Coherent Wigner Dynamics of a Superposition State in a Tunable Barrier Quantum Dot

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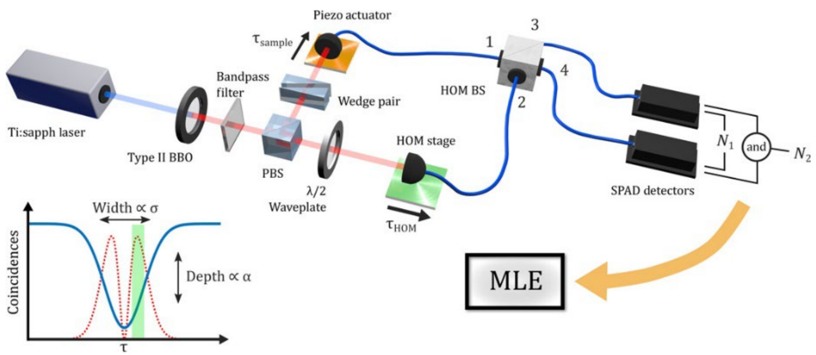
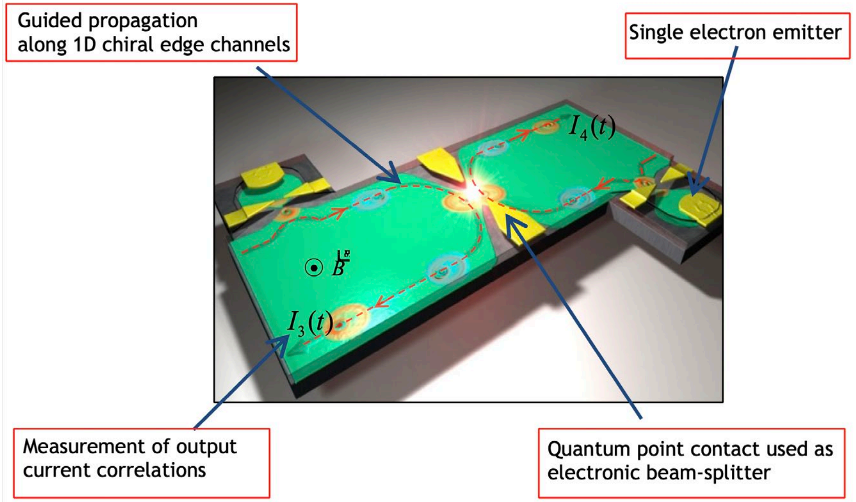
FWF Austrian Science Fund

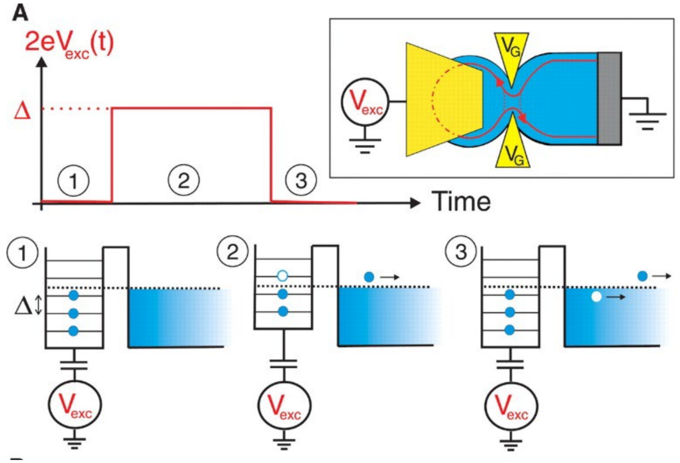
IWCN BARCELONA 2023

Electron Quantum Optics

Wave nature of electron → Interferometers, electron sources etc.







Quantum Optics

Lyons *et al.*, Sci. Adv. 4 (2018)

Electron Quantum Optics

Bäuerle *et al.*, Rep. Prog. Phys. 81 (2018)

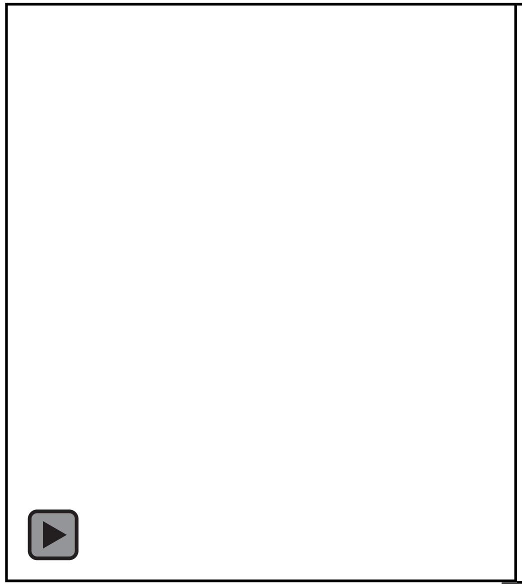
Coherent Single Electron Sources

Feve *et al.*, Science 316 (2007)

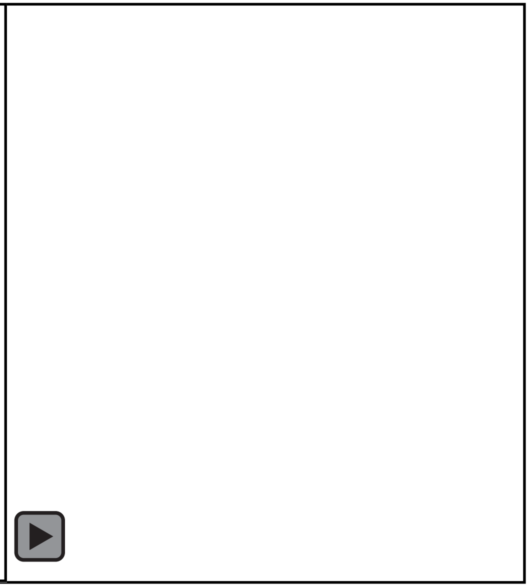
Particle Wigner transport dynamics is a natural choice!

Weinbub and Kosik, J. Phys. Condens. Matt. 34 (2022)

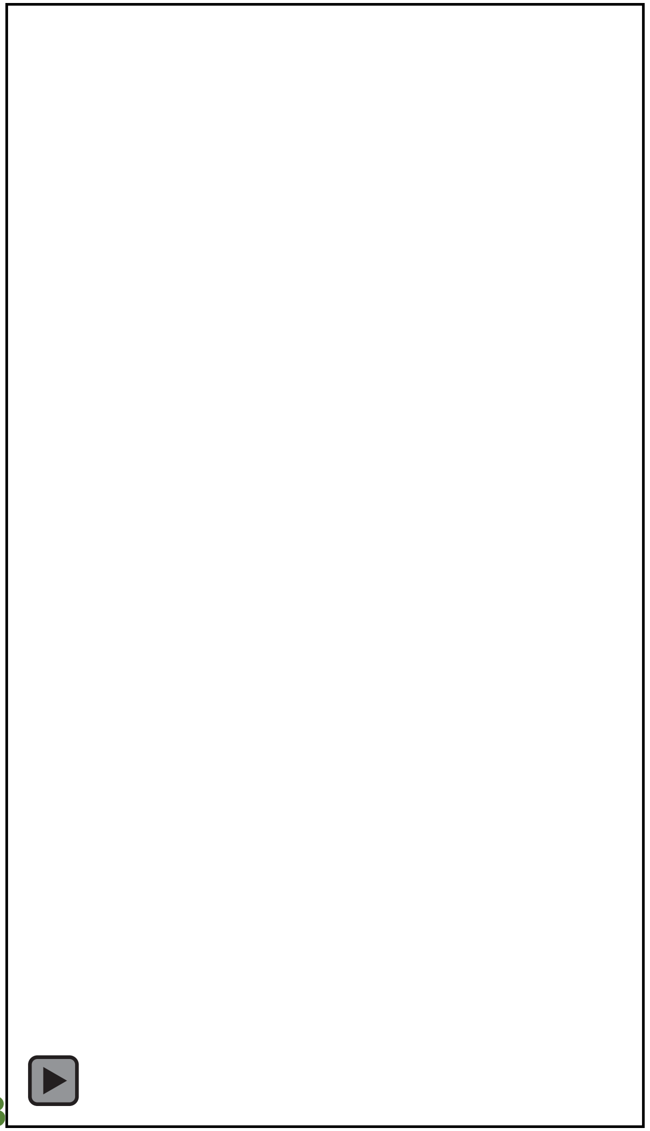
Wigner Modelling of Single-Electron Dynamics



Ballicchia *et al.*
IEEE Nano 2020



Ferry *et al.*
Entropy 22 (2020)



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Nedjalkov *et al.* Phys. Rev. A (2022)
Nedjalkov *et al.* Phys. Rev. B (2019)

TOPICAL REVIEW • OPEN ACCESS

Computational perspective on recent advances in quantum electronics: from electron quantum optics to nanoelectronic devices and systems

Josef Weinbub[3,1] and Robert Kosik[2]

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DOI 10.1088/1361-648X/ac49c6

Motivation

Coherent dynamics of interest!

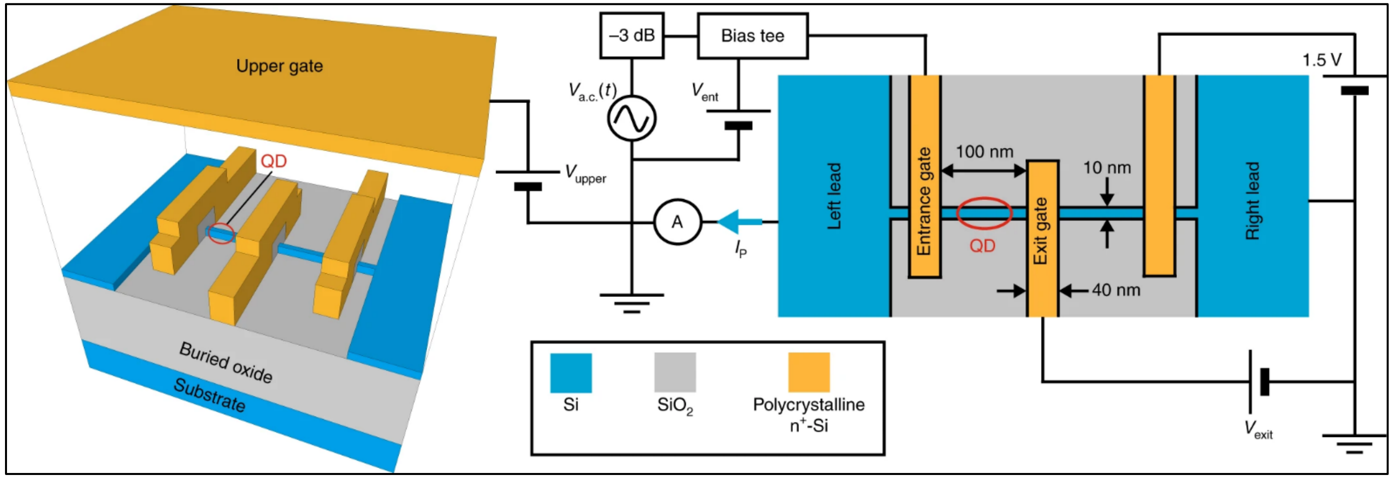
Letter | Published: 04 November 2019

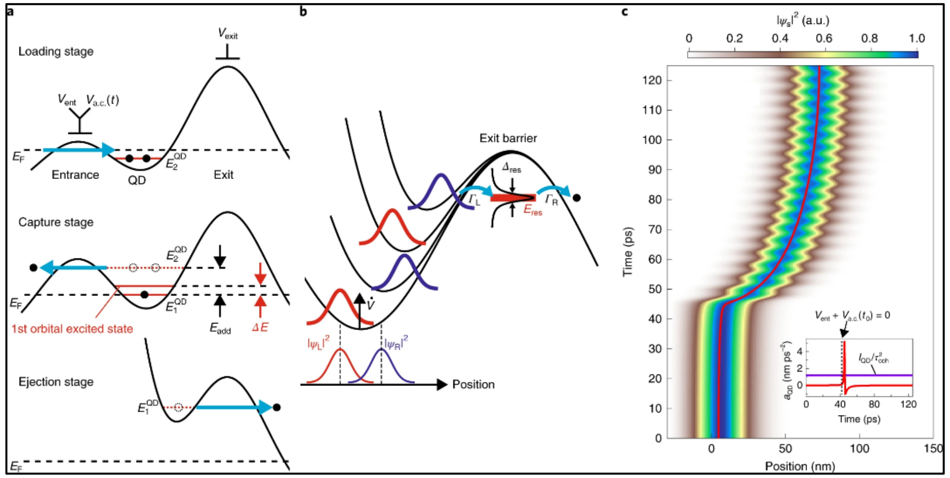
Picosecond coherent electron motion in a silicon single-electron source

Gento Yamahata, Sungguen Ryu, Nathan Johnson, H.-S. Sim, Akira Fujiwara & Masaya Kataoka

Nature Nanotechnology **14**, 1019–1023 (2019) | Cite this article

This talk:
Wigner modeling: oscillation/exit
Impact of timing on wave packet shape
First step into single-electron sources





Yamahata et al., Nature Nanotechnology 14 (2019)

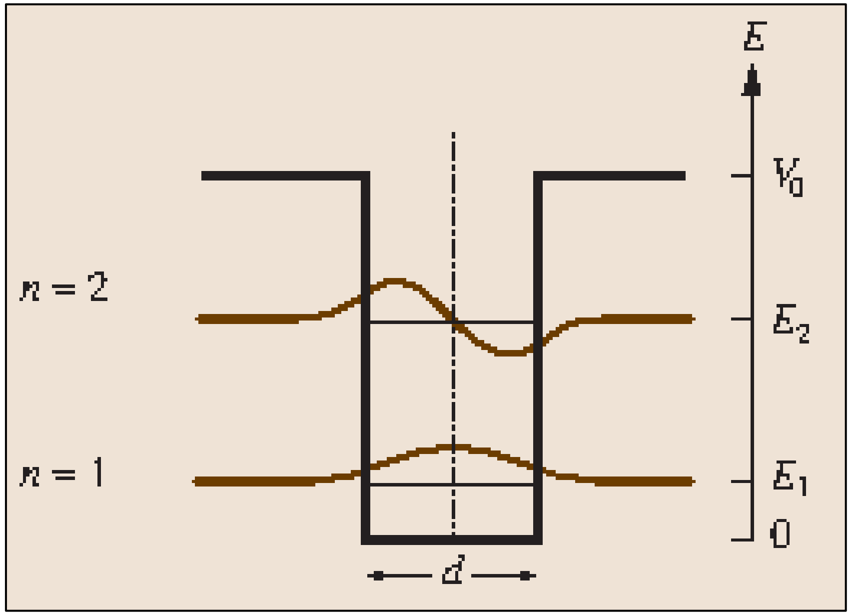
Confined States & Energy Quantization

Stationary Schrödinger equation

$$H(\boldsymbol{r})\psi_n(\boldsymbol{r}) = \epsilon_n \psi_n(\boldsymbol{r})$$

Hamiltonian

$$H(\boldsymbol{r}) = \frac{1}{2m}(-i\hbar\nabla_r)^2 + V(\boldsymbol{r})$$



Eigenvalues

ϵ_1

ϵ_2

ϵ_3

$\vdots$

Eigenfunctions

$\psi_1(\boldsymbol{r})$

$\psi_2(\boldsymbol{r})$

$\psi_3(\boldsymbol{r})$

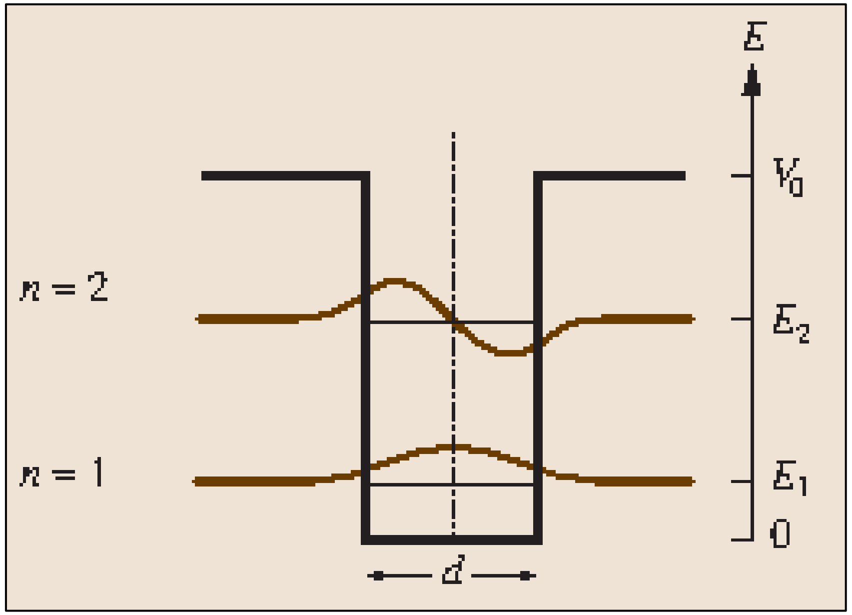
$\vdots$

Electron Quantum Superposition States

Set of Eigenfunctions represents electron state

$$\Psi(r,t) = \sum_n a_n \psi_n(r) e^{-\frac{i}{\hbar}\epsilon_n t}$$

$$\sum_n |a_n|^2 = 1$$



Two energy levels considered: ϵ_1 and ϵ_2

$$\Psi(r,t) = a_1 \psi_1(r) e^{-\frac{i}{\hbar}\epsilon_1 t} + a_2 \psi_2(r) e^{-\frac{i}{\hbar}\epsilon_2 t}$$

Yamahata *et al.*, Nature Nanotechnology 14 (2019)

Electron Quantum Superposition States

Density matrix

$$\rho(r,r',t) = \Psi(r,t)\Psi^*(r',t) = \left(a_1\psi_1(r)e^{-\frac{i}{\hbar}\epsilon_1 t} + a_2\psi_2(r)e^{-\frac{i}{\hbar}\epsilon_2 t}\right)\cdot$$
$$\left(a_1^*\psi_1^*(r)e^{\frac{i}{\hbar}\epsilon_1 t} + a_2^*\psi_2^*(r)e^{\frac{i}{\hbar}\epsilon_2 t}\right)$$

Time evolution probability density at given position based on stationary densities $n_1 = |\psi_1|^2, n_2 = |\psi_2|^2$ of the two Eigenstates

$$n(x,t) = \rho(x,x,t) = |a_1|^2\, n_1(x) + |a_2|^2\, n_2(x) + \Phi(x)cos(\phi(x) - \Delta_\epsilon t)$$

$$x = r = r'$$

$$\Phi(x)e^{i\phi(x)} = a_1\psi_1(x)a_2^*\psi_2^*(x)$$

Probability density of electron quantum superposition state oscillates with a period $T = 2\pi/\Delta_\epsilon$ with $\Delta_\epsilon = (\epsilon_2 - \epsilon_1)/\hbar$

Wigner Dynamics

The Wigner Function $f_w(x,p,t)$ is unitarily equivalent to $\rho(r,r',t) = \Psi(r,t)\Psi^*(r',t)$ after center-of-mass transform

$$x = \frac{r+r'}{2} \qquad x' = r - r'$$

and Fourier transform

$$f_w(x,p,t) = \int \rho\left(x + \frac{x'}{2}, x - \frac{x'}{2}, t\right) e^{-i\frac{sp}{\hbar}}\, ds$$

The initial Wigner function $f_w(x,p,0)$ at $t = 0$ can be obtained from $\rho(r,r',0)$

Wigner Dynamics

Wigner dynamics $f_w(x,p,t)$ in a potential $V(r)$ is obtained from the

- **Initial condition $f_w(x,p,0)$ and**
- **Wigner transport equation**

$$\frac{\partial f_w(x,p,t)}{\partial t} + \frac{p}{m}\frac{\partial f_w(x,p,t)}{\partial x} = \int dp' V_w(x,p-p') f_w(x,p',t)$$

$$V_w(x,p) = \frac{1}{(2\pi\hbar)^3}\int \frac{ds}{i\hbar} e^{-\frac{i}{\hbar}s\cdot p}\left(V\left(x+\frac{s}{2}\right) - V\left(x-\frac{s}{2}\right)\right)$$

Solved by Wigner signed-particle Ensemble Monte Carlo

ViennaWD: https://www.iue.tuwien.ac.at/software/viennawd/

Comparing Probability Density: Schrödinger vs Wigner

Schrödinger

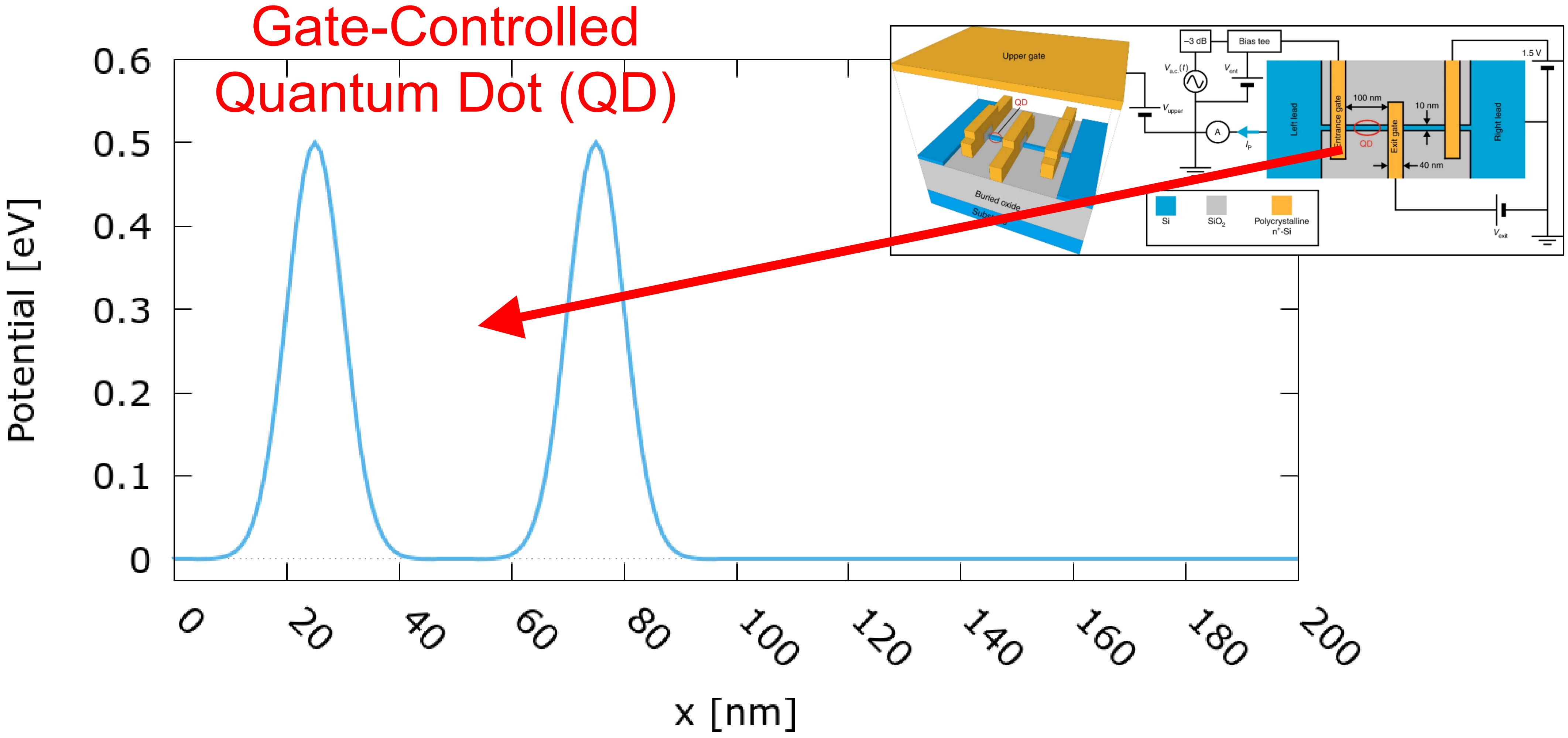
$$n(x,t) = |a_1|^2 n_1(x) + |a_2|^2 n_2(x) + \Phi(x)\cos(\phi(x) - \Delta_\epsilon t)$$

Wigner

$$\frac{\partial f_w(x,p,t)}{\partial t} + \frac{p}{m}\frac{\partial f_w(x,p,t)}{\partial x} = \int dp' V_w(x,p-p') f_w(x,p',t)$$

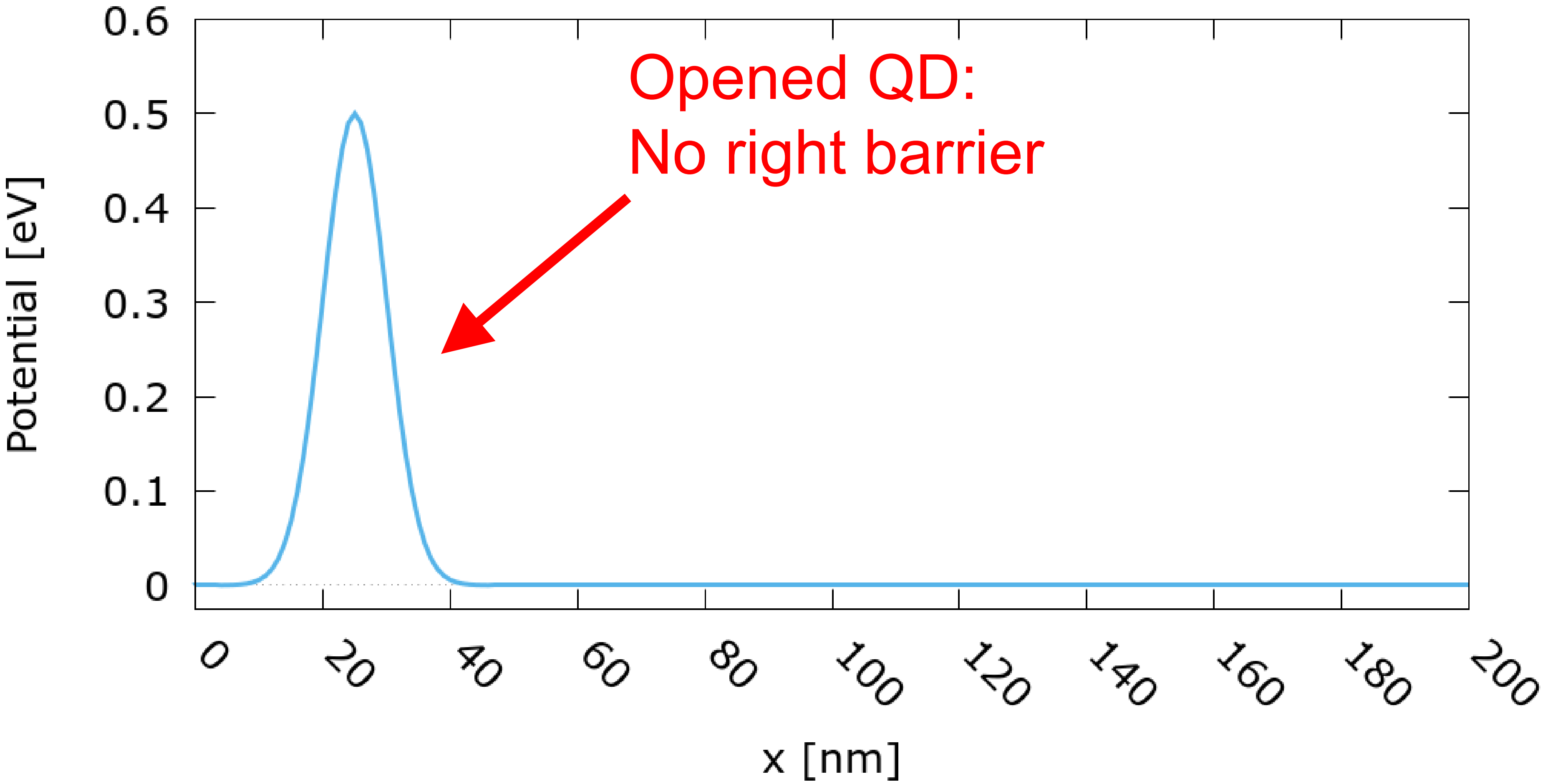
$$n(x,t) = \int f_w(x,p,t)\, dp$$

Simulation Setup: Potential Profiles



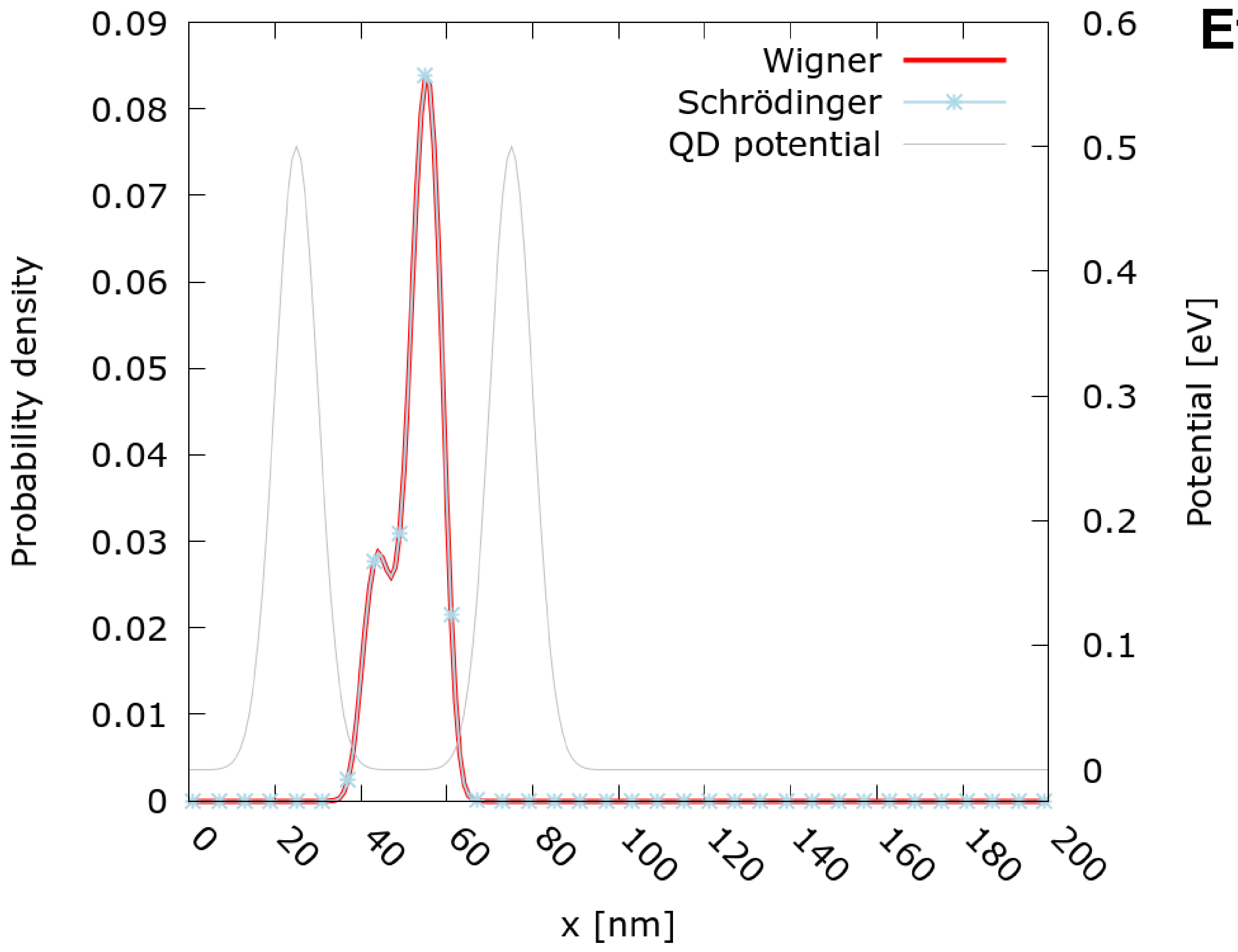
QD is localized by two potential barriers (Gaussians): Height 0.5eV and centered at 25 nm and 75 nm

Simulation Setup: Potential Profiles



The right barrier of the QD can be removed at a specific time instant t_1 (opening time)

Simulation Setup: Initial State



Effective mass of electrons in Si

$$m = 0.19\, m_{\mathrm{el}}$$

Superposition coefficients

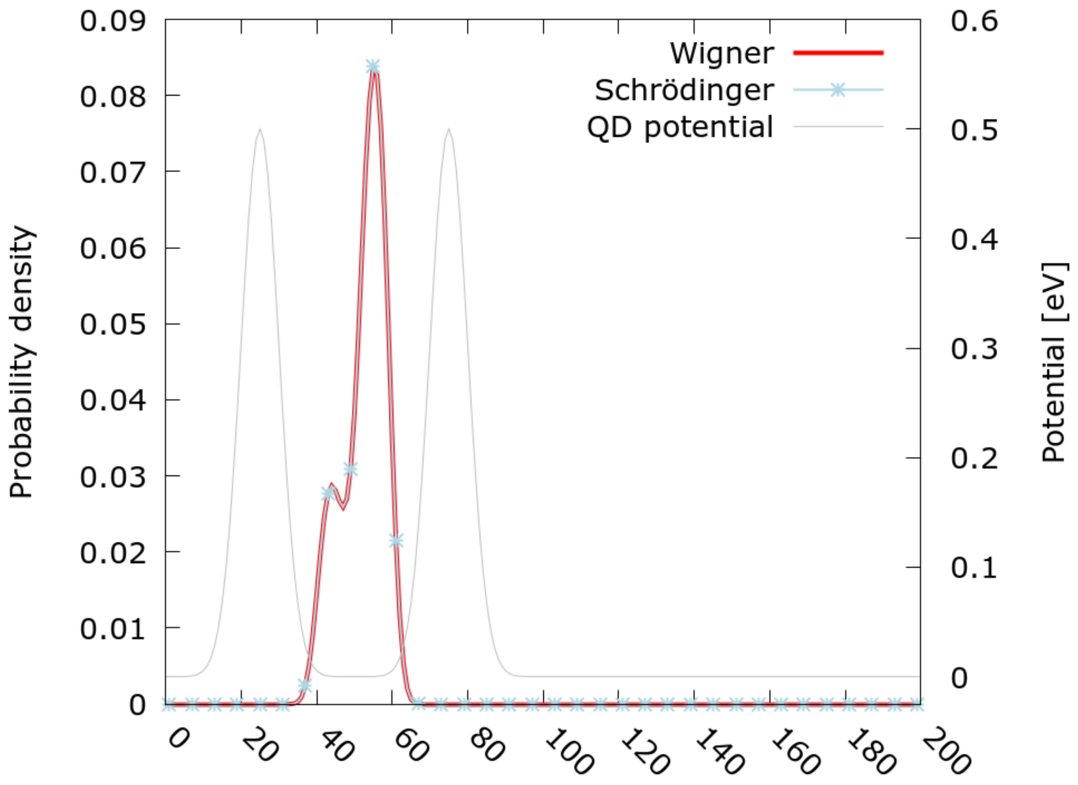
$$a_1 = a_2 = \frac{1}{\sqrt{2}}$$

$$\sum_n |a_n|^2 = 1$$

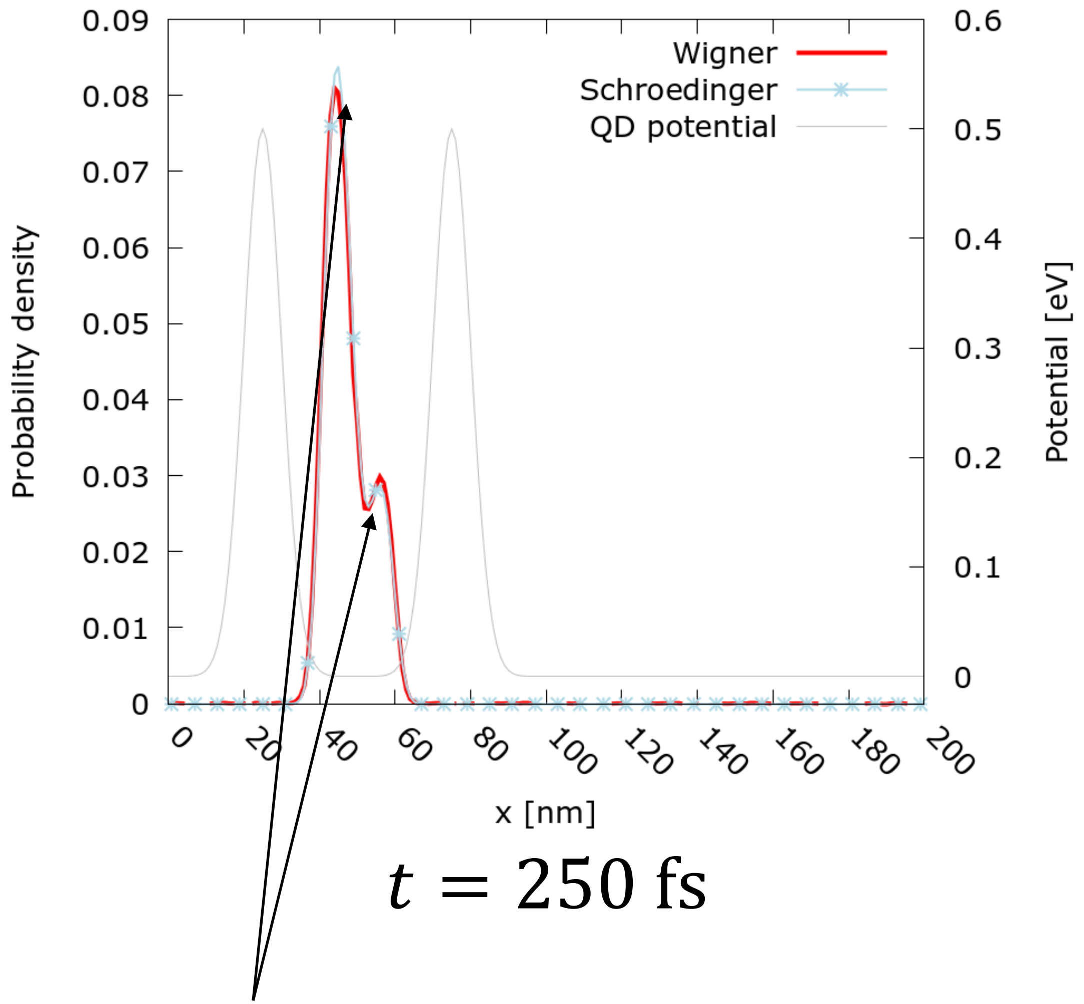
Oscillation period

$$T = \frac{2\pi}{\Delta_\epsilon} = 500\ \mathrm{fs}$$

Coherent Oscillations in QD: Schrödinger vs Wigner



$t = 0$ fs



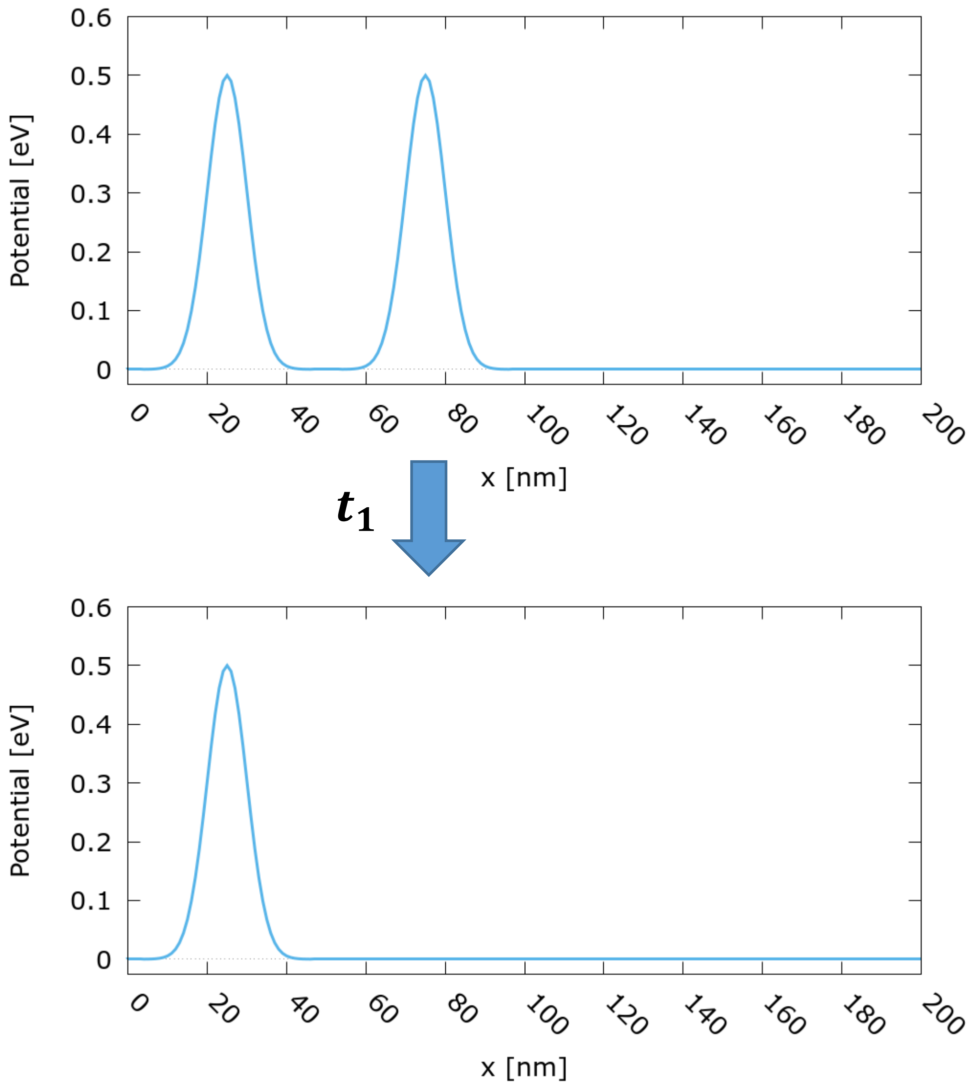
$t = 250$ fs

Monte Carlo sampling approximation

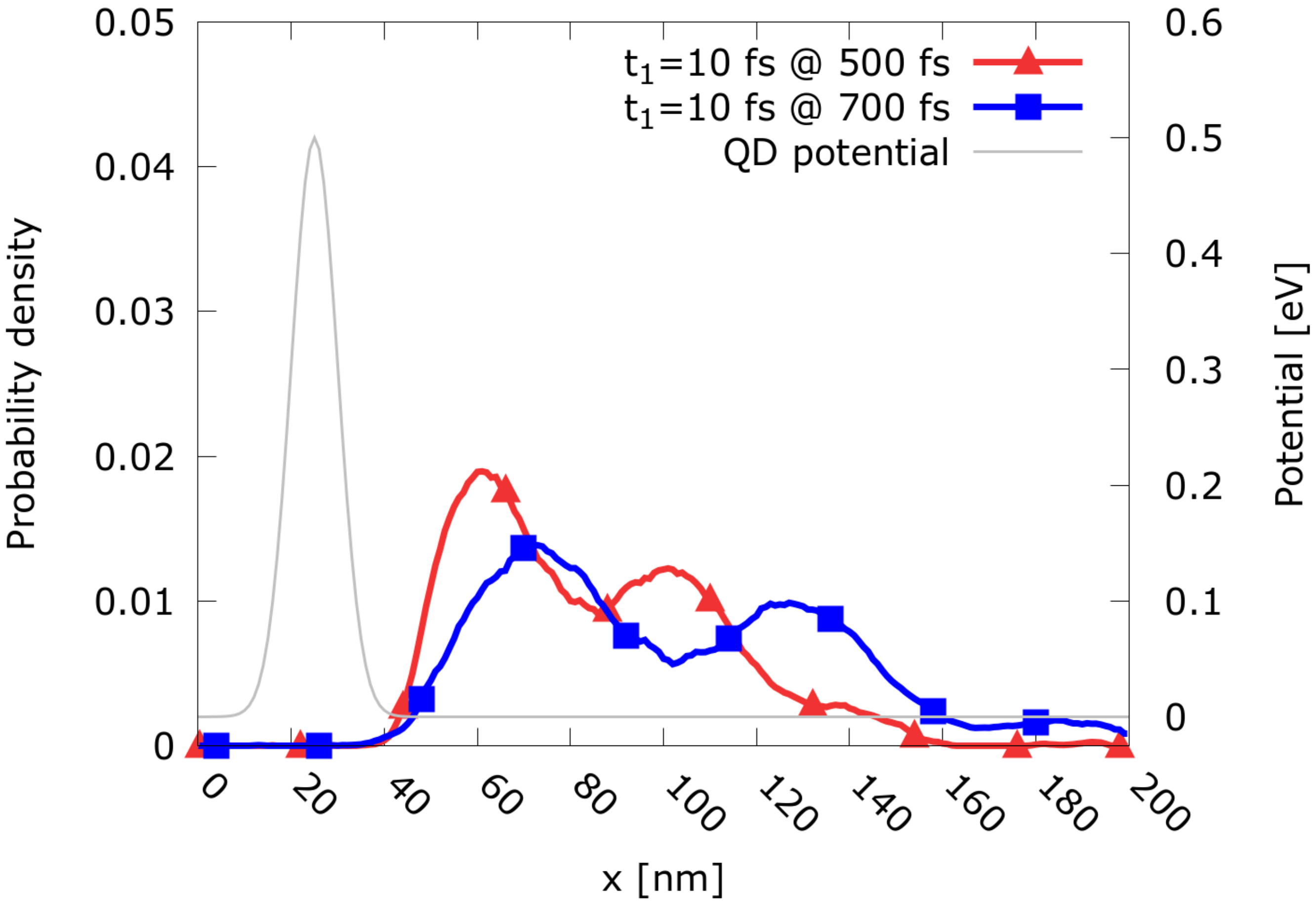
Coherent Evolution Outside of QD

Experiments consider different opening times t_1:

- **CASE I : $t_1 = 10\ \mathrm{fs}$**
- **CASE II : $t_1 = 400\ \mathrm{fs}$**



Coherent Evolution Outside of QD – Case I : $t_1 = 10\ \mathrm{fs}$



Right barrier opened right after start

Different opening times influence shape

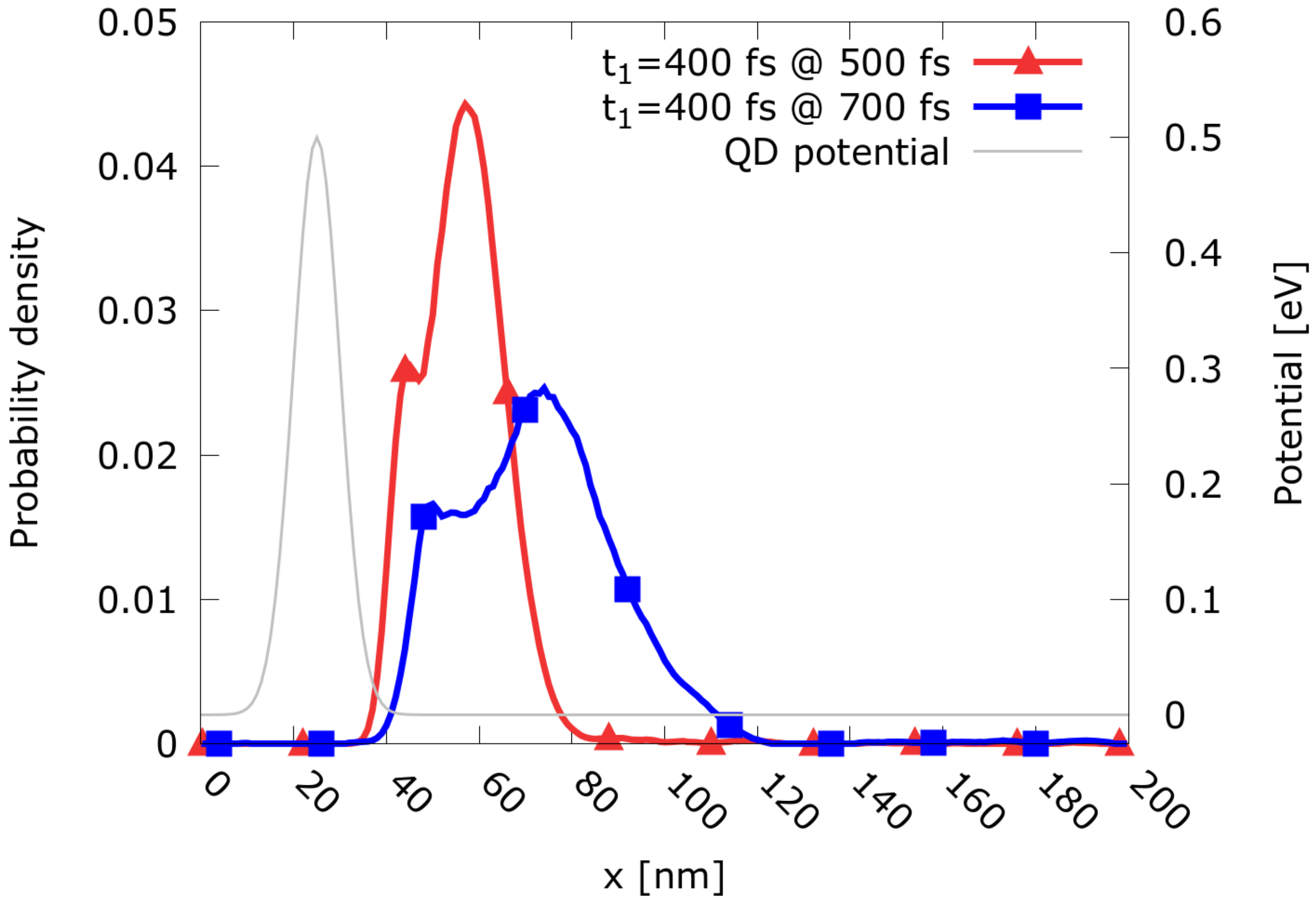
Leading to separation/superposition.

Highest peak before right barrier

Two peaks manifest:

- **Different velocities**
- **Right peak is faster**

Coherent Evolution Outside of QD – Case II : $t_1 = 400\ \mathrm{fs}$



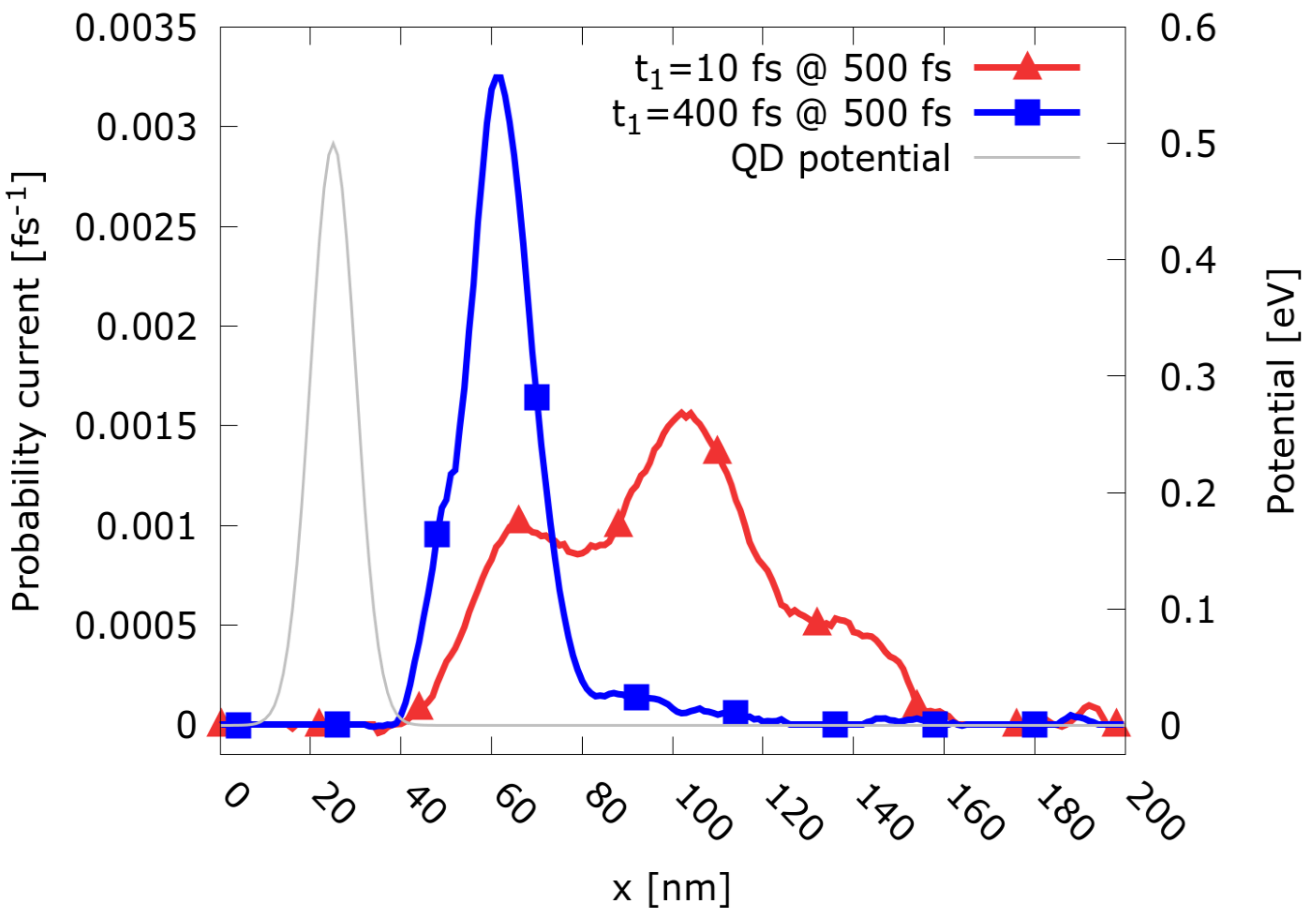
After approximately ¾ of a period

Pronounced right peak

State is compressed before exit:

Exiting peaks are closer together

Probability Current



$$J(x) = \left(\frac{1}{m_{eff}}\right) \int p f_w(x,p) \mathrm{d}p$$

Different opening times clearly result in different probability current

Peak separation (different velocities/energies) vs much stronger localization/magnitude

Summary

These are first steps

Particle Wigner approach ideal for studying electron dynamics

New tool to further optimize design and operation of single electron sources

Next steps

Determining ideal scenario and optimize: Is compressed even ideal?

Extended parameter study

Experimental verification

Free Webinar Series of TC-10

https://tinyurl.com/26j3uf5m

Date: June 27, 2023 Time: 8:00 PDT, 17:00 CEST, 00:00 JST Philippe Blaise, Silvaco *Atomistic TCAD Simulations*	Date: October 12, 2023 Time: 16:00 PDT, 1:00 CEST, 08:00 JST Gerhard Klimeck, Purdue University *nanoHUB for Research and Education in Nanoelectronics*	Date: December 12, 2023 Time: 23:00 PDT, 8:00 CEST, 15:00 JST Tue Gunst, Synopsys *QuantumATK Applied to Nanoelectronics*