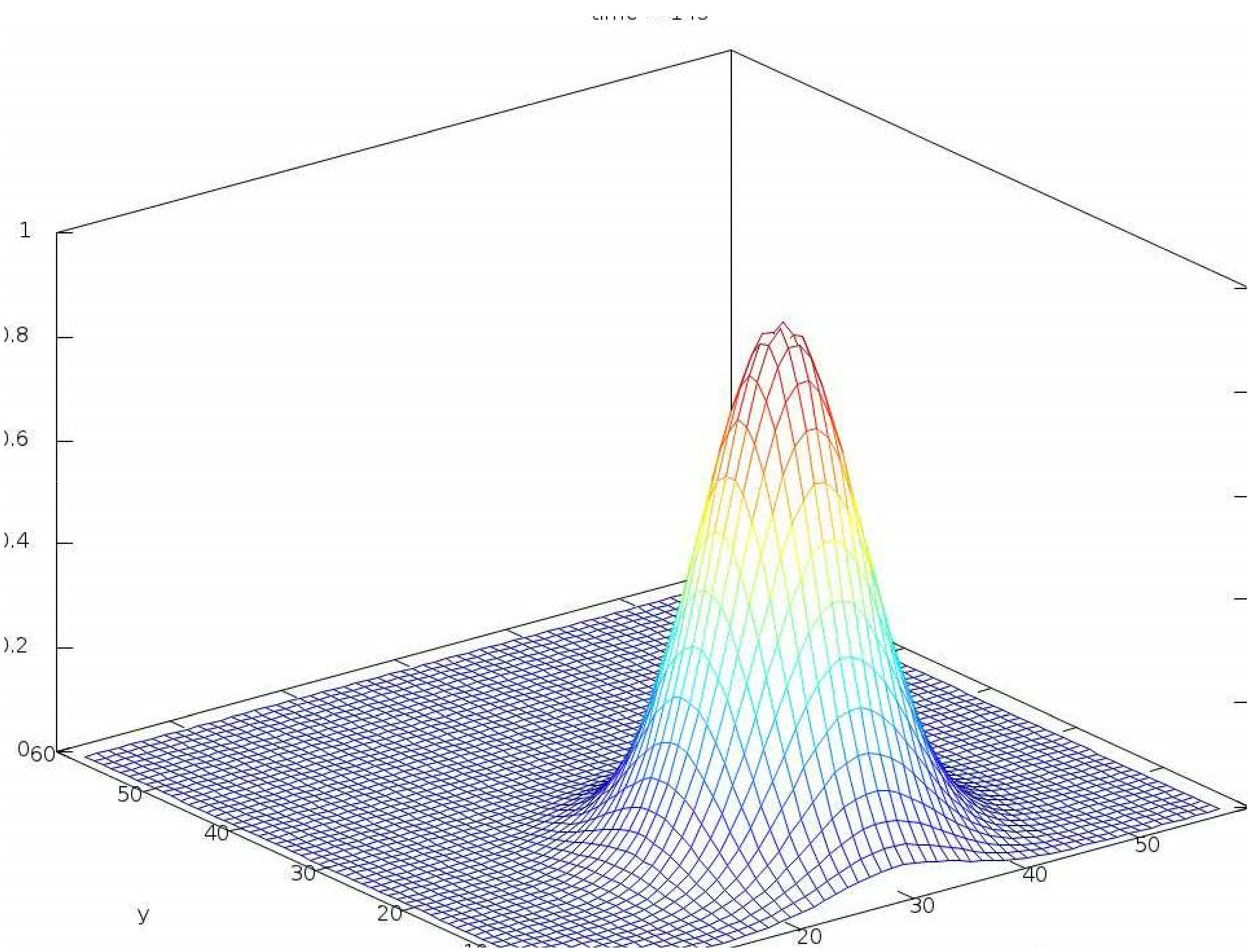
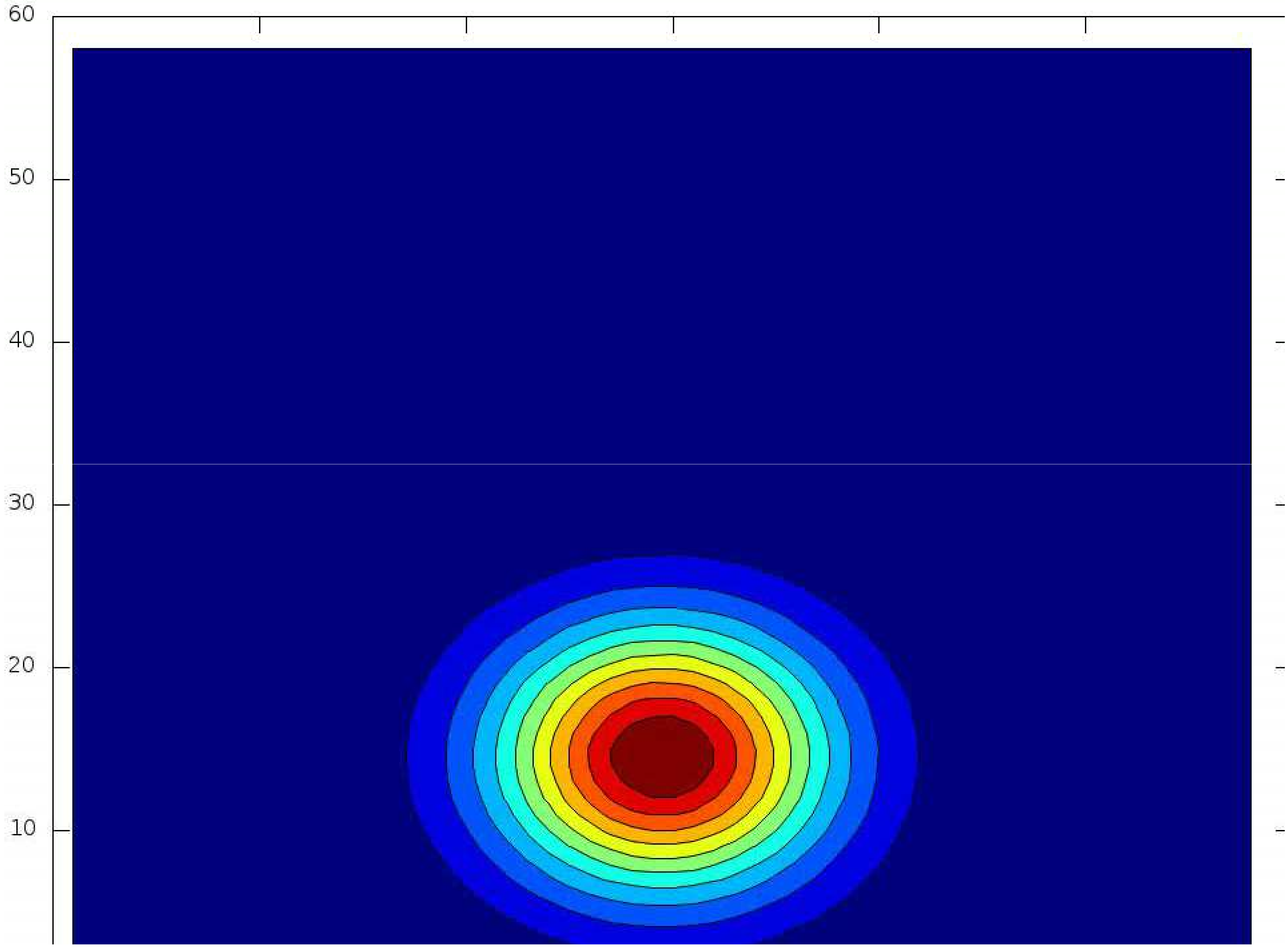


Figure 1
potential wall
0.1
0.08
0.06
0.04
0.02
0
60
50
40
30
20
10
0
0
10
20
30
40
50
60
view: 60.0000, 322.500 scale: 1.00000, 1.00000



1
0.8
0.6
0.4
0.2
0
60
50
40
30
20
y
20
30
40
50


60
50
40
30
20
10

Conclusions and Future works

- *Quantum effects are now dominating but scattering is still important. It needs to be included in the previous simulation prototypes.*

- *2D Transport needs to be investigated further.*

- *Self-consistent simulations. Coupling with Poisson equation to simulate real semiconductor devices.*