Title: Quantum Mechanics without Wave Functions: a Signed Particle Formulation

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Abstract: <p>Recently, a new formulation of quantum mechanics was suggested which is based on the evolution of classical particles, provided with a sign, rather than standard wave functions. This allows several advantages over other approaches: from a theoretical perspective, it offers a more intuitive framework while, from a numerical point of view, it allows the simulation of complex systems with relatively small computational resources. In this talk, I will first go through the tenets of this new approach. In particular, I will focus on the derivation of such theory and the peculiar view it provides in the passage from the quantum to the classical regime. Then, I will discuss the various applications which have been performed so far, especially for systems of Fermions. Finally, a list of possible future works will be presented and discussed.</p>

Quantum Mechanics Without Wave Functions: A Signed Particle Formulation

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Topics

- *Standard Quantum Mechanics*
- *The Wigner Monte Carlo method*
- *The Signed Particle Formulation of Quantum Mechanics*
- *Benchmarks and Applications*
- *Conclusions*

References

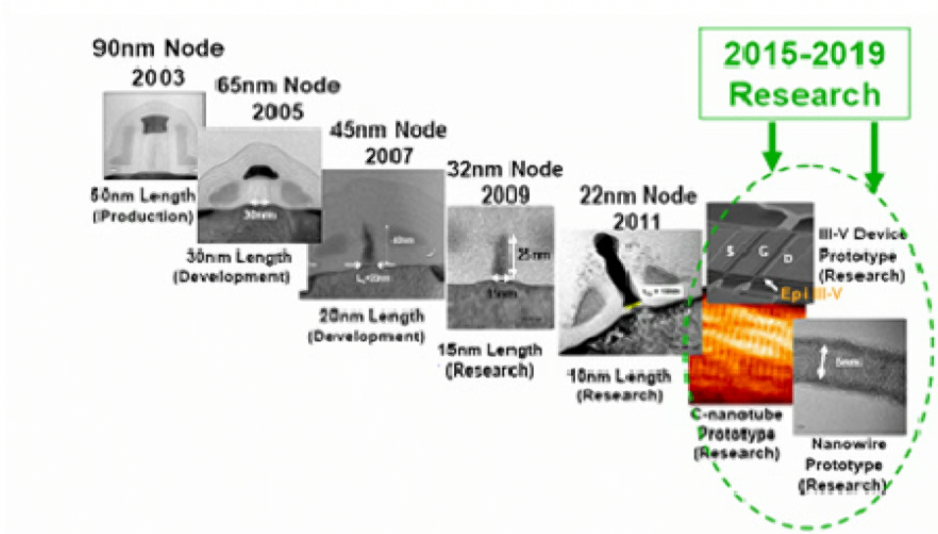
- Link to list of publications (more than 30 papers):

  http://www.nano-archimedes.com/publications

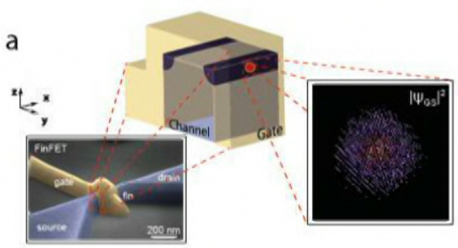
- Source code:

  http://www.nano-archimedes.com/download.php

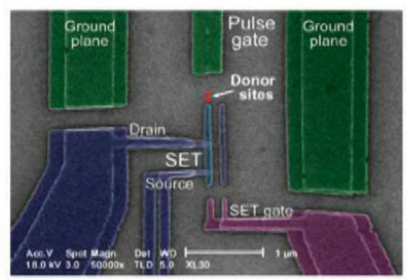
nano-archimedes



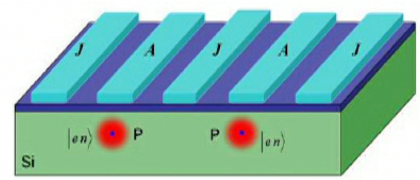
Acknowledgement : Robert Chau, Intel



Lansbergen, Delft



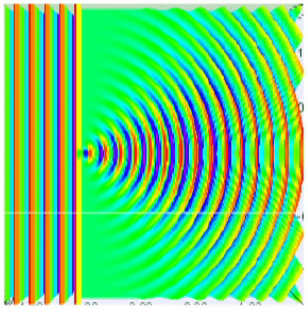
Andresen, UNSW



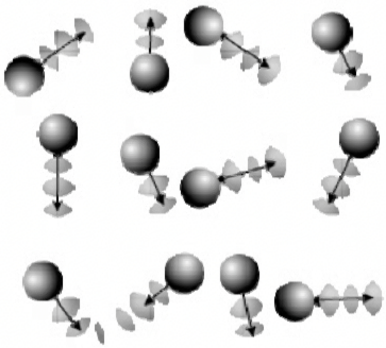
Kane Qubit

The challenges

- *Wave-Particle duality appears*
- *A Full-Quantum approach is required*



- *Inclusion of Phonon Scattering effects*
- *Time-dependent phenomena*



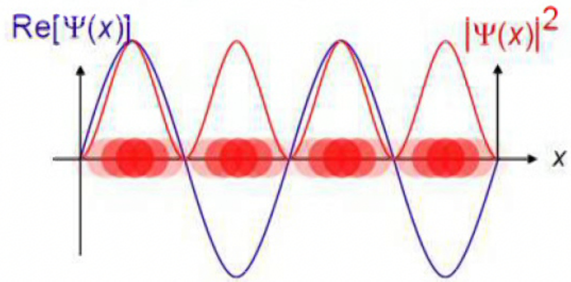
(*) Pictures from wikipedia.

Wave function formulation - I

- Systems are described in terms of (complex) wave functions

$$\Psi = \Psi(x_1, y_1, z_1, \ldots, x_N, y_N, z_N)$$

- Born rule (heuristic)



- Observables are represented by operators
$\hat{O} = \hat{O}(\hat{x}; \hat{p})$

(*) Picture from wikipedia.

Wave function formulation - II

- Time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi$$

- Time-independent Schrödinger equation

$$\hat{H}\Psi = E\Psi$$

Available formalisms

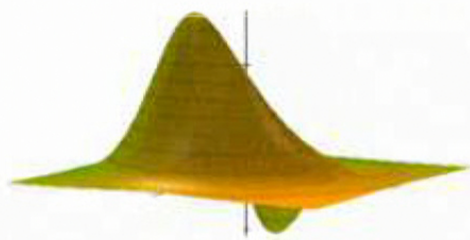
• Heisenberg	Density matrix	1925
• Schrödinger	Wave-functions	1926
• Wigner	Quasi-distributions	1932
• Feynman	Path integrals	1948
• Keldysh	Green functions	1964

- Signed Particle Formulation 2015

Wigner formulation - I

- Systems are described in terms of (complex) quasi-distribution functions

$$f_W = f_W\left(x_1, y_1, z_1, p_1^x, p_1^y, p_1^z \ldots, x_N, y_N, z_N, p_1^x, p_1^y, p_1^z\right)$$



- Observables are represented exactly as in classical statistical physics.

(*) Picture from wikipedia.

Wigner formulation - II

- Time-dependent Wigner equation

$$\frac{\partial f_W}{\partial t}(\mathbf{x};\mathbf{p}) = -\frac{\mathbf{p}\cdot\nabla_{\mathbf{x}}}{\mathbf{m}} f_W(\mathbf{x};\mathbf{p}) + \int_{-\infty}^{+\infty} d\mathbf{q} f_W(\mathbf{x};\mathbf{p}+\mathbf{q}) V_W(\mathbf{x};\mathbf{p})$$

- Time-independent Wigner equation

$$H(x;p) * f_W(x;p) = E \cdot f_W(x;p)$$

Wigner-Weyl transform

$$\hat{A}(\hat{q},\hat{p}) \mapsto V_{\mathrm{W}}(\hat{A}) = A(x,p) = \\ = \frac{\hbar}{2\pi}\int \mathrm{d}\xi \int \mathrm{d}\eta\, \mathrm{Tr}\left\{\hat{A}(\hat{q},\hat{p})\mathrm{e}^{\mathrm{i}\xi\hat{q}+\mathrm{i}\eta\hat{p}}\right\}\mathrm{e}^{-\mathrm{i}\xi x-\mathrm{i}\eta p}$$

$$\begin{cases} A * B & \equiv V_{\mathrm{W}}\left(\hat{A}\cdot\hat{B}\right) \\ [A,B]_M & \equiv \frac{1}{\mathrm{i}\hbar}(A * B - B * A) \end{cases}$$

N.C. Dias, J.N. Prata / Annals of Physics 313 (2004) 110–146

Advantages

- *Intuitive language, very close to classical statistical physics*
- *Natural inclusion of inelastic effects*
- *General boundary conditions*

The Wigner Monte Carlo Method

The Wigner equation

- *The Wigner equation reads*

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

- *where*

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

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

Comment

- The Wigner equation is a VERY difficult task in a finite difference framework.

- The distribution is known to be rapidly varying and the diffusion term cannot be calculated correctly.

$$\nabla_{\vec{r}} f_W\left(\vec{r},\vec{k},t\right)$$

Fredholm Equation of 2nd Kind

- Given a function $f = f(t)$ and a kernel $K = K(t,s)$ the problem is to find the unknown

$$\varphi(t) = f(t) + \lambda \int_a^b K(t,s)\varphi(s)ds$$

- Its solution can be written formally as (Liouville – von Neumann series)

$$\varphi(x) = \sum_{n=0}^{\infty} \lambda^n \varphi_n(x)$$

Wigner equation in semi-discrete form

- *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

- *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 involves a process of creation of two particles, one positive and one negative, and the sign carries the quantum information.

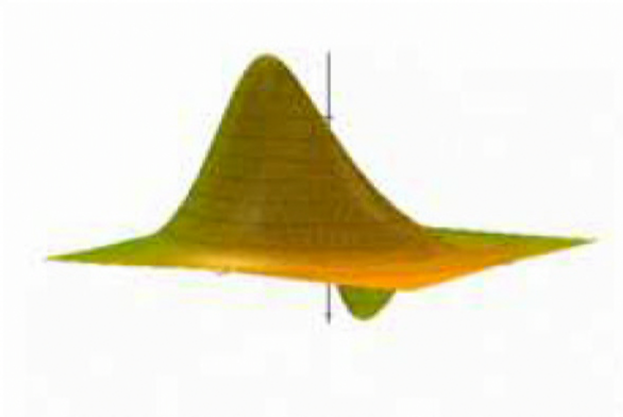
  Particles are Newtonian. Dynamics is field-less.

  → *Postulates I, II and III.*

Postulates

Postulate I. *Physical systems can be described by means of (virtual) Newtonian particles, i.e. provided with a position* $\mathbf{x}$ *and a momentum* $\mathbf{p}$ *simultaneously, which carry a sign which can be positive or negative.*

Postulate III. *Two particles with opposite sign and same phase-space coordinates* $(\mathbf{x}, \mathbf{p})$ *annihilate.*



Postulates

Postulate II. *A signed particle, evolving in a potential $V = V(\mathbf{x})$, behaves as a field-less classical point-particle which, during the time interval dt, creates a new pair of signed particles with a probability $\gamma(\mathbf{x}(t))\, dt$ where*

$$\gamma(\mathbf{x}) = \int_{-\infty}^{+\infty} \mathcal{D}\mathbf{p}' V_W^+(\mathbf{x};\mathbf{p}') \equiv \lim_{\Delta\mathbf{p}'\to 0^+} \sum_{\mathbf{M}=-\infty}^{+\infty} V_W^+(\mathbf{x};\mathbf{M}\Delta\mathbf{p}'), \qquad (1)$$

and $V_W^+(\mathbf{x};\mathbf{p})$ is the positive part of the quantity

$$V_W(\mathbf{x};\mathbf{p}) = \frac{i}{\pi^d \hbar^{d+1}} \int_{-\infty}^{+\infty} d\mathbf{x}' e^{-\frac{2i}{\hbar}\mathbf{x}'\cdot\mathbf{p}} \left[V(\mathbf{x}+\mathbf{x}') - V(\mathbf{x}-\mathbf{x}')\right], \qquad (2)$$

known as the Wigner kernel (in a d-dimensional space) [2]. If, at the moment of creation, the parent particle has sign s, position $\mathbf{x}$ and momentum $\mathbf{p}$, the new particles are both located in $\mathbf{x}$, have signs $+s$ and $-s$, and momenta $\mathbf{p}+\mathbf{p}'$ and $\mathbf{p}-\mathbf{p}'$ respectively, with $\mathbf{p}'$ chosen randomly according to the (normalized) probability $\frac{V_W^+(\mathbf{x};\mathbf{p})}{\gamma(\mathbf{x})}$.

Postulates (many-body)

Postulate I. *Physical systems can be described by means of (virtual) signed particles defined in the ($2 \times n \times d$-dimensional) phase-space, i.e. provided with a ($n \times d$-dimensional) position* $\mathbf{x}$ *and a ($n \times d$-dimensional) momentum* $\mathbf{p}$ *simultaneously, and which carry a sign which can be positive or negative.*

Postulate III. *Two particles with opposite sign and same phase-space coordinates* $(\mathbf{x}, \mathbf{p})$ *annihilate.*

Postulates (many-body)

Postulate II. *A signed particle, evolving in a potential* $V = V\left(\mathbf{x}^1, \ldots, \mathbf{x}^n\right)$, *behaves as a field-less classical point-particle which, during the time interval* dt, *creates a new pair of signed particles with a probability* $\gamma\left(\mathbf{x}^1(t), \ldots, \mathbf{x}^n(t)\right) dt$ *where*

$$\gamma\left(\mathbf{x}^1, \ldots, \mathbf{x}^n\right) = \int_{-\infty}^{+\infty} \mathcal{D}\mathbf{p}_1{}' \ldots \int_{-\infty}^{+\infty} \mathcal{D}\mathbf{p}_n{}' V_W^+\left(\mathbf{x}^1, \ldots, \mathbf{x}^n; \mathbf{p}_1{}', \ldots, \mathbf{p}_n{}'\right) \quad (2)$$

is the many-body momentum integral defined as

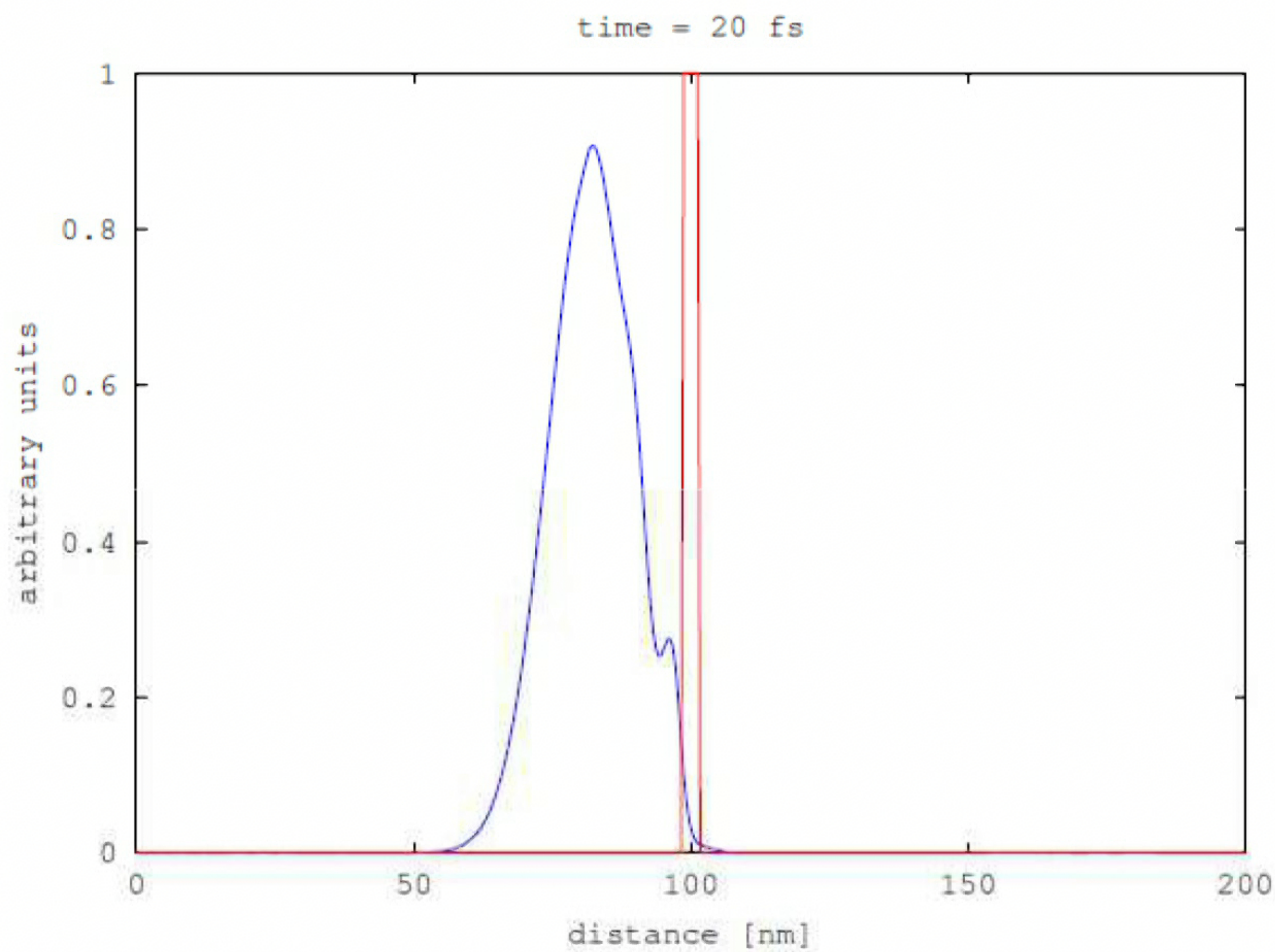
$$\lim_{\Delta\mathbf{p}_1{}' \to 0^+} \cdots \lim_{\Delta\mathbf{p}_n{}' \to 0^+} \sum_{\mathbf{M}_1=-\infty}^{+\infty} \cdots \sum_{\mathbf{M}_n=-\infty}^{+\infty} V_W^+\left(\mathbf{x}^1, \ldots, \mathbf{x}^n; \mathbf{M}_1\Delta\mathbf{p}_1{}', \ldots, \mathbf{M}_n\Delta\mathbf{p}_n{}'\right), \quad (3)$$

and $V_W^+\left(\mathbf{x}^1, \ldots, \mathbf{x}^n; \mathbf{p}^1, \ldots, \mathbf{p}^n\right)$ *is the positive part of the many-body Wigner kernel [12], [14]. If, at the moment of creation, the parent particle has sign* s, *position* $\mathbf{x} = \left(\mathbf{x}^1, \ldots, \mathbf{x}^n\right)$ *and momentum* $\mathbf{p} = \left(\mathbf{p}^1, \ldots, \mathbf{p}^n\right)$, *the new particles are both located in* $\mathbf{x}$, *have signs* $+s$ *and* $-s$, *and momenta* $\mathbf{p} + \mathbf{p}'$ *and* $\mathbf{p} - \mathbf{p}'$ *respectively, with* $\mathbf{p}'$ *chosen randomly according to the (normalized) probability*

$$\frac{V_W^+\left(\mathbf{x}^1, \ldots, \mathbf{x}^n; \mathbf{p}^1, \ldots, \mathbf{p}^n\right)}{\gamma\left(\mathbf{x}^1, \ldots, \mathbf{x}^n\right)}.$$

Classical Limit (summary)

- Creation of signed particles is prohibited.
- Particles are not field-less anymore.
- Negative particles are not allowed any longer.
- Equations of motion coincide with Newton's law.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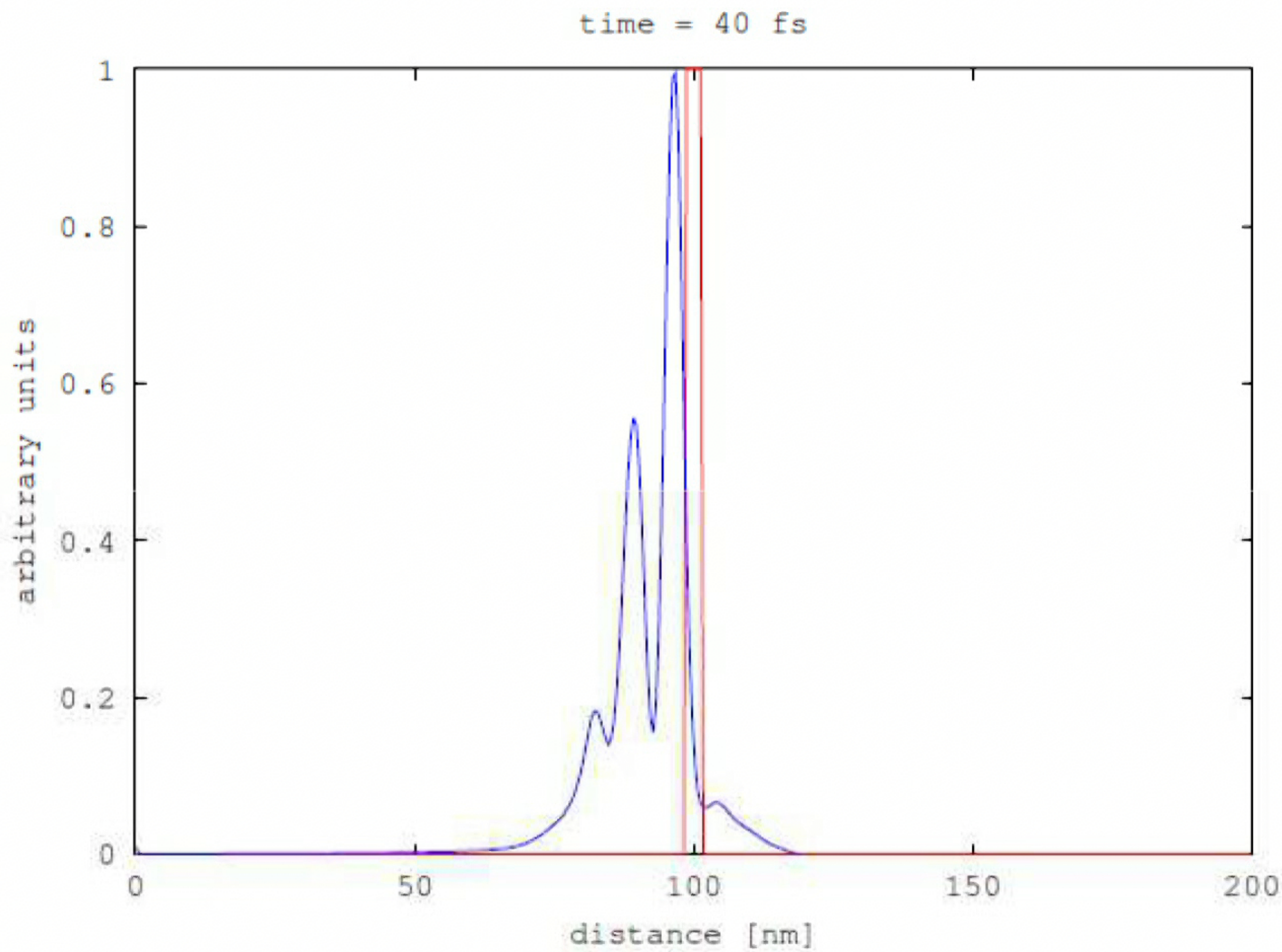
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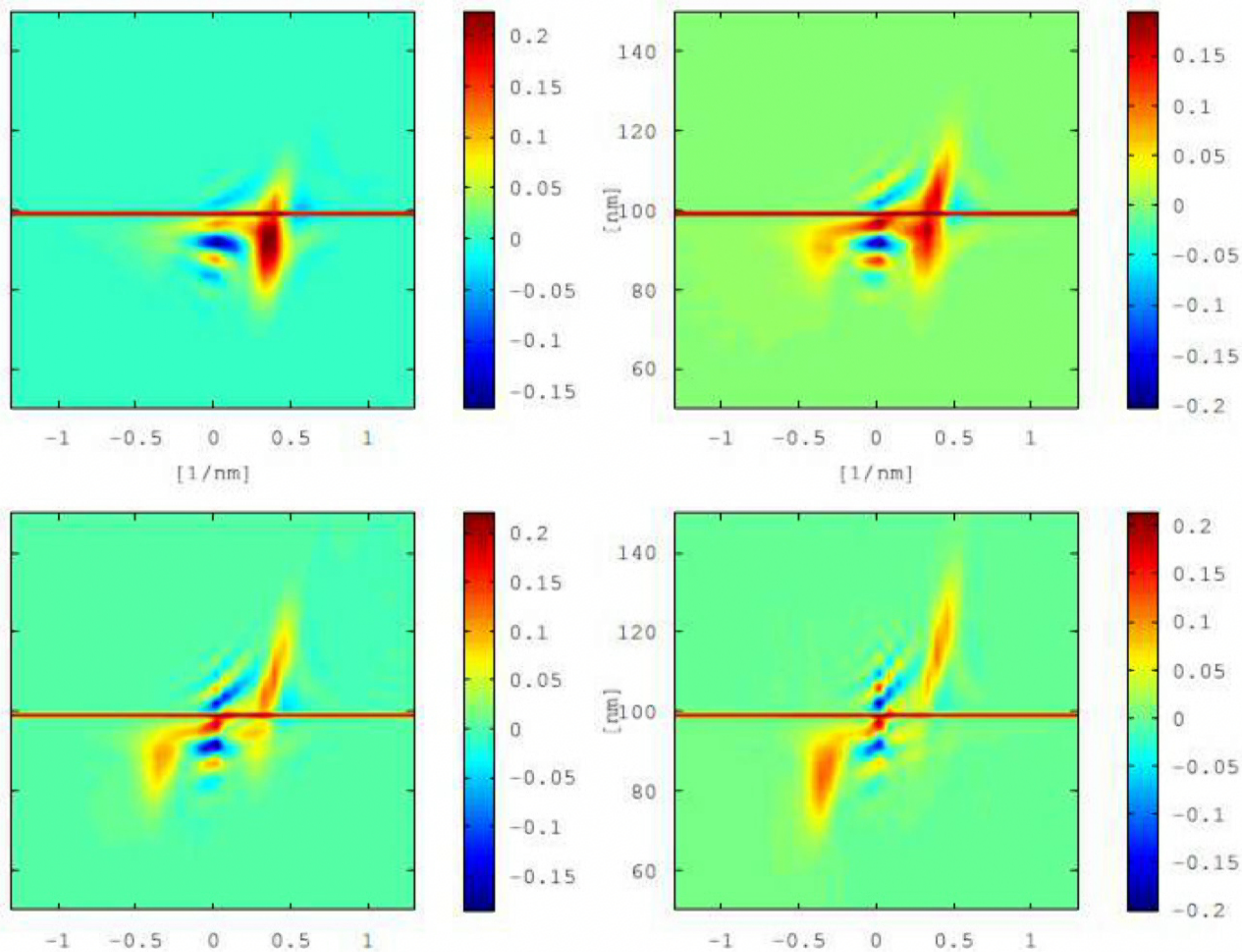
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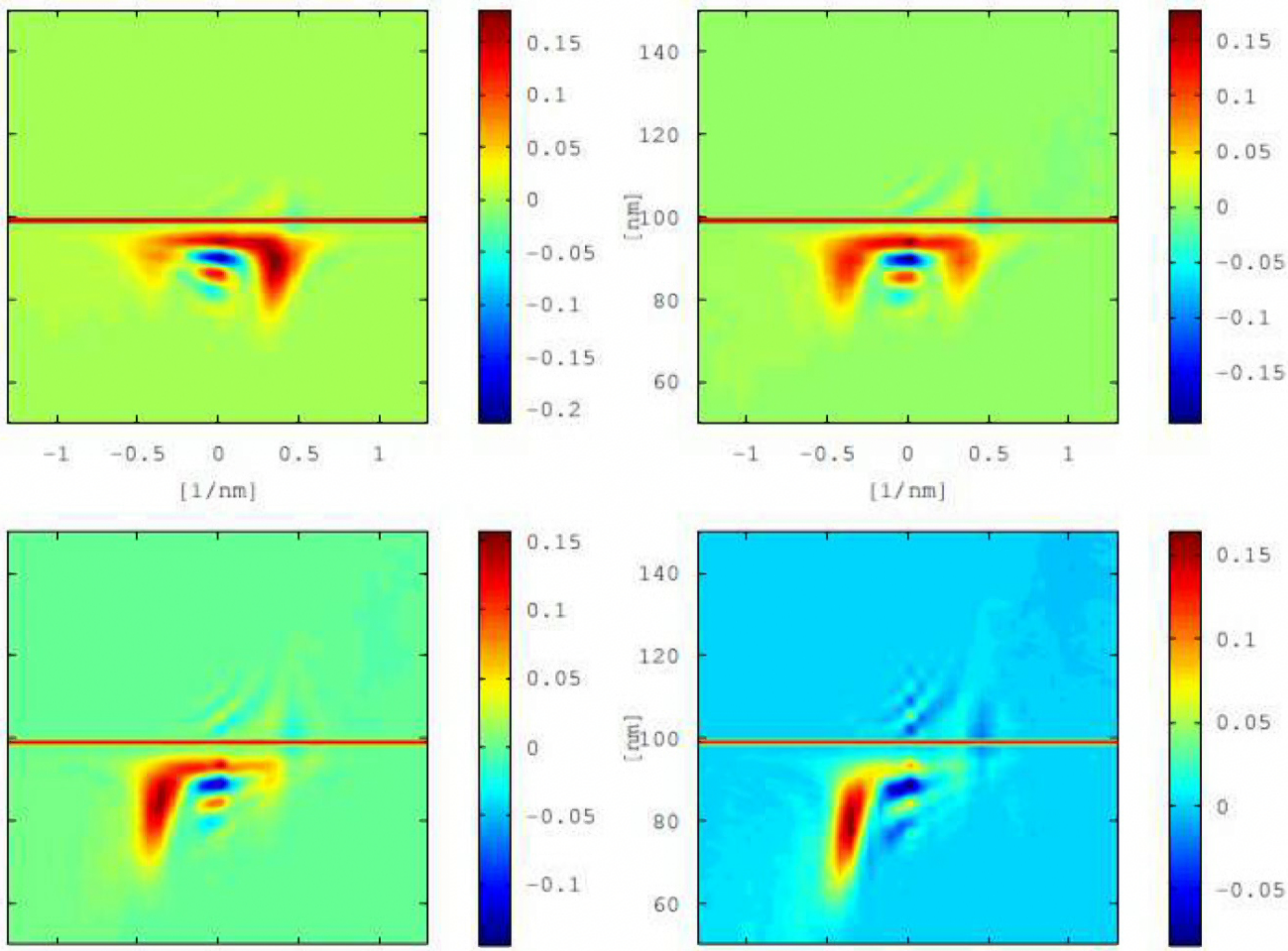
-0.2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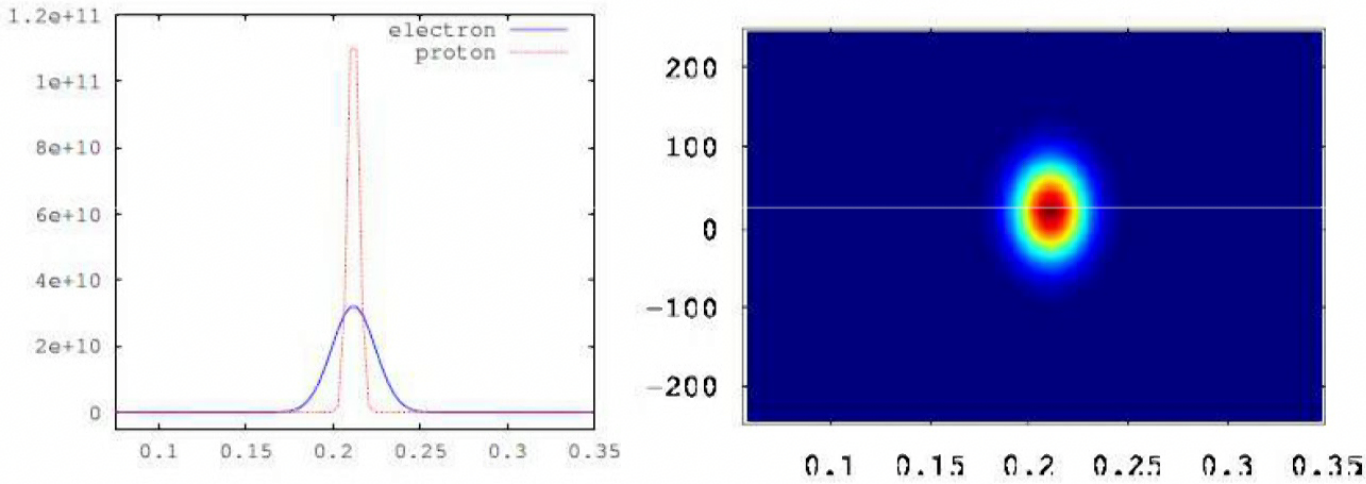
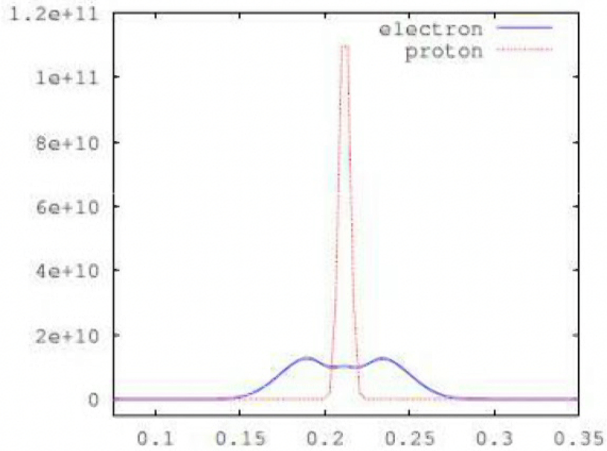
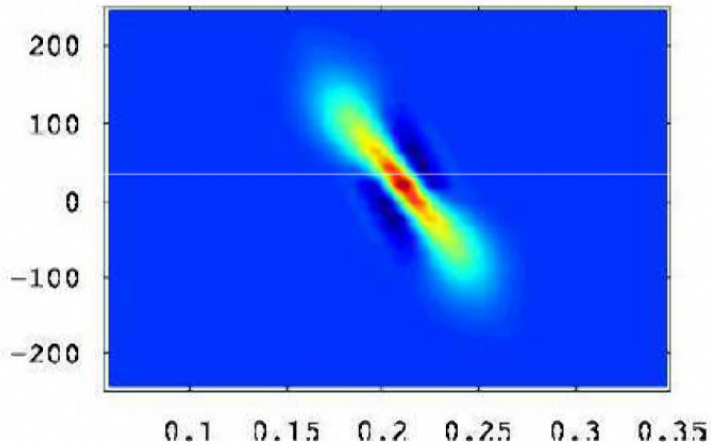
Hydrogen atom: 0as

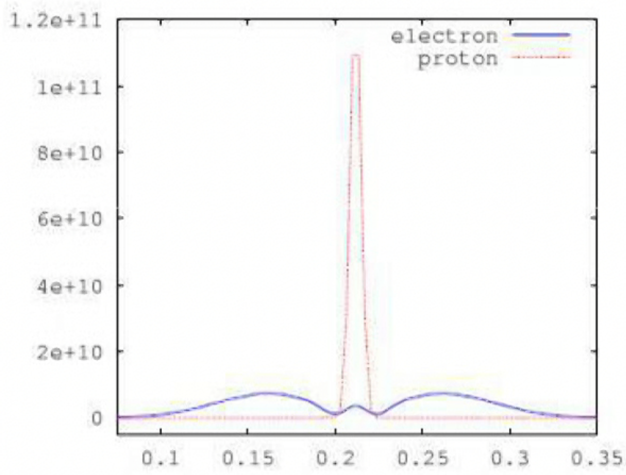


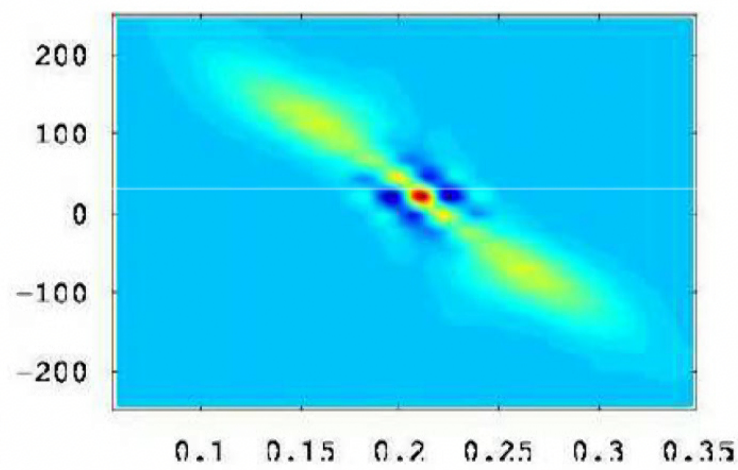
Hydrogen atom: 3as



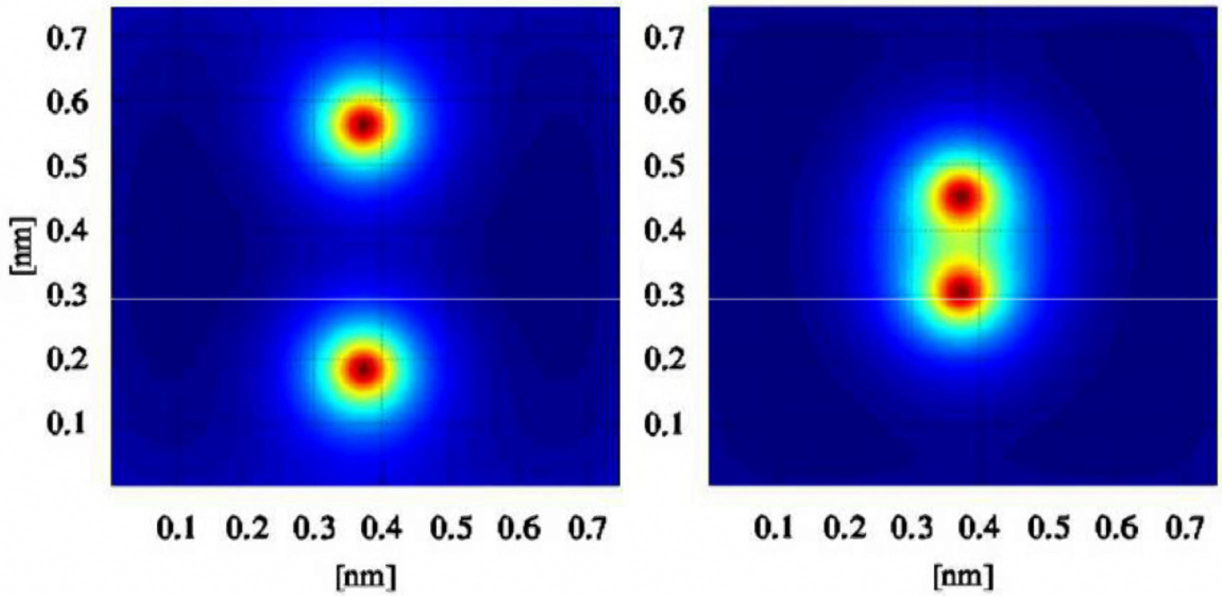


Hydrogen atom: 6as

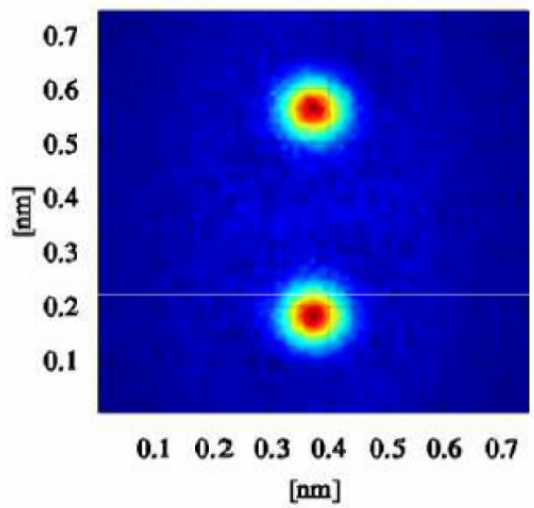


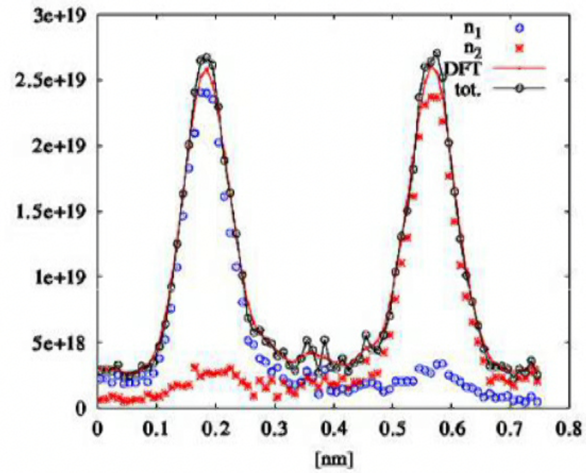


The H_2 molecule

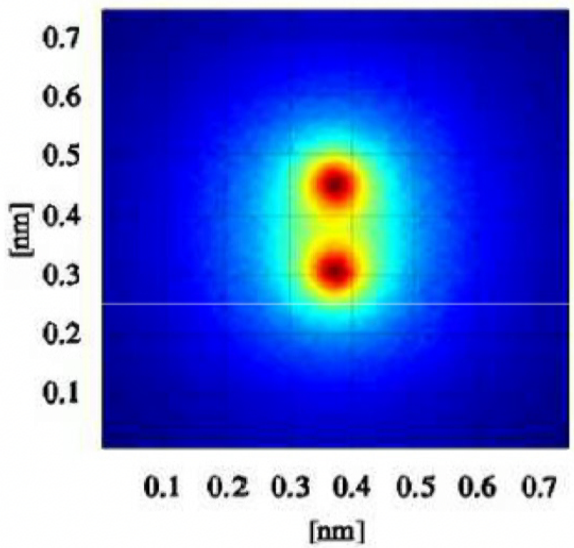


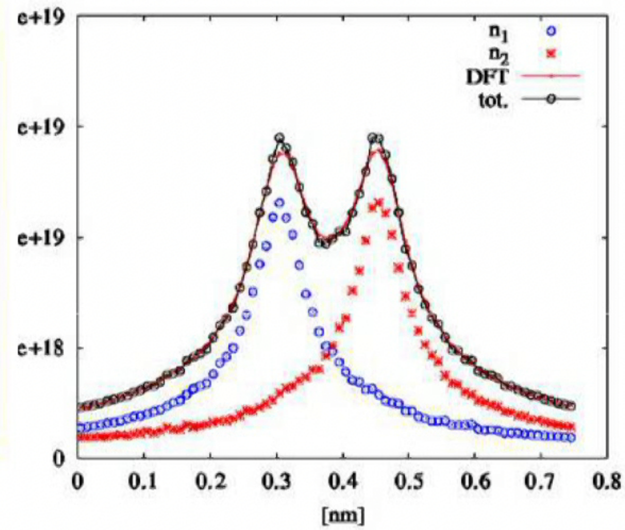
The H_2 molecule



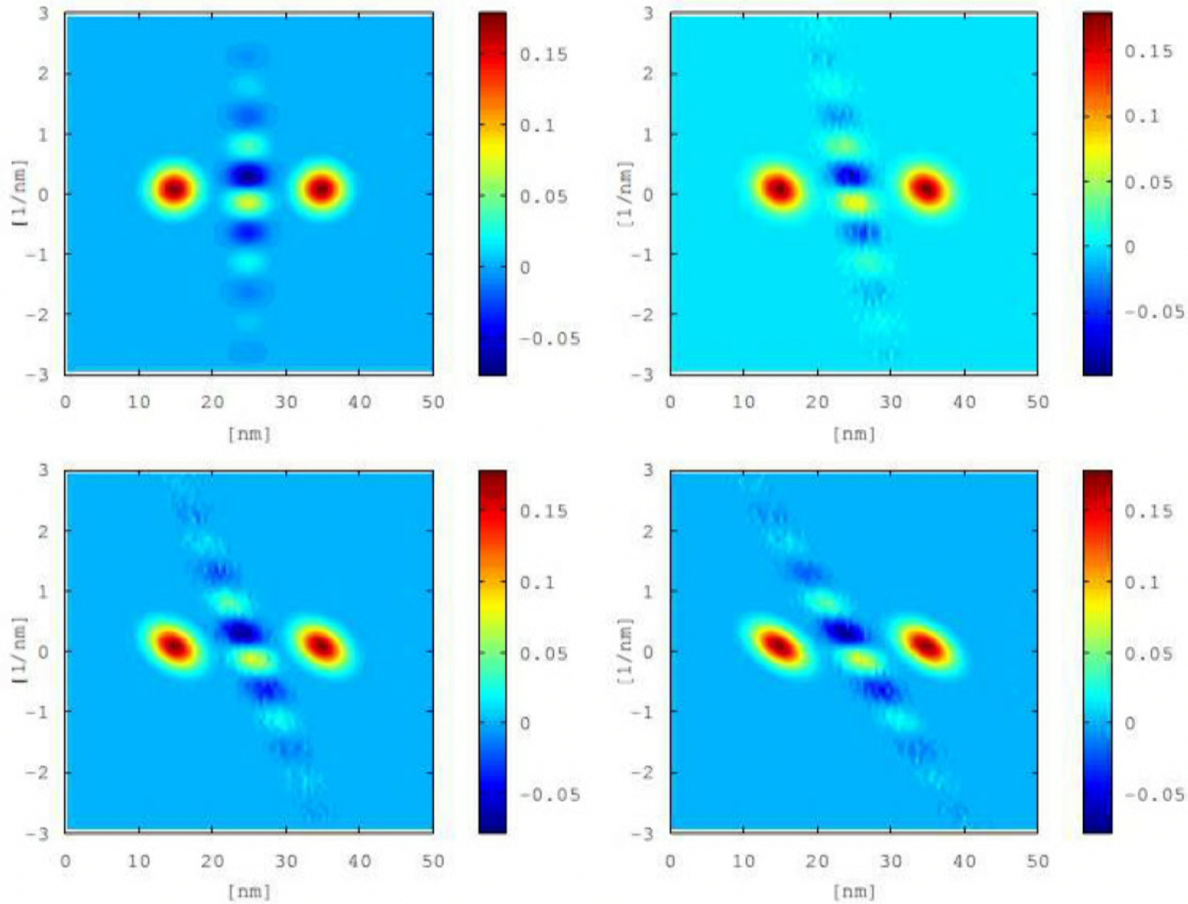


The H_2 molecule

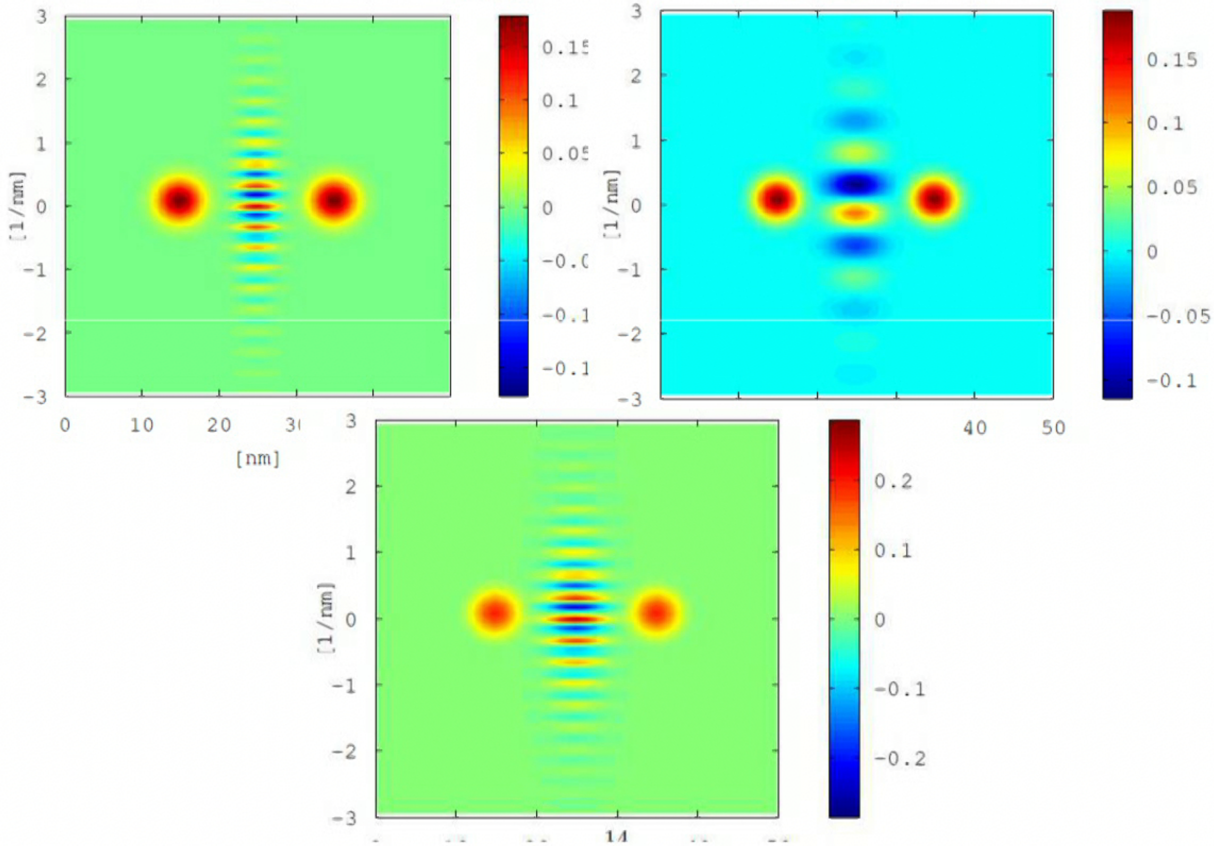




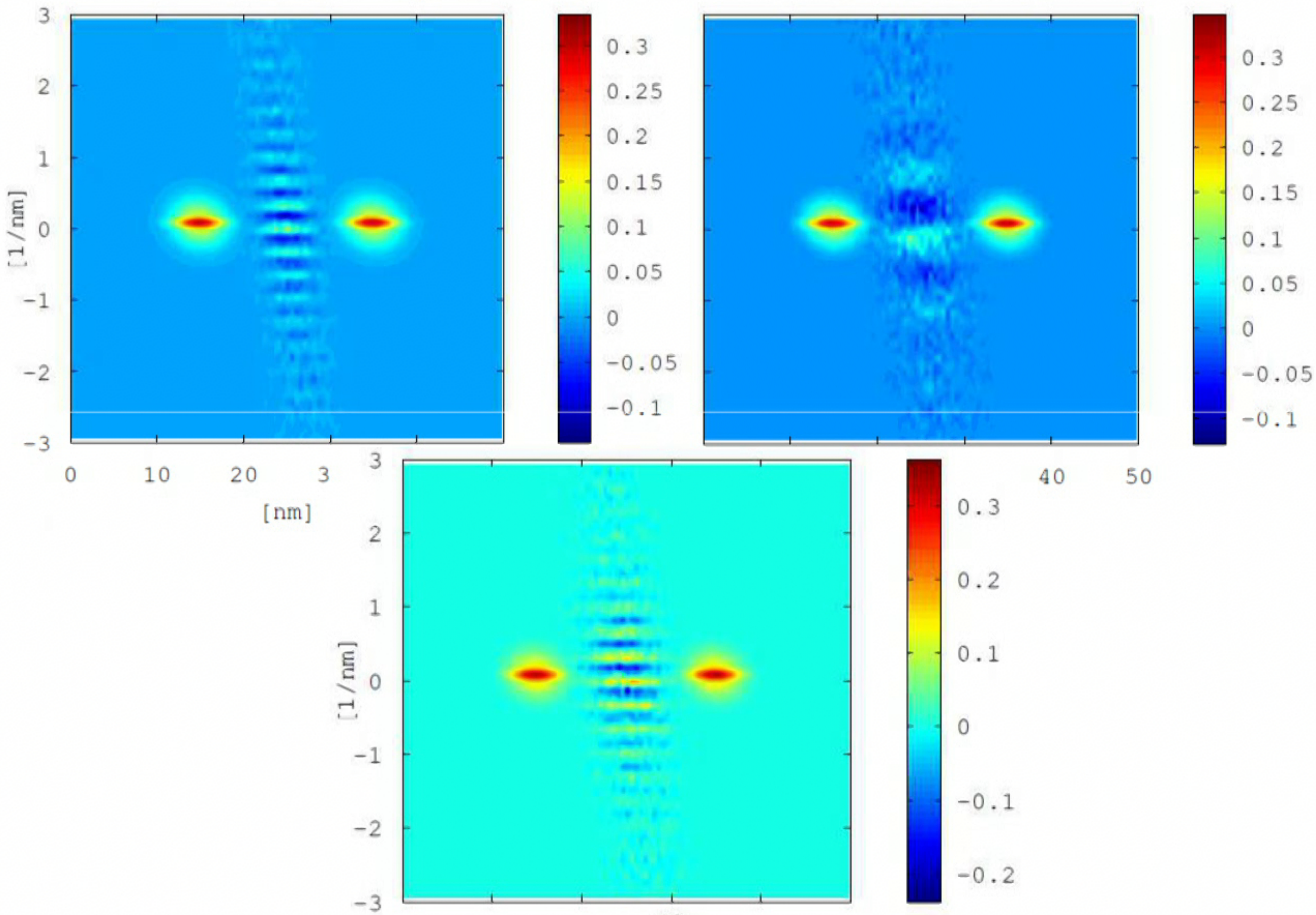
Ballistic, 0, 1, 2, 3 fs

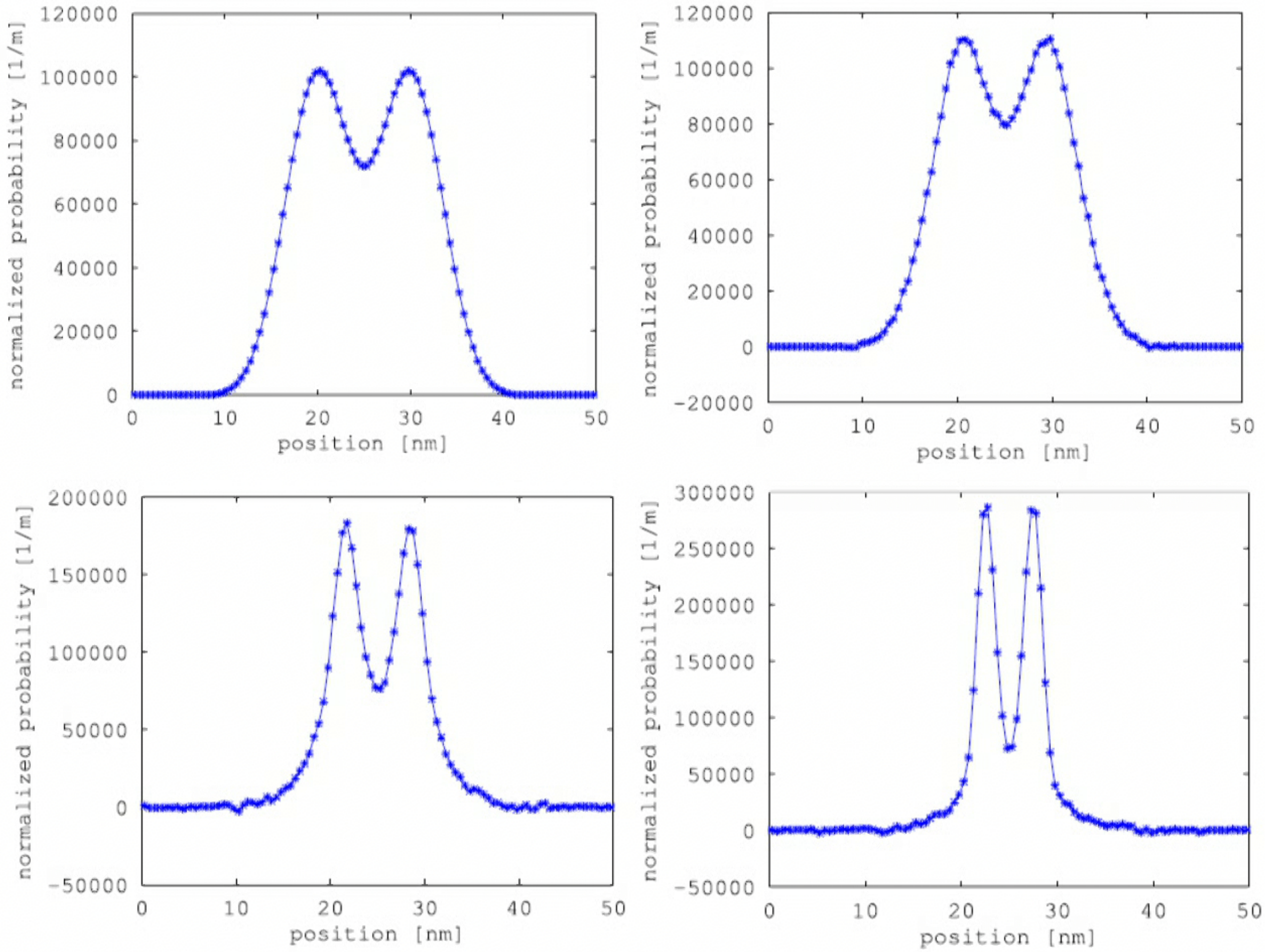


Different Initial Conditions, 1% scattering, 5% energy removed



Comparison – final state

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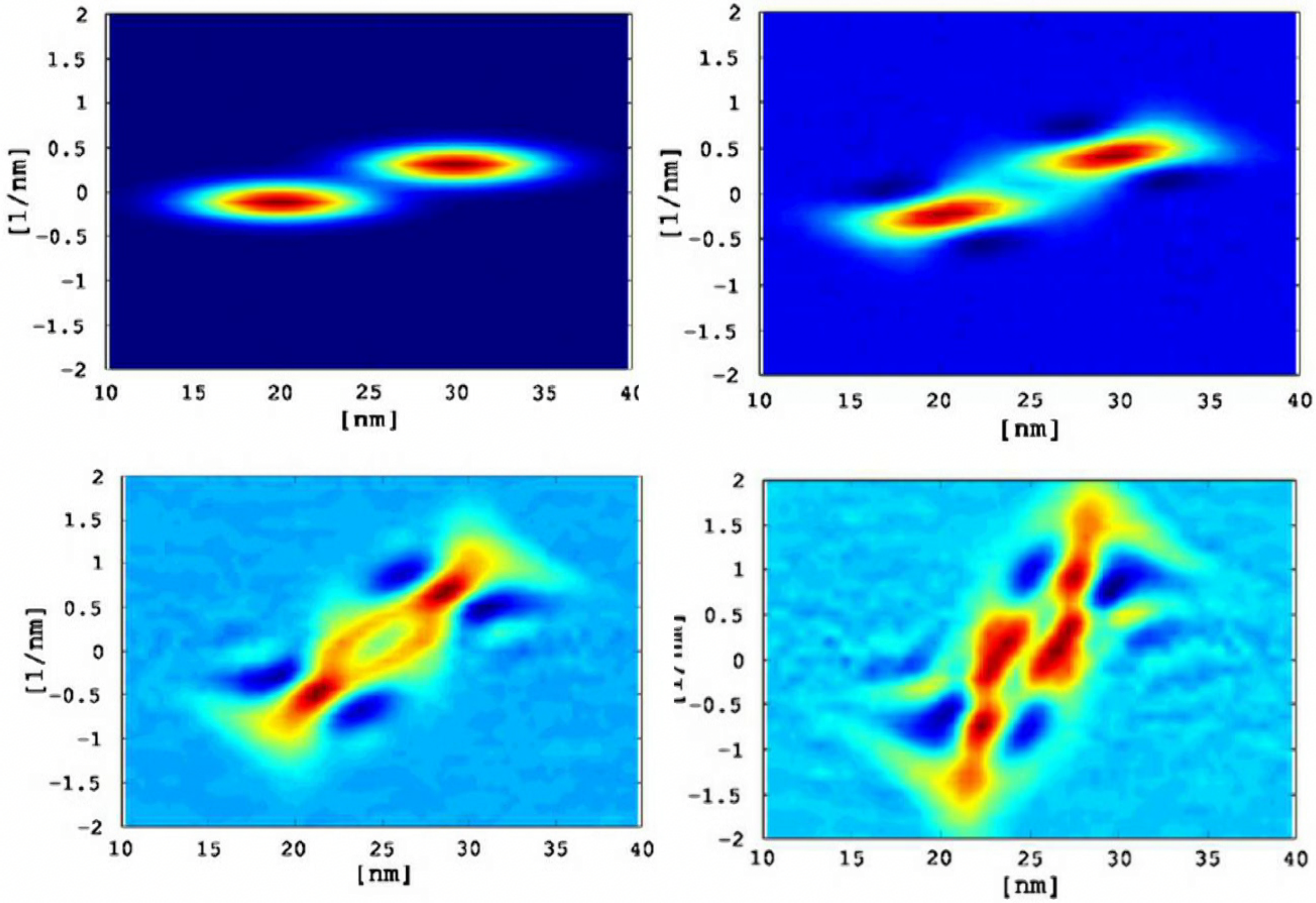
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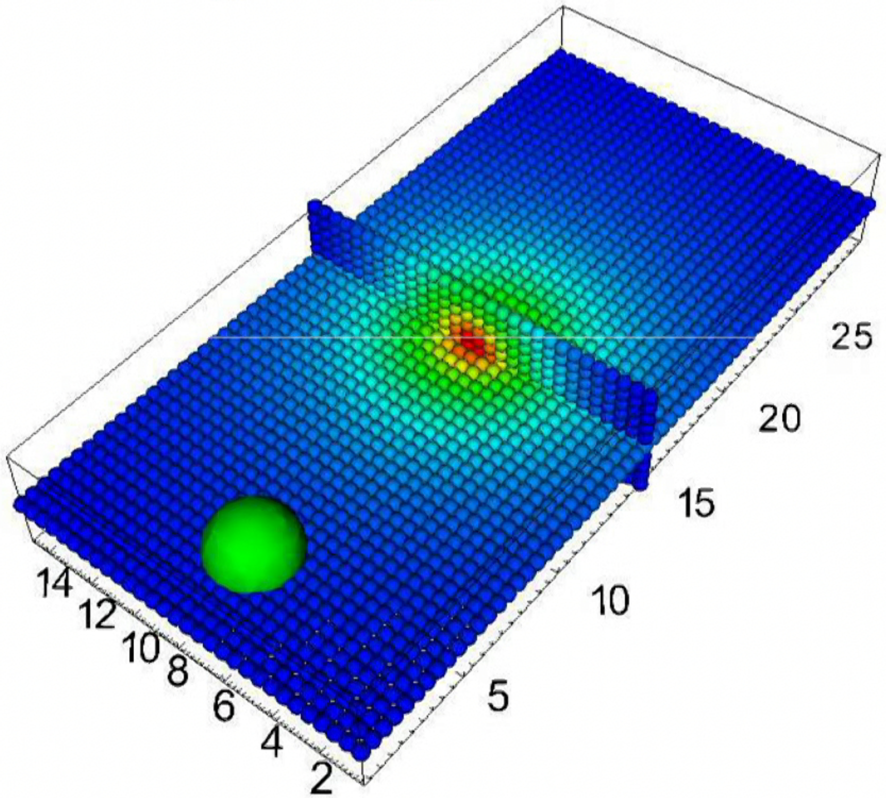
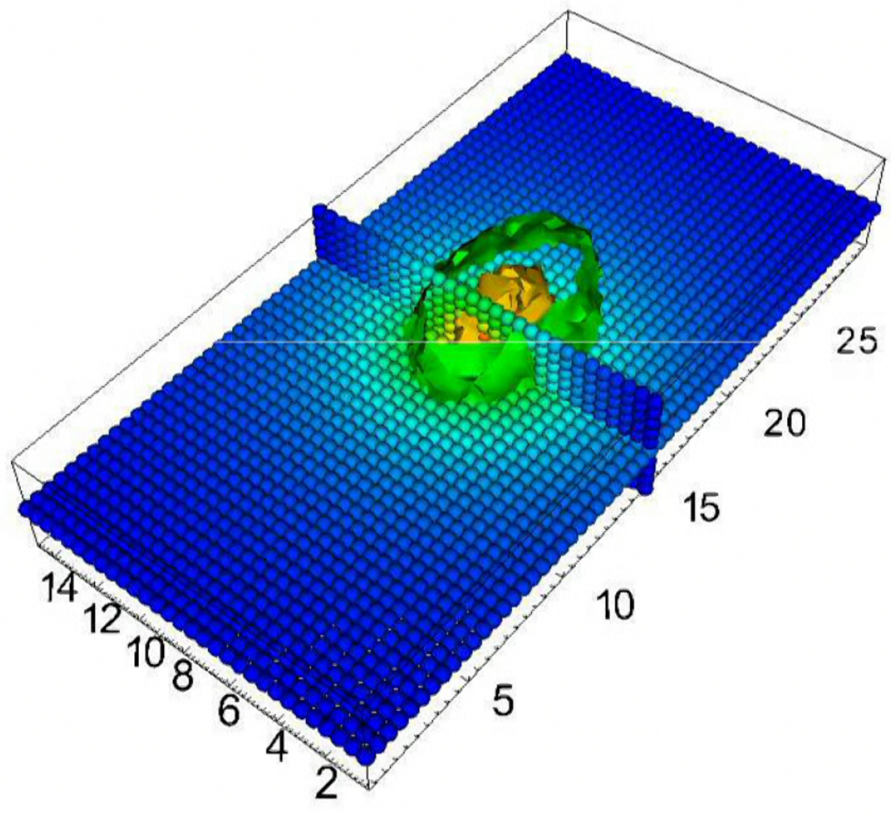
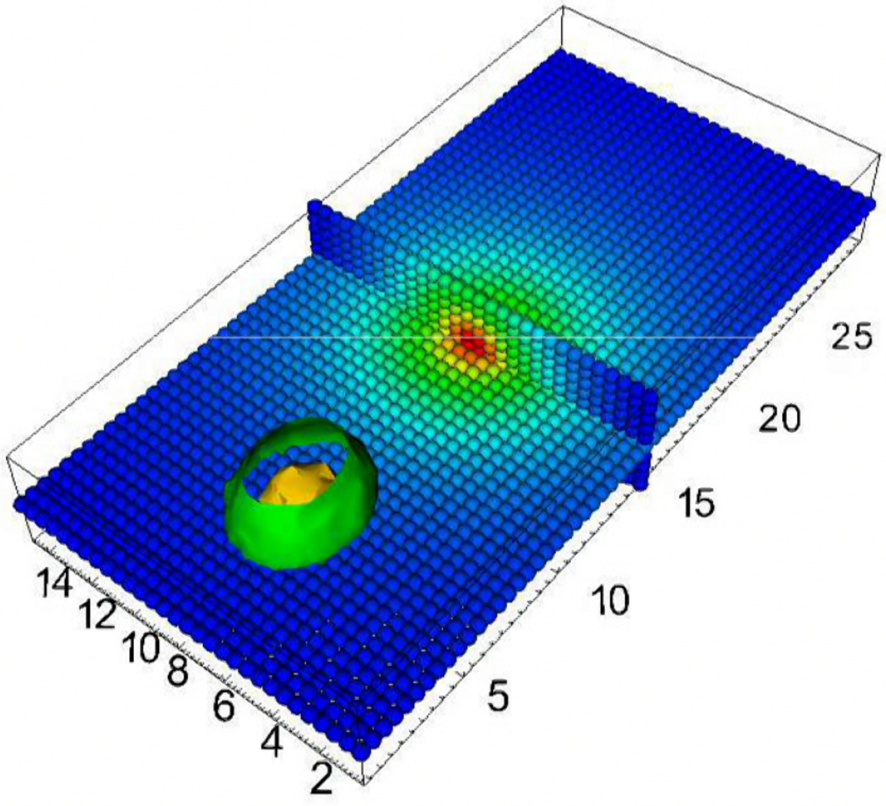
Single dopant devices



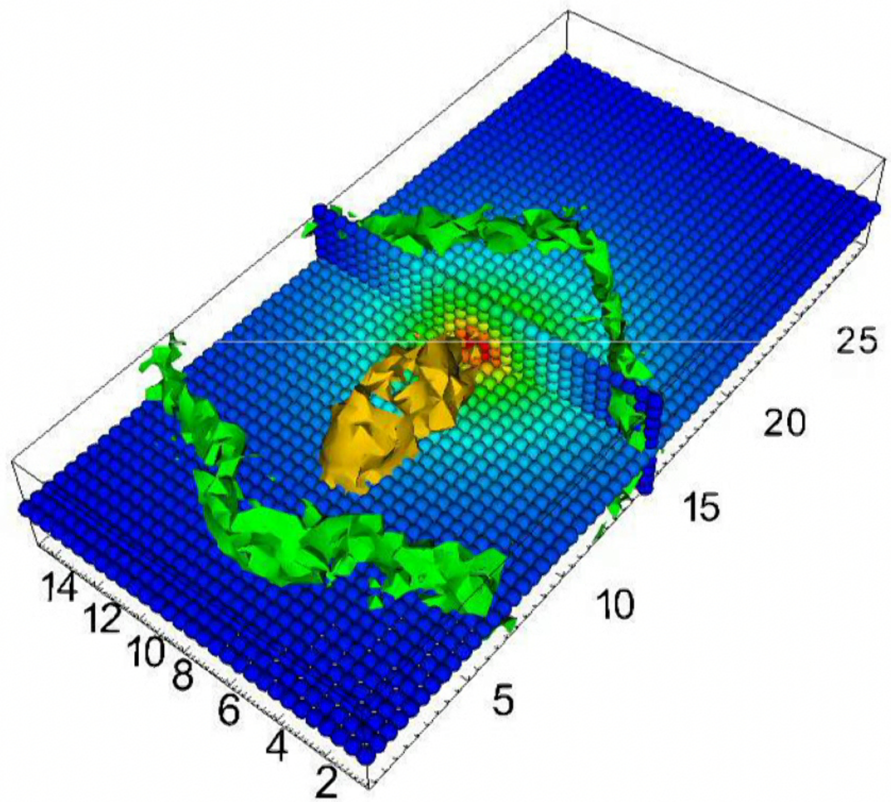
20mK – 20fs



300K – 10fs



300K – 30fs



Conclusions

- More applications, (quantum computing and chemistry)
- Theoretical investigations: inclusion of spin, connection to the Feynman formulation, etc.
- Collaborations!
- Spread the word!