Simulation of laser-induced rectification in a nano-scale diode

Presenter: XJ Xu

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Modern age of electronics

ENIAC (1956)

- 20,000 vacuum-tubes
- 5,000 Hz operations on 10 digit numbers
- Power: 150 kW

Sunway TaihuLight (2017)

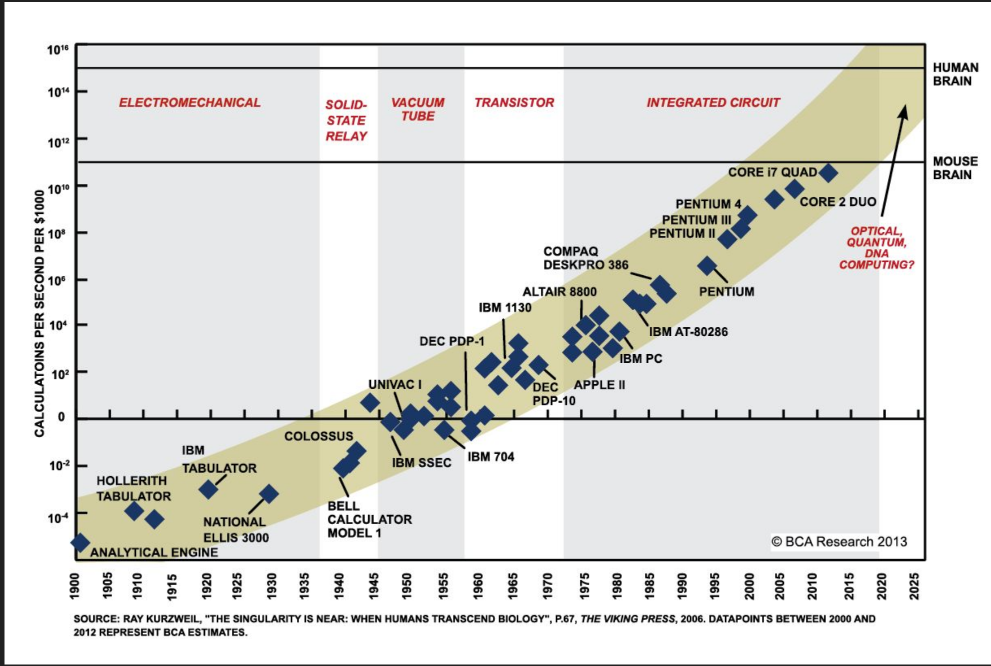
- 40,960 SW26010 processors
- 3.06 TFLOPS per processor
- Power: 15 MW

Lower power consumption by scale, higher reliability, and more intuitive circuit design.

Weik, Martin H. (December 1955).
https://www.top500.org/

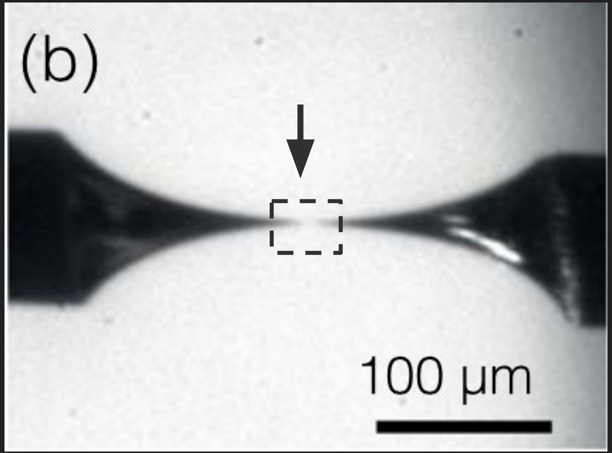
Pushing for the petahertz range

- Limited electron transport velocity in semiconductor transistors.
- Recent interest in electron photoemission from metal nanotips.
- Ultrafast laser-guidance of electrons.
- This inspired research pointing back to vacuum transport to take advantage of higher vacuum transport velocities.

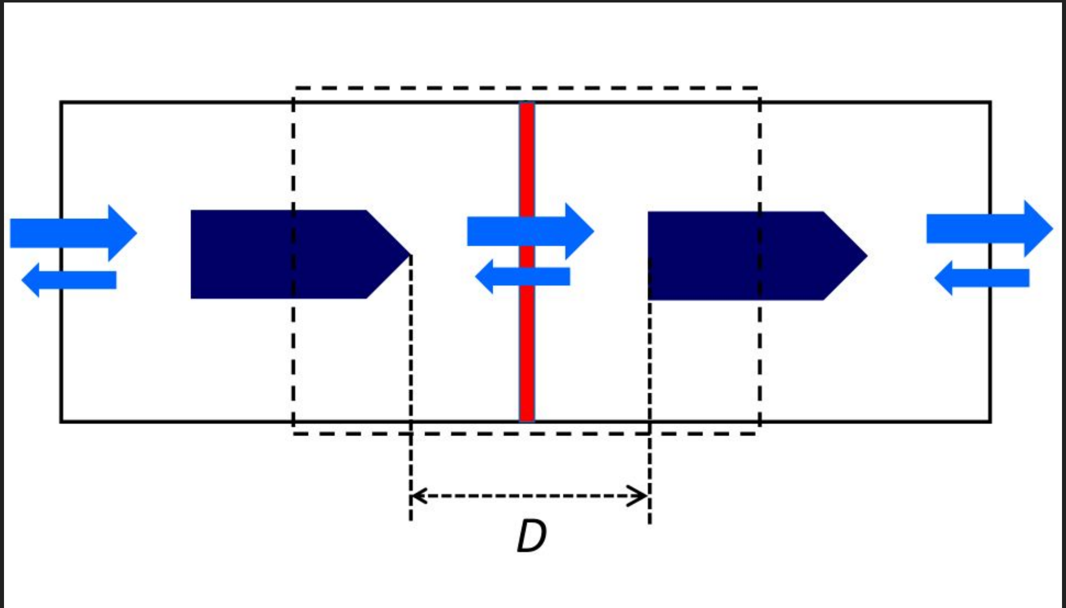


Diamant, E. Halahmi, L. Kronik, J. Levy, R. Naaman, and J. Roulston, Appl. Phys. Lett. **92**, 262903 (2008).
J.-W. Han, J. S. Oh, and M. Meyyappan, Appl. Phys. Lett. **100**, 213505 (2012).
J.-W. Han, D.-I. Moon, and M. Meyyappan, Nano Lett. **17**, 2146 (2017).

Jellium model



Optical microscopic image of opposing tungsten nanotips.
Higuchi et al. (2015)



D = 30 Å

T. Higuchi, L. Maisenbacher, A. Liehl, P. Dombi, and P. Hommelhoff, Appl. Phys. Lett. **106**, 051109 (2015).

Homogeneous laser field

The form of the laser field is a variation of the smooth turn-on pulse.

- Wavelength of 780 nm
- Polarized parallel to the axis of symmetry

$$\mathbf{E}_{\text{laser}}(t) = \begin{cases} -\mathbf{E}_0 \sin\left(\dfrac{\pi t}{2T_{\text{r}}}\right) \sin(\omega t + \varphi), & \text{if } 0 \leq t \leq T_{\text{r}}, \\ -\mathbf{E}_0 \sin(\omega t + \varphi), & \text{otherwise,} \end{cases}$$

Where **φ** is the phase of the laser and $\mathbf{T_r}$ is the ramping time.
The vector potential is then:

$$\mathbf{A}(t) = -\int_0^t \mathbf{E}_{\text{laser}}(t')dt'$$

RT-TDDFT

We solve the time-dependent Kohn-Sham equation

$$i\hbar \frac{\partial \phi_j(\mathbf{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{KS}}[\rho](\mathbf{r},t) \right] \phi_j(\mathbf{r},t)$$

The Kohn-Sham potential is a functional of the density and consists of 3 terms:

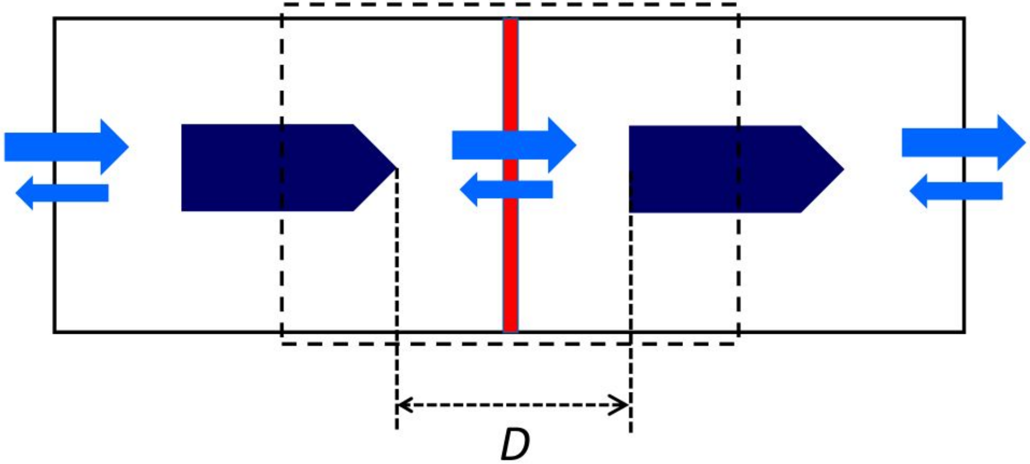
1) the Hartree potential
2) the exchange-correlation potential (using LDA)
3) the external potential (includes V_{laser})

$$V_{\mathrm{laser}}(\mathbf{r},t) = \frac{1}{2m}|\mathbf{A}(t)|^2 - \frac{i\hbar}{m}\mathbf{A}(t)\cdot\nabla$$

Time propagation using split-operator:

$$\Psi(t+\triangle t) = e^{i\hat{H}\triangle t/\hbar}\Psi(t)$$

Induced current **j** and flux $\mathbf{\Phi}$



The induced oscillating current is:

$$\mathbf{j}(\mathbf{r},t) = 2\sum_{j=1}^{N} \frac{\hbar}{2mi}(\phi_j^* \nabla \phi_j - \phi_j \nabla \phi_j^*) + \frac{1}{m}\mathbf{A}\rho$$

The resulting flux at the plane bisecting the two edges of the jellium model:

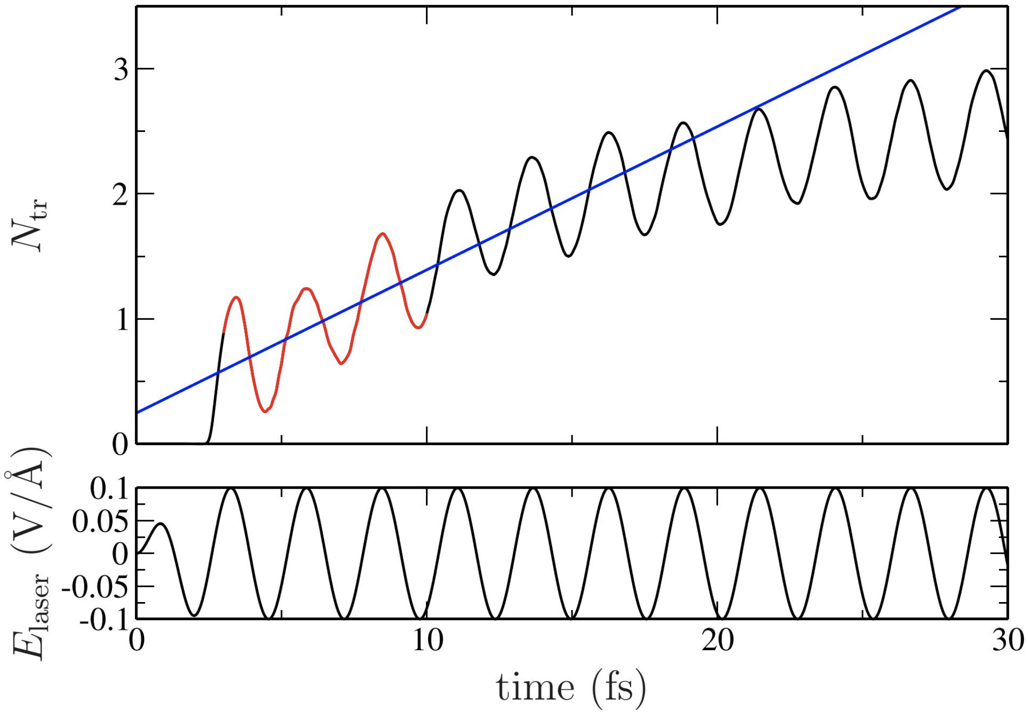
$$\Phi(z_0,t) = \int \mathbf{j}(\mathbf{r},t)\delta(z-z_0)d\mathbf{r}$$

Calculating the results

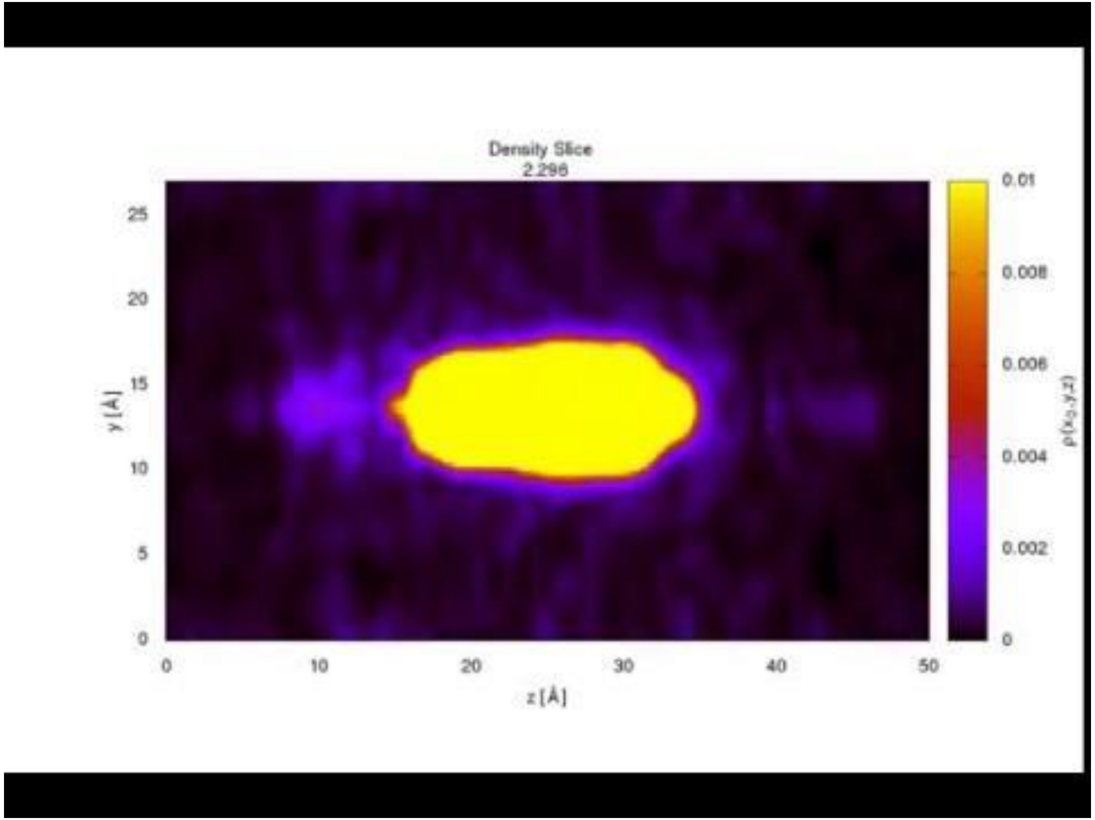
- The flux at the boundary of is integrated with respect to time

$$N_{\mathrm{tr}}(t) = \int_0^t \Phi(t')dt'$$

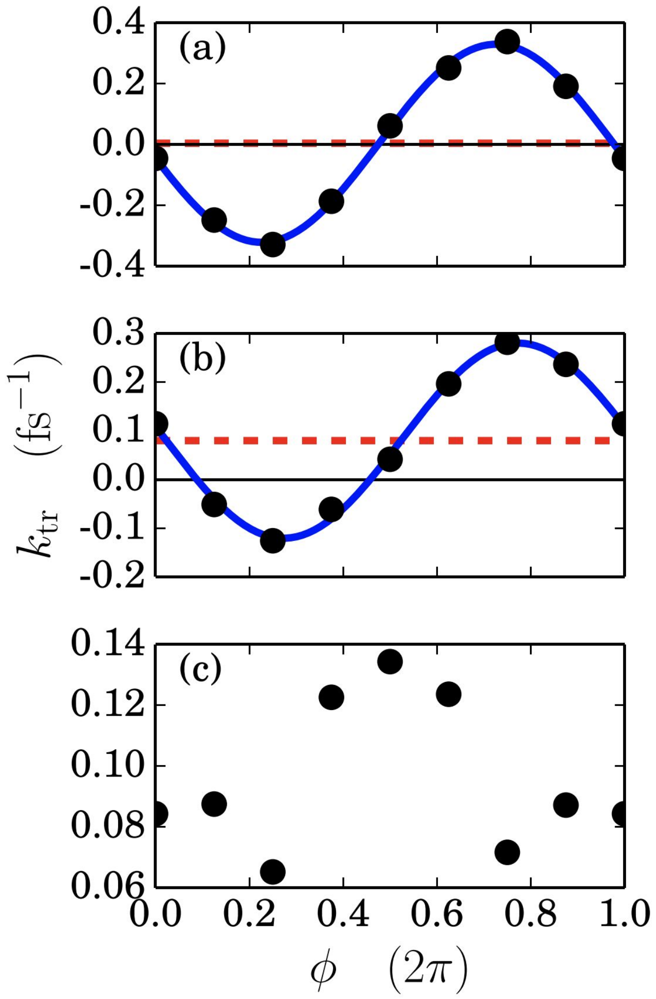
- We find the **probability density transferred N_{tr}**
- The **probability density transfer rate k_{tr}** is determined with linear regression of $t \leq 15$ fs
- k_{tr} levels off $15 \leq t \leq 50$
- Parameters:
  - Separation distance: 30 Å
  - Field intensity: 1.33×10^{13} W/cm^2
  - Ramping time $T_r = 2.48$ fs



20 Å diode with 30 Å separation



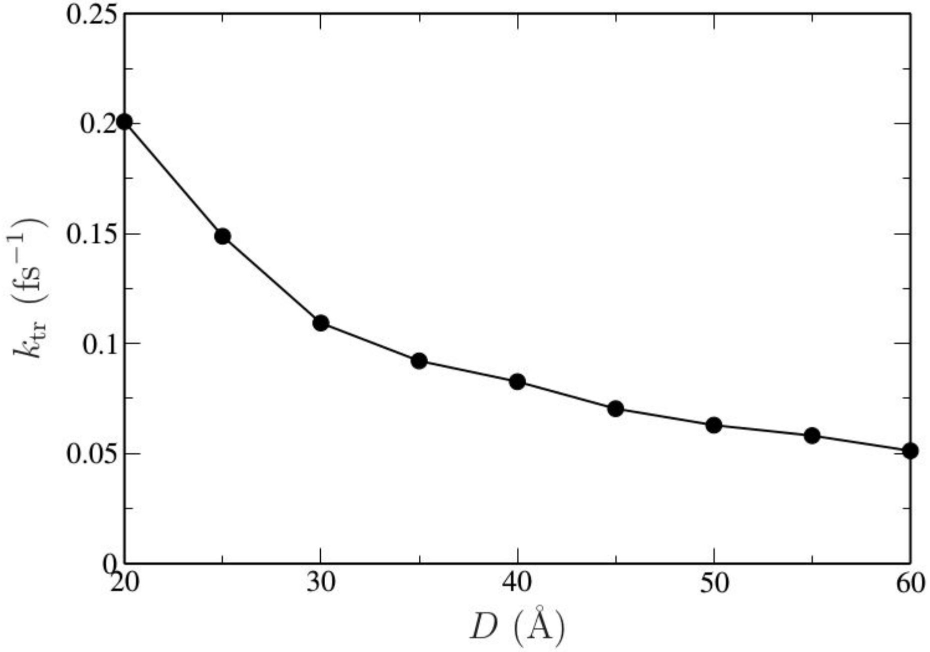
Phase shift dependence



a) Symmetric cylinder jellium model with ramping time (control run)
   T_r = 2.48 fs
b) Diode jellium model with ramping time
   T_r = 2.48 fs
c) Diode jellium model with ramping time
   T_r = 9.94 fs

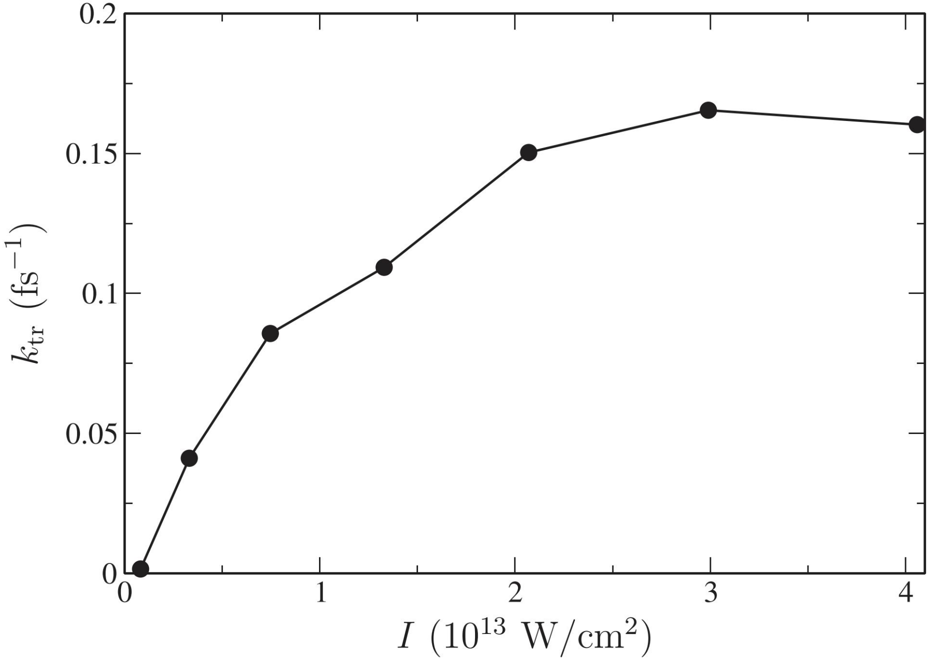
- In fig (a), the short ramping time makes the system sensitive to phase shifts.
- Positive offset in fig (b) as opposed to negligible offset in fig (a)
- Phase shift becomes insignificant if the ramping time is long enough.

Dependence of separation distance, D



- We simply change the size of the computational box to vary D
- Parameters kept constant:
  $I = 1.33 \times 10^{13}$ W/cm^2
  $T_r = 9.94$ fs
- Results from simulations with phases of 0 and π were averaged to **eliminate phase dependence**
- Approximately exponential decay

Dependence of intensity, I



- Phase shift dependence is eliminated in a similar fashion
- Parameters kept constant:
  - D = 30 Å
  - T_r = 9.94 fs
- For sufficiently high intensities, the local near-field enhancement becomes negligible.

Conclusions

- We have computationally demonstrated laser-induced rectification by simulating the effects of increased electron emission due to near-field enhancement within a periodic jellium system with geometrical asymmetry.
- Opening new doors for new nanoscale "vacuum-tube-based" devices
- Approximately exponential increase in transport rate for small separations
- Convergence of transport rate for higher laser intensities
- The paper is available at:

Daniel Kidd, Xiaojia Xu, Cody Covington, Kazuyuki Watanabe, Kalman Varga.

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