Tight-Binding Ehrenfest Molecular Dynamics Studies of Electronic Stopping in Metals

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Joint ICTP-IAEA Workshop on Non-Adiabatic Dynamics and Radiation Damage in Nuclear Materials

Imperial College London

Outline

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Basis Sets

- Most of the methods used to solve the one-electron Schrödinger equation use a basis set.
- Having chosen a set of basis functions $\{\phi_1(\mathbf{r}), \phi_2(\mathbf{r}), \ldots\}$, the wavefunction is expanded as

$$\psi_i(\mathbf{r}) = \sum_\alpha c_{i\alpha}\phi_\alpha(\mathbf{r})$$

and the Schrödinger equation becomes

$$\left[-\frac{1}{2}\nabla^2 + V_{\text{eff}}\right]\sum_\alpha c_{i\alpha}\phi_\alpha(\mathbf{r}) = \varepsilon_i \sum_\alpha c_{i\alpha}\phi_\alpha(\mathbf{r})$$

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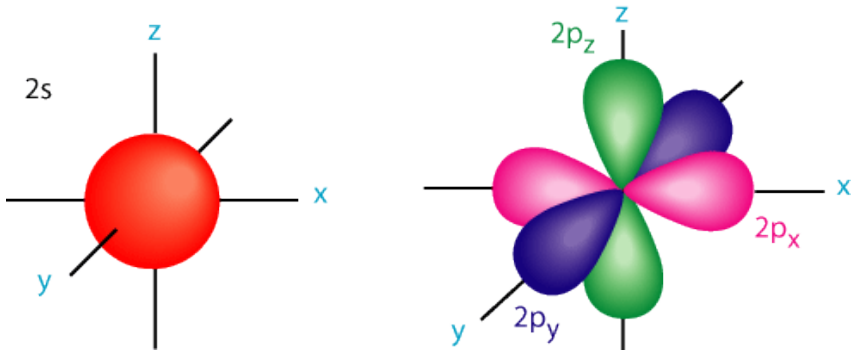
- Multiplying both sides by $\phi^*_\beta(\mathbf{r})$ and integrating over $\mathbf{r}$ yields the matrix version of the Schrödinger equation

$$\sum_\alpha H_{\beta\alpha} c_{i\alpha} = \varepsilon_i \sum_\alpha S_{\beta\alpha} c_{i\alpha}$$

where

$$\begin{aligned} H_{\beta\alpha} &= \langle\phi_\beta| \left(-\frac{1}{2}\nabla^2 + V_{\text{eff}}\right) |\phi_\alpha\rangle \\ S_{\beta\alpha} &= \langle\phi_\beta|\phi_\alpha\rangle \end{aligned}$$

Tight-Binding Models



- Choose a basis set of atomic or atomic-like orbitals. This makes good sense in the tight-binding limit, when the atoms are far apart and the orbital overlap is small.
- By using more orbitals per atom, the basis can be made arbitrarily accurate.
- Matrix elements between orbitals on different atoms decrease exponentially as the interatomic separation increases.
- The tight-binding **H** and **S** matrices are sparse.

Ab-Initio Tight-Binding

In ab initio tight-binding calculations

- The Hamiltonian and overlap matrix elements are evaluated numerically.
- If the basis is good enough, this can yield accurate results even for solids that are nowhere near the tight-binding limit.

Semi-Empirical Tight-Binding

In semi-empirical tight-binding calculations

- The Hamiltonian and overlap matrix elements are fitted to various physical properties (band structures, total energies of various crystal and molecular structures, phonon frequencies, defect formation energies, . . .).
- The matrix elements between orbitals on different atoms decay in some simple way (which is also fitted) with inter-atomic distance.
- The underlying orbitals (which are never used directly) are often assumed to be orthogonal, so that the overlap matrix is the identity.

The SETB Total Energy

- The eigenvalues ϵ_i are calculated by solving the matrix eigenvalue problem for the solid. The total energy is then

$$\begin{aligned} E &= \sum_{i \text{ occ}} \epsilon_i + \frac{1}{2} {\sum_{a,b}}' V_{ab}^{\text{pair}}(|\mathbf{R}_a - \mathbf{R}_b|) \\ &= \sum_{i \text{ occ}} \sum_{\alpha,\beta} c_{i\alpha}^* H_{\alpha\beta} c_{i\beta} + \frac{1}{2} {\sum_{a,b}}' V_{ab}^{\text{pair}}(|\mathbf{R}_a - \mathbf{R}_b|) \end{aligned}$$

  where $V_{ab}^{\text{pair}}(|\mathbf{R}_a - \mathbf{R}_b|)$ is a repulsive pair potential between atoms a and b, meant to represent the ion-ion repulsion and double-counting contributions.

- This fitting-based approach is similar in style to the methods used to construct classical interatomic potentials, but SETB is better because it offers a more plausible treatment of QM bond formation.

Ordinary Ehrenfest Dynamics

In ordinary Ehrenfest dynamics, the conserved total energy is

$$\frac{P^2}{2M} + \int \Phi \left(-\frac{1}{2}\nabla_{\mathbf{r}}^2 + V(\mathbf{r}, \mathbf{R}) \right) \Phi \, d\mathbf{r}$$

and the equations of motion are

$$\begin{aligned} i\frac{\partial \Phi}{\partial t} &= \left[-\frac{1}{2m}\boldsymbol{\nabla}_{\mathbf{r}}^2 + V(\mathbf{r}, \mathbf{R}(t)) \right] \Phi \\ \frac{dP}{dt} &= \int \Phi^* \left(-\boldsymbol{\nabla}_{\mathbf{R}} V \right) \Phi \, d\mathbf{r} \end{aligned}$$

Tight-Binding Ehrenfest Dynamics

In TB Ehrenfest dynamics, the conserved total energy is

$$\frac{P^2}{2M} + \sum_{i \text{ occ}} \sum_{\alpha,\beta} c_{i\alpha}^* H_{\alpha\beta} c_{i\beta} + \frac{1}{2} \sum_{a,b}{}' V_{ab}^{\text{pair}}(|\mathbf{R}_a - \mathbf{R}_b|)$$

and the equations of motion are

$$\begin{aligned} i\frac{dc_{i\alpha}}{dt} &= \sum_{\beta} H_{\alpha\beta} c_{i\beta} \\ \frac{d\mathbf{P}}{dt} &= \sum_{i \text{ occ}} \sum_{\alpha,\beta} c_{i\alpha}^* \left(-\nabla_{\mathbf{R}} H_{\alpha\beta}\right) c_{i\beta} \end{aligned}$$

- We have assumed that the basis set is orthonormal ($\mathbf{S} = \mathbf{I}$).
- The solution vectors $\mathbf{c}_i(t)$ can be evolved using a finite difference approximation (e.g., RK4).

The Density Matrix

In practice, we work with the density matrix

$$\rho_{\beta\alpha} = \sum_{i \text{ occ}} c_{i\beta} c^*_{i\alpha}$$

- The equation of motion of the density matrix is

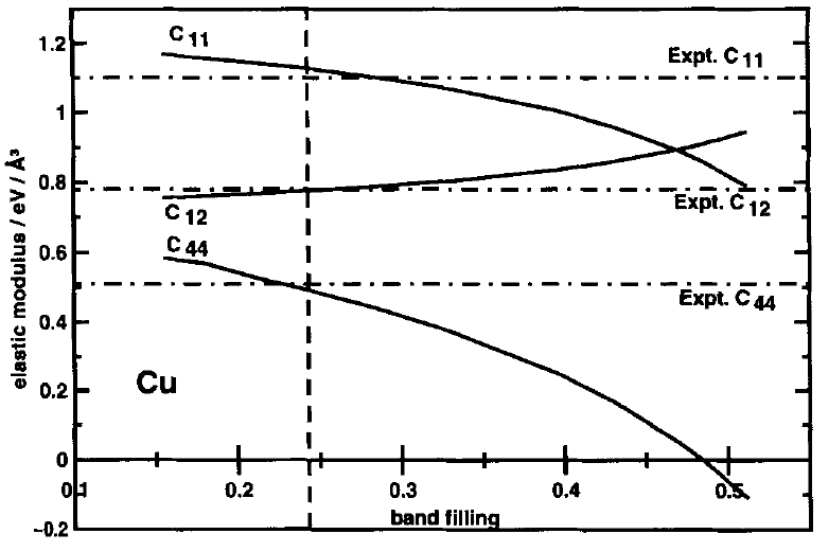
$$\frac{d\boldsymbol{\rho}}{dt} = -i[\mathbf{H}, \boldsymbol{\rho}]$$

  Solving this matrix ODE evolves all of the one-electron orbitals simultaneously.
- Setting the initial electronic temperature is easy:

$$\rho_{\beta\alpha} = \sum_{\text{all } i} f(\epsilon_i) c_{i\beta} c^*_{i\alpha}$$

Bolonium

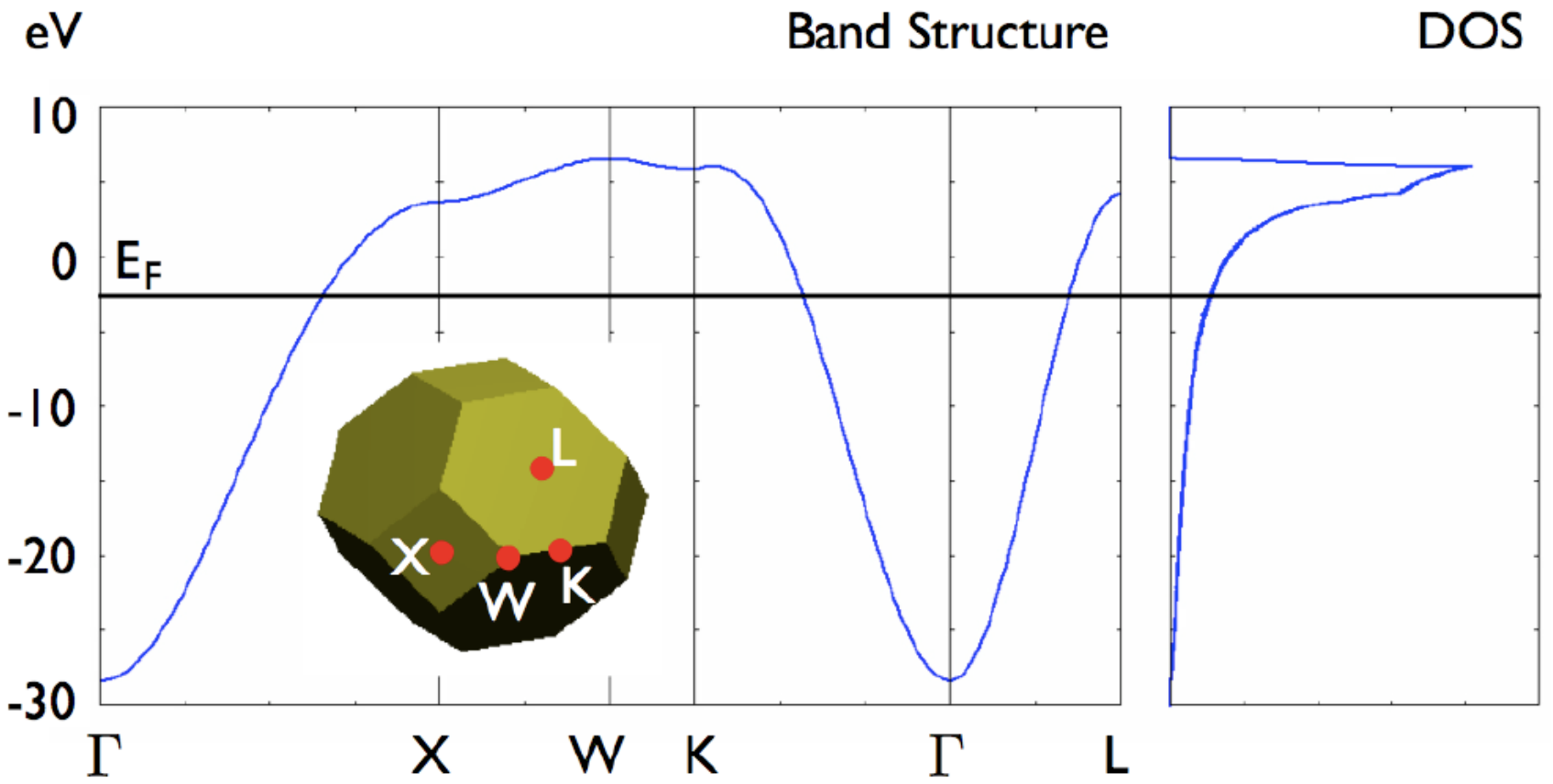
- Orthogonal TB model with one *s* orbital per atom
  - Inverse power laws for matrix elements and pair repulsion.
  - Parameters fitted to FCC volume, cohesive energy, bulk modulus.
  - Band filling is a parameter.



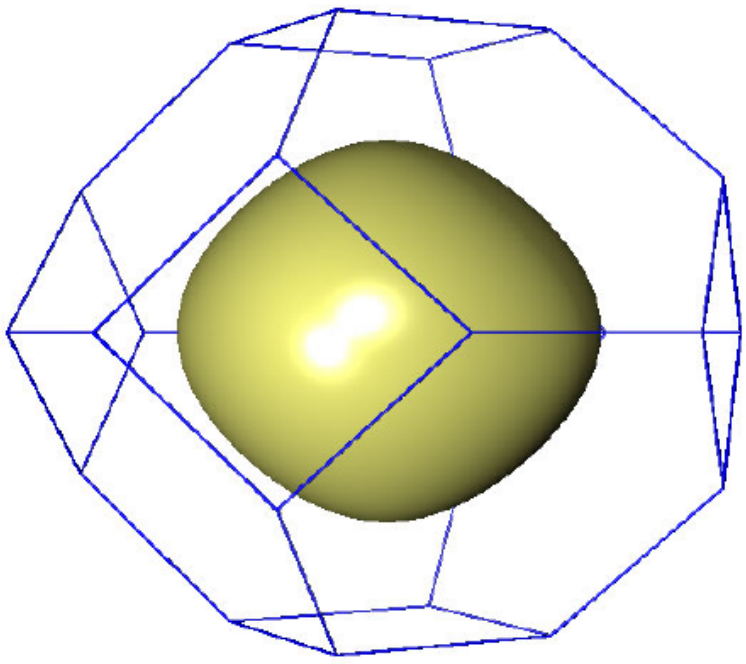
  - Surprisingly good description of structural properties of Cu.
  - Hartree terms are included in most of our calculations.

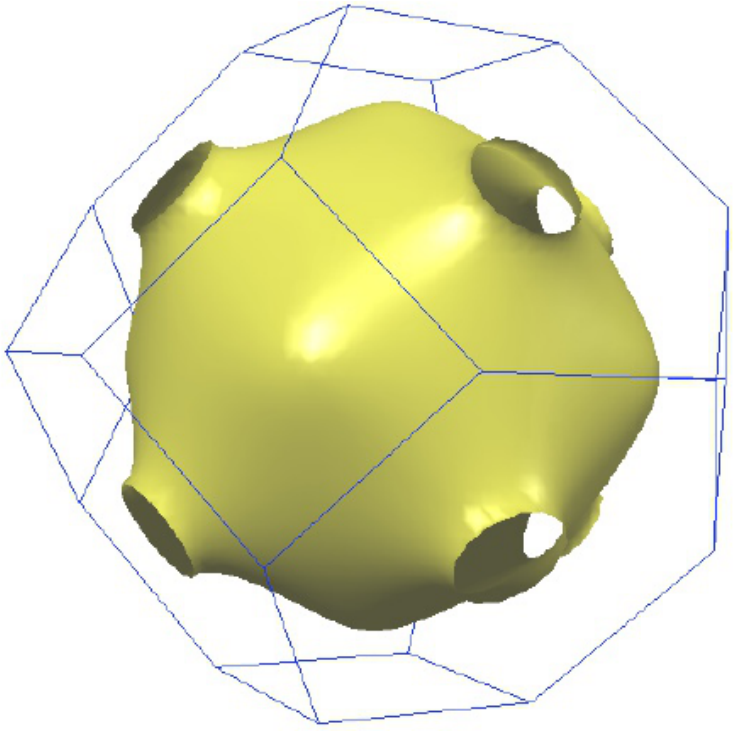
(Sutton *et al.*, Phil. Mag. **81**, 1833 (2001))

Bolonium Bandstructure



Bolonium Fermi Surface





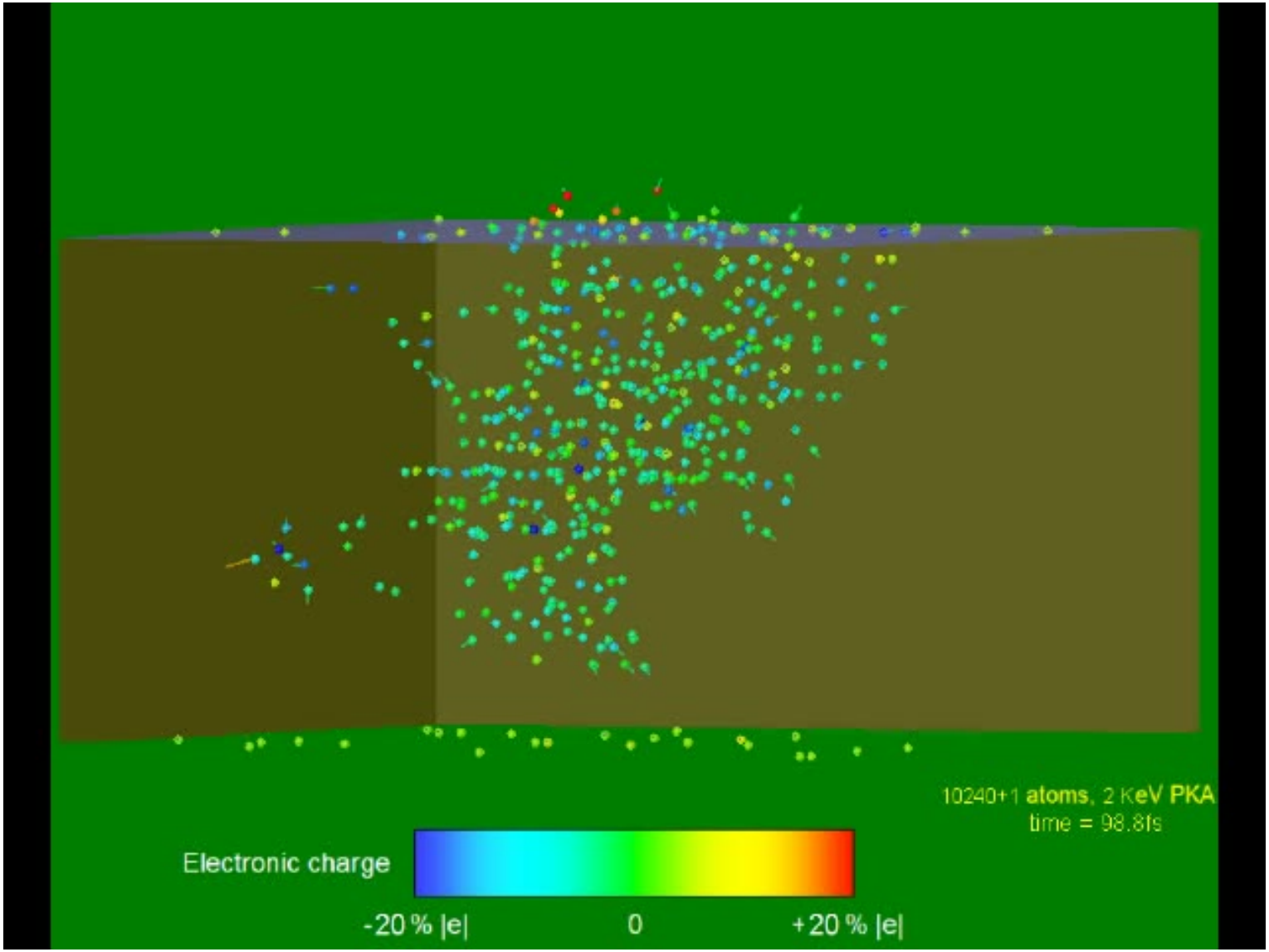
spICED

sparse parallel Imperial College Ehrenfest Dynamics

- Written by Daniel Mason
- Density matrix formalism
- The density matrix itself is *not* sparse
- F95
- MPI
- RK4

(www.cmth.ph.ic.ac.uk/people/d.mason/RadiationDamage/index.html)

Sputtering Simulation



Outline

Testing the Ehrenfest Approximation

How can we test the Ehrenfest approximation?

Apply it to a system simple enough to be solved exactly

A system of harmonic phonons interacting weakly with a bath of non-interacting electrons is an obvious choice.

Validity of the Ehrenfest Approximation

Consider a system of electrons (initially at temperature T_{el}) weakly coupled to a system of phonons (initially at temperature T_{ion}). The energy transferred to the electrons

$$\Delta E_e(t) \;=\; \langle \Psi(t)|\hat{H}_{\mathrm{QM}}|\Psi(t)\rangle - \langle \Psi(t=0)|\hat{H}_{\mathrm{QM}}|\Psi(t=0)\rangle$$

may be calculated both in exact QM and in the Ehrenfest approximation using perturbation theory (FGR).

$$\mathrm{QM} \;=\; \frac{2\pi t}{\hbar}\sum_{\mathbf{q},\lambda}\hbar\omega_\lambda(\mathbf{q})\left\{\langle N_{\mathbf{q},\lambda}\rangle\mathfrak{A}(\omega_\lambda(\mathbf{q})) - \left(\langle N_{\mathbf{q},\lambda}\rangle + 1\right)\mathfrak{E}(\omega_\lambda(\mathbf{q}))\right\}$$

$$\mathrm{Ehr} \;=\; \frac{2\pi t}{\hbar}\sum_{\mathbf{q},\lambda}\hbar\omega_\lambda(\mathbf{q})\left\{\langle N_{\mathbf{q},\lambda}\rangle\mathfrak{A}(\omega_\lambda(\mathbf{q})) - \langle N_{\mathbf{q},\lambda}\rangle\mathfrak{E}(\omega_\lambda(\mathbf{q}))\right\}$$

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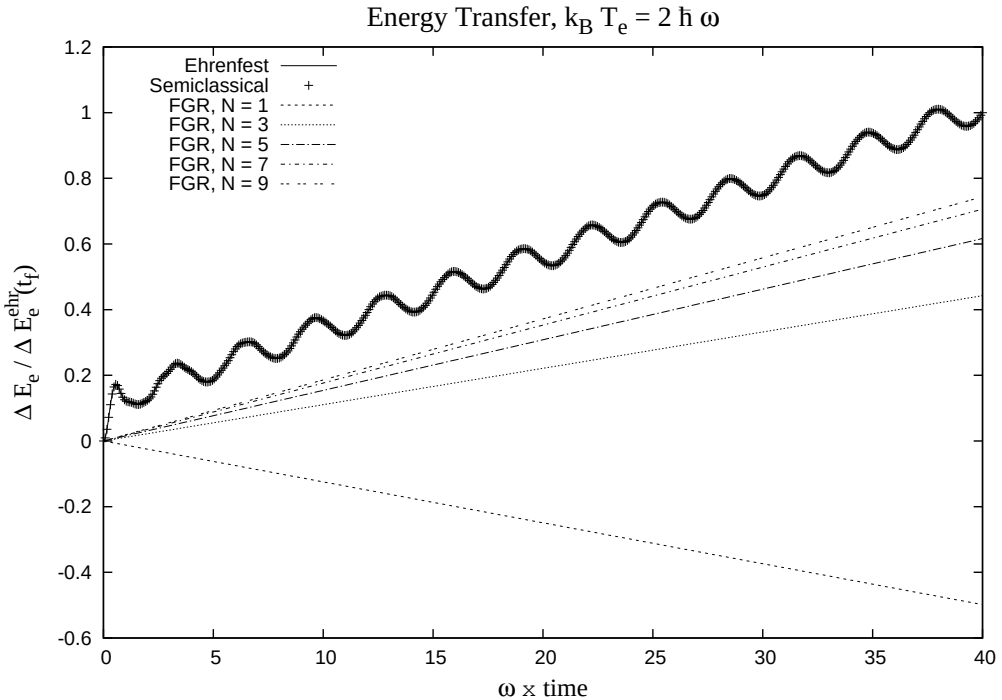
Only difference is spontaneous phonon emission term

Validity of the Ehrenfest Approximation

- For a system of electrons and phonons, can calculate energy transferred to electrons exactly using FGR.
- Ehrenfest neglects spontaneous emission of phonons by electrons; stimulated emission and absorption treated properly.
- Spontaneous phonon emission negligible when $T_{ion} \gg T_{el}$.



- Ehrenfest phonons do not equilibrate with the electrons; the ions lose KE continuously and eventually come to rest.

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Outline

Electronic Friction

Several attempts have been made to model electronic stopping in the low-energy regime by adding a drag to MD simulations:

$$M\ddot{\mathbf{R}} = -\nabla V - \beta\dot{\mathbf{R}}$$

Then

$$\frac{d\left(\frac{1}{2}M\dot{R}^2 + V\right)}{dt} = M\ddot{\mathbf{R}}\cdot\dot{\mathbf{R}} + (\nabla V)\cdot\dot{\mathbf{R}} = -\beta\dot{R}^2.$$

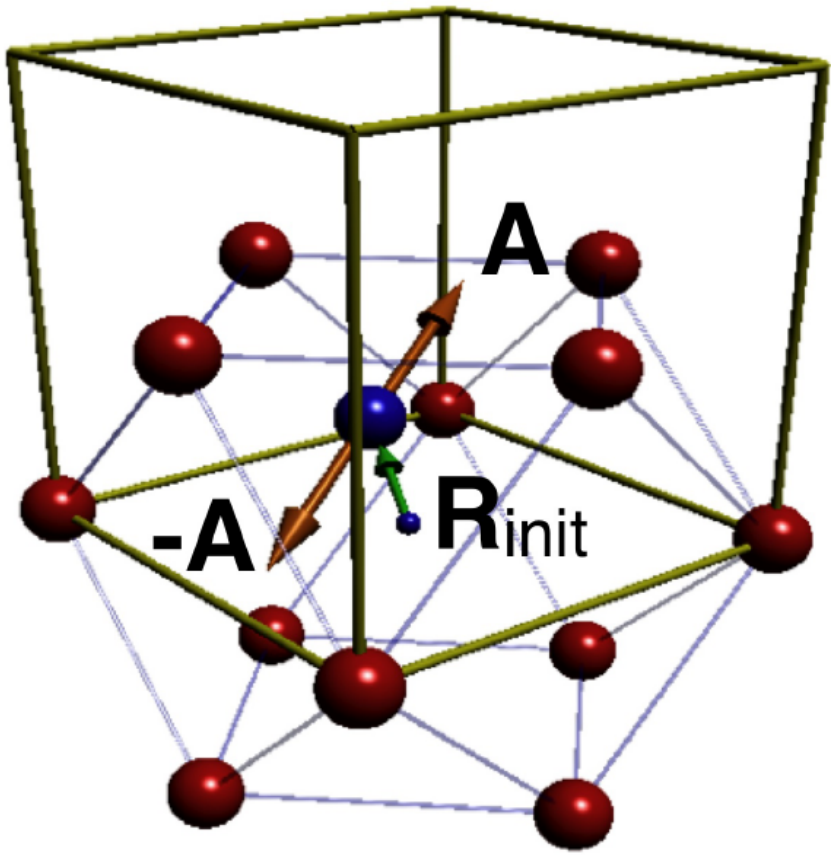
Equivalent Statements

- Drag force $\propto \dot{\mathbf{R}}$
- Stopping power $\propto \dot{\mathbf{R}}$
- Rate of transfer of energy to electrons $\propto$ KE

Vibrating Atom

Displace and then vibrate one atom with small amplitude

$$\mathbf{R}_{\text{osc}}(t) = \mathbf{R}_{\text{init}} + \mathbf{A}\sin(\Omega t)$$



Fermi Golden Rule

Start system in thermal state at temperature T and apply FGR to work out energy transfer to electrons. Obtain

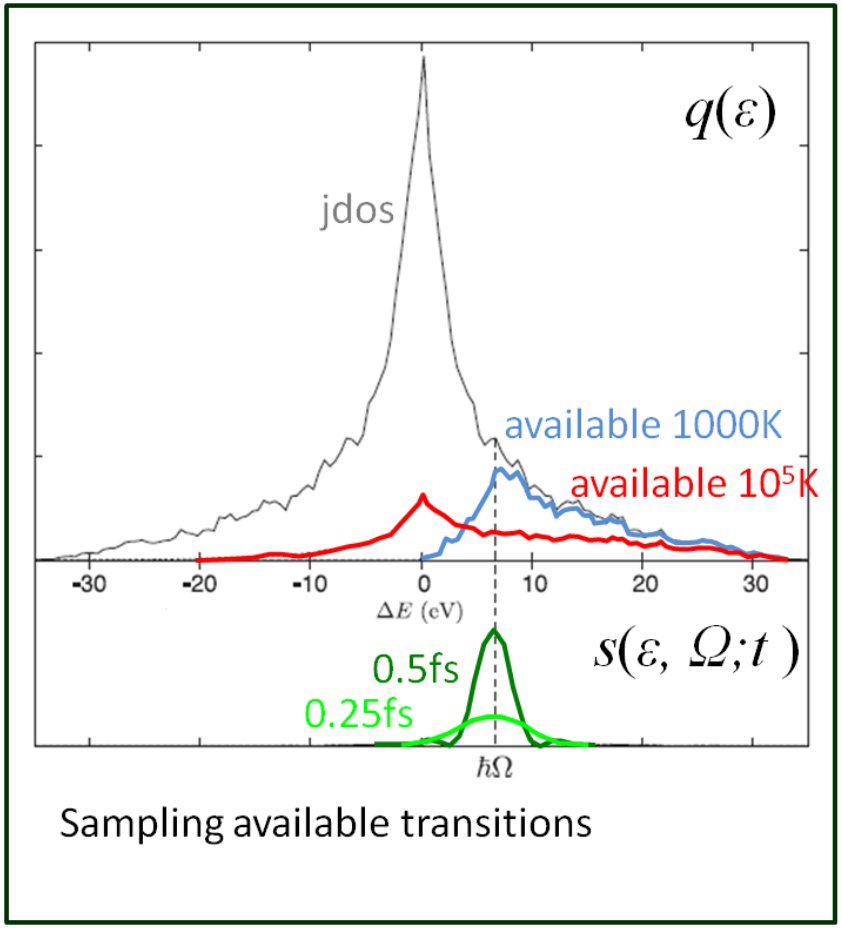
$$\Delta E(t) = \int \varepsilon \, q(\varepsilon) \, s(\varepsilon, \Omega, t) \, d\varepsilon$$

where

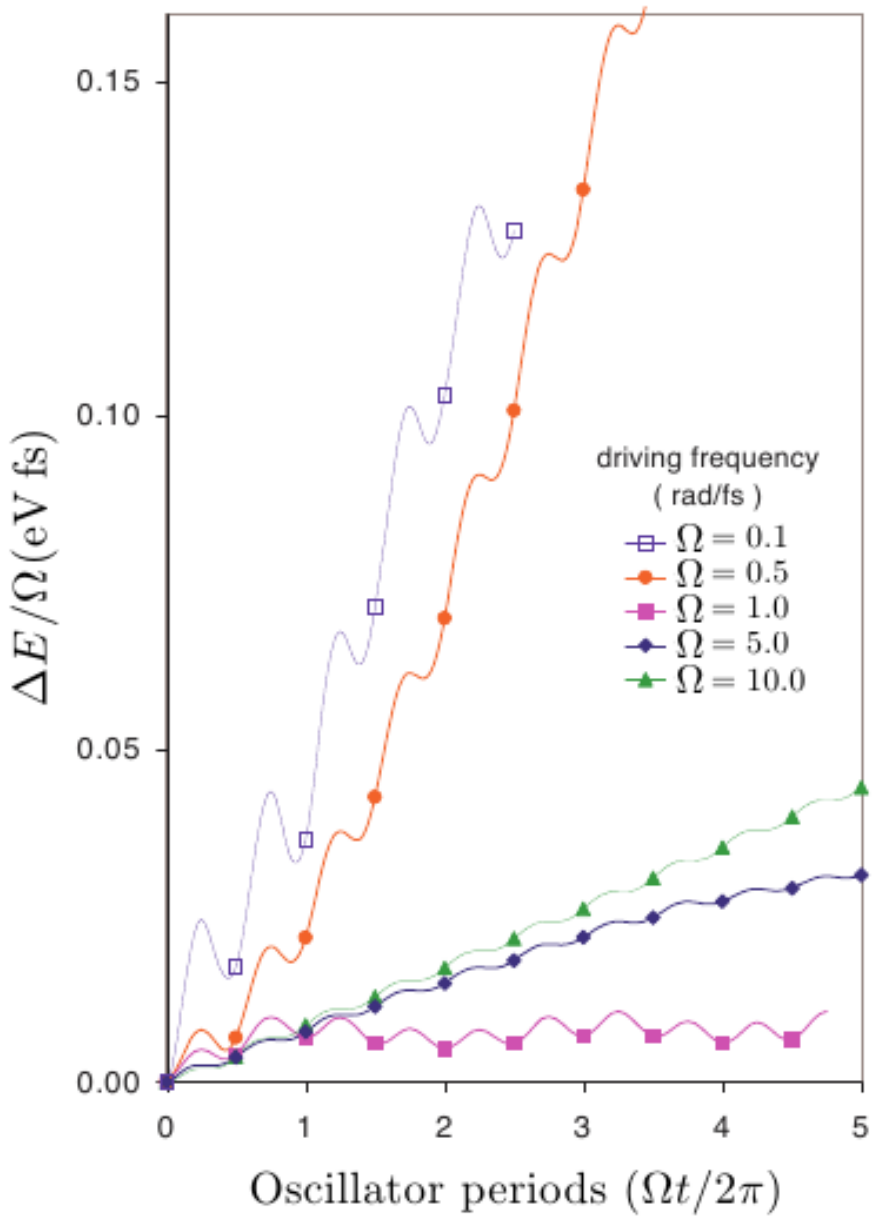
- $q(\varepsilon) = \dfrac{1}{2\hbar^2} \sum_{i,j}{}' |V_{ij}|^2 f(\epsilon_i)(1 - f(\epsilon_i + \varepsilon))\delta(\varepsilon - \epsilon_j + \epsilon_i)$
- $s(\varepsilon, \Omega, t) = t^2 \left\{ \mathrm{sinc}^2 \left[\dfrac{(\varepsilon - \hbar\Omega)t}{2\hbar} \right] + \mathrm{sinc}^2 \left[\dfrac{(\varepsilon + \hbar\Omega)t}{2\hbar} \right] \right\}$

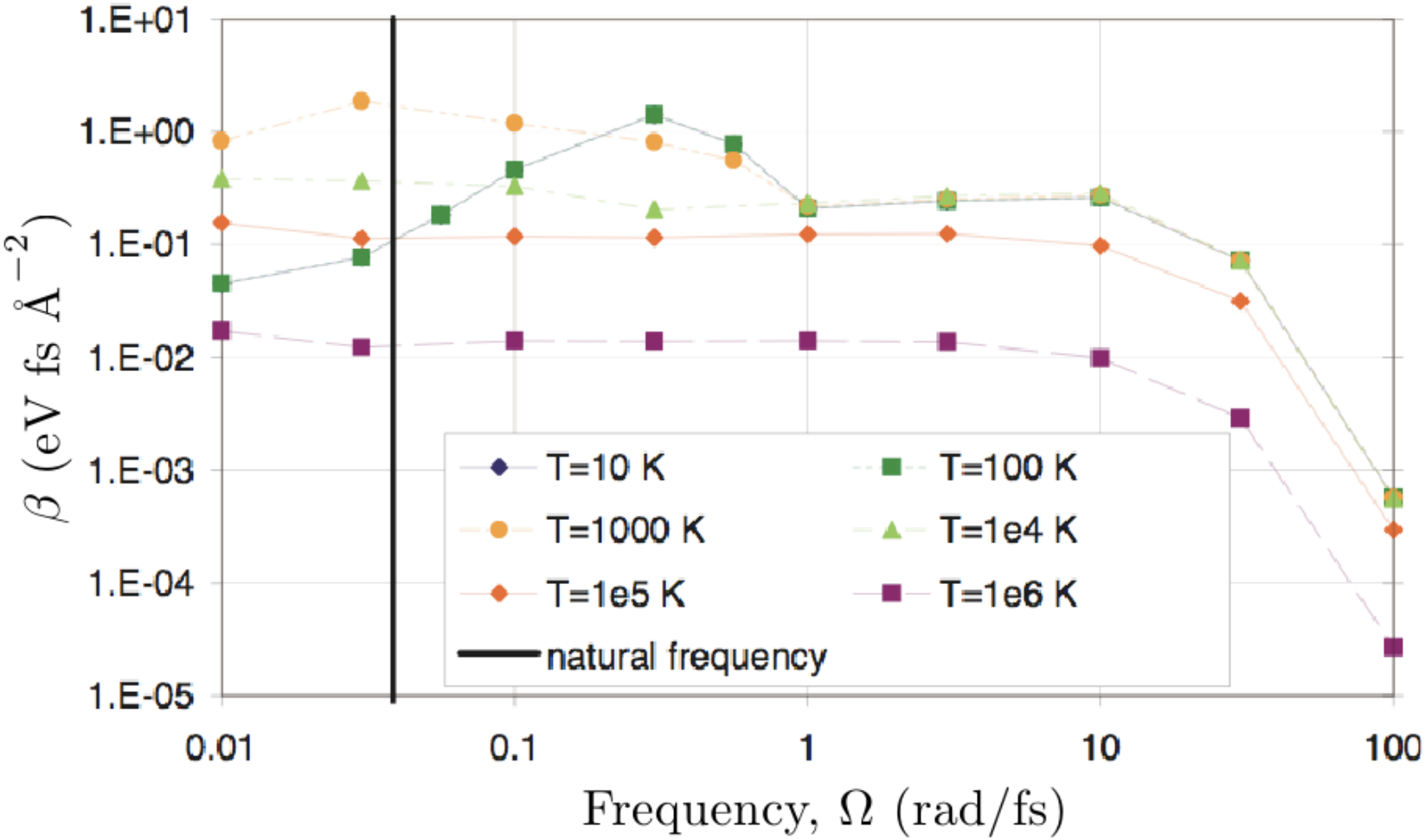
Size Effects

- At short times, the sinc^2 function samples many available transitions.
- At long times, the sinc^2 function tends to a δ function.
- Granularity of available transitions most apparent at low T, large t.

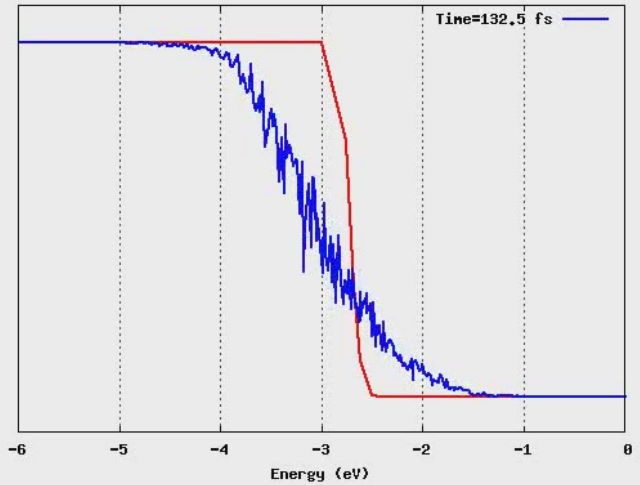


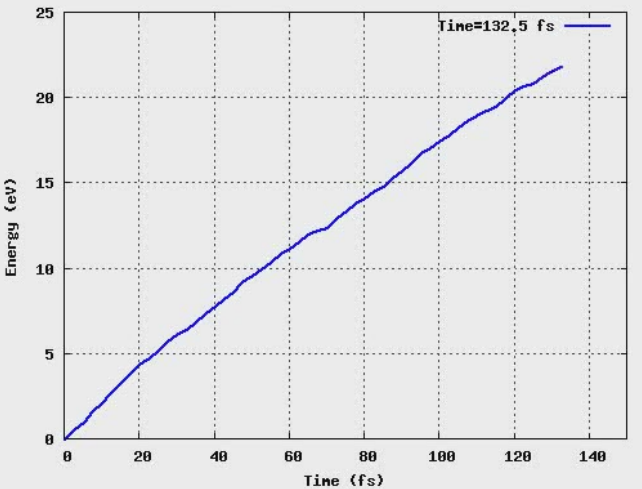
Sampling available transitions

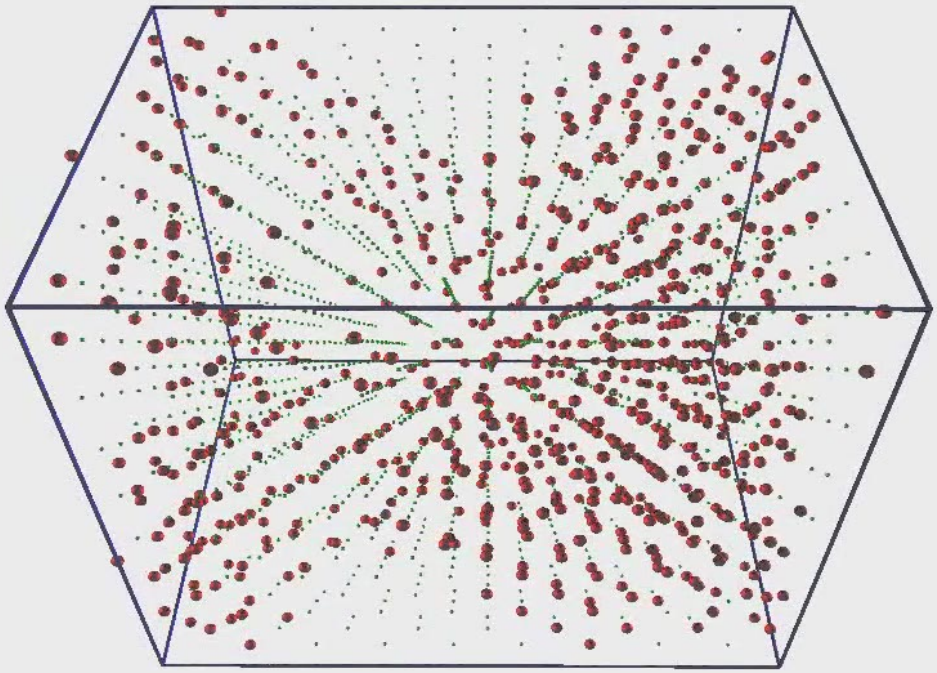




Energy Loss Simulation







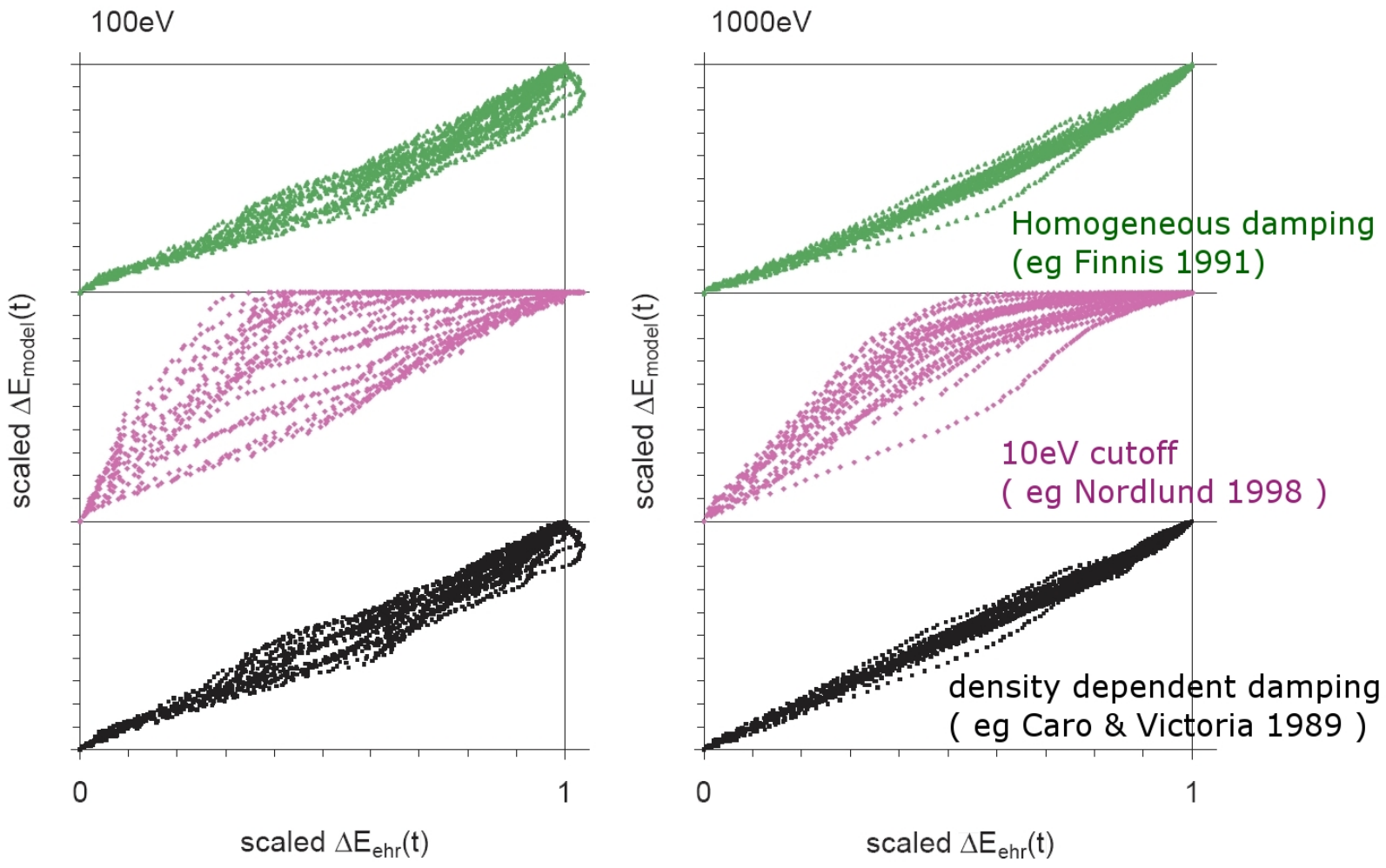
Three Classical Models

Model	Damping	Reference
1	$\beta_n(t) = \beta$	Finnis *et al.* PRB **44**, 567 (1991)
2	$\beta_n(t) = \begin{cases} \beta & \text{KE} > 10\text{eV} \\ 0 & \text{otherwise} \end{cases}$	Nordlund *et al.* PRB **57**, 7556 (1998)
3	$\beta_n(t) = \beta\ F(\rho_n(t))$	Caro and Victoria PRA **40**, 2287 (1989)

Ehrenfest Simulations

- $9 \times 8 \times 7$ fcc cells (2016 atoms) evolved for 200fs.
- 24 PKA directions in irreducible 1/48th of sphere.
- 10 PKA energies (100eV – 1keV).
- Electrons initially in thermal state at temperature T_e.

Comparison of Damping Models



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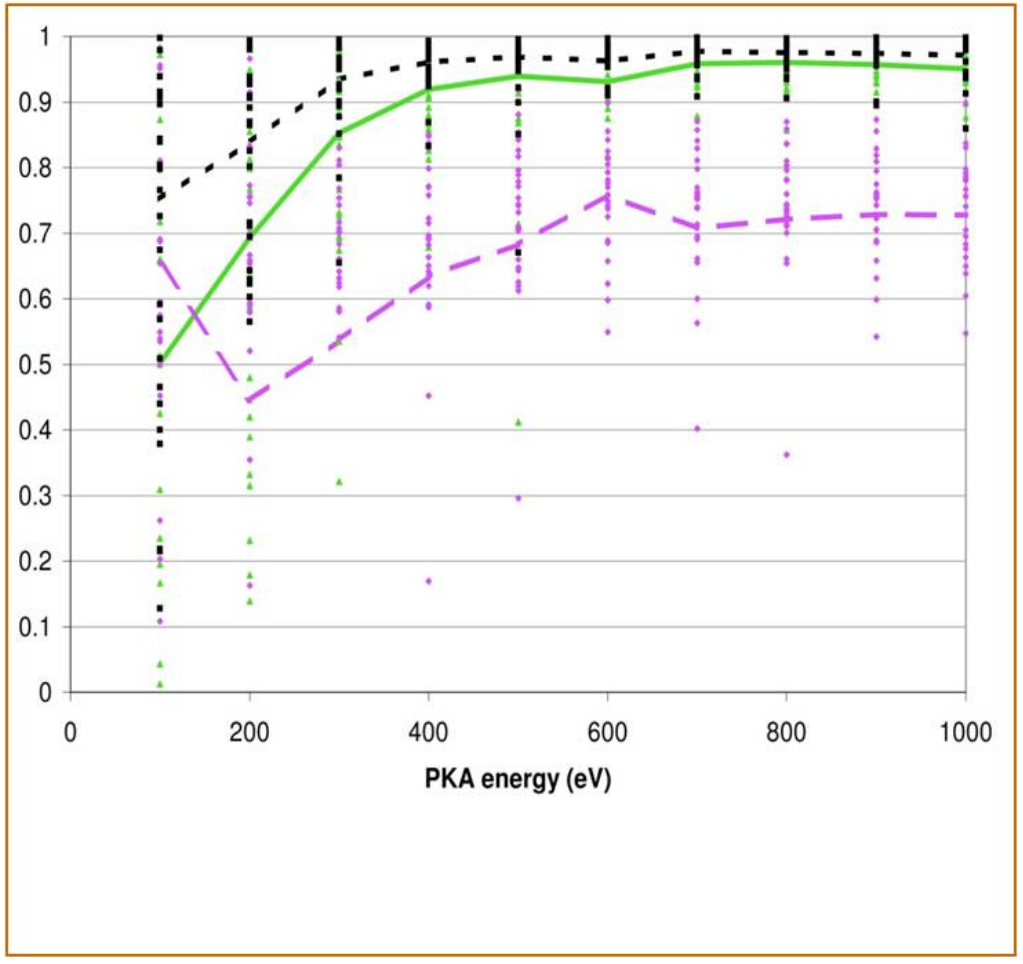
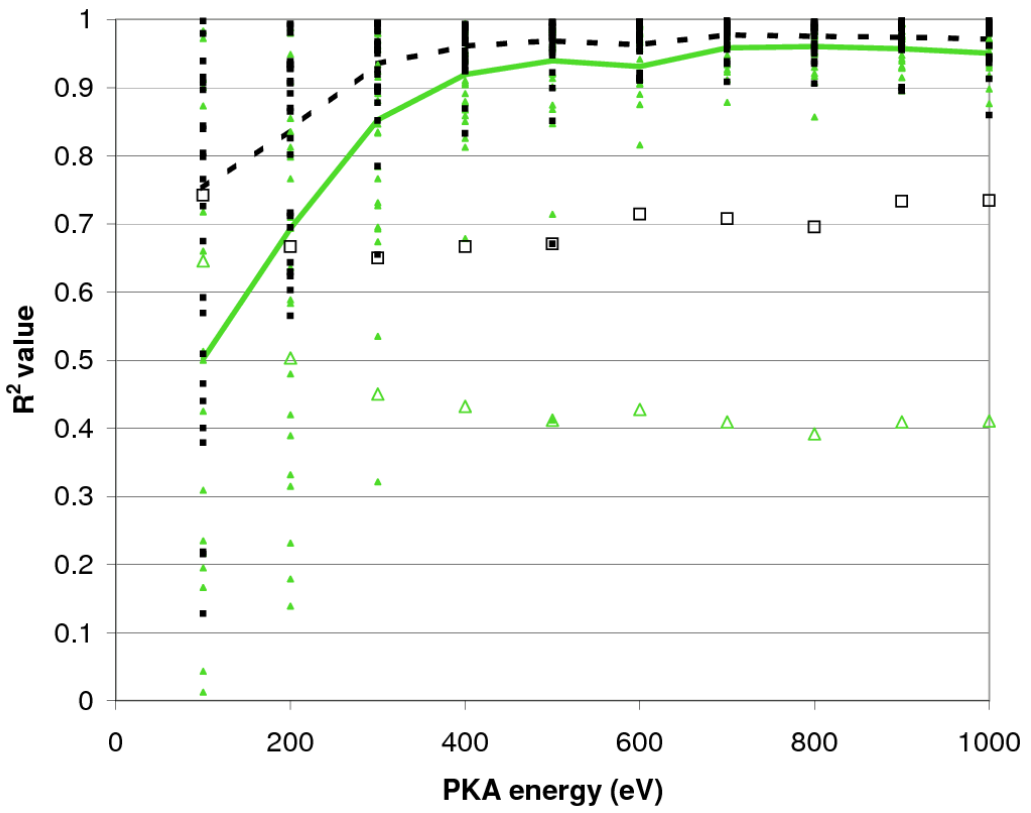
R^2 Goodness of Fit



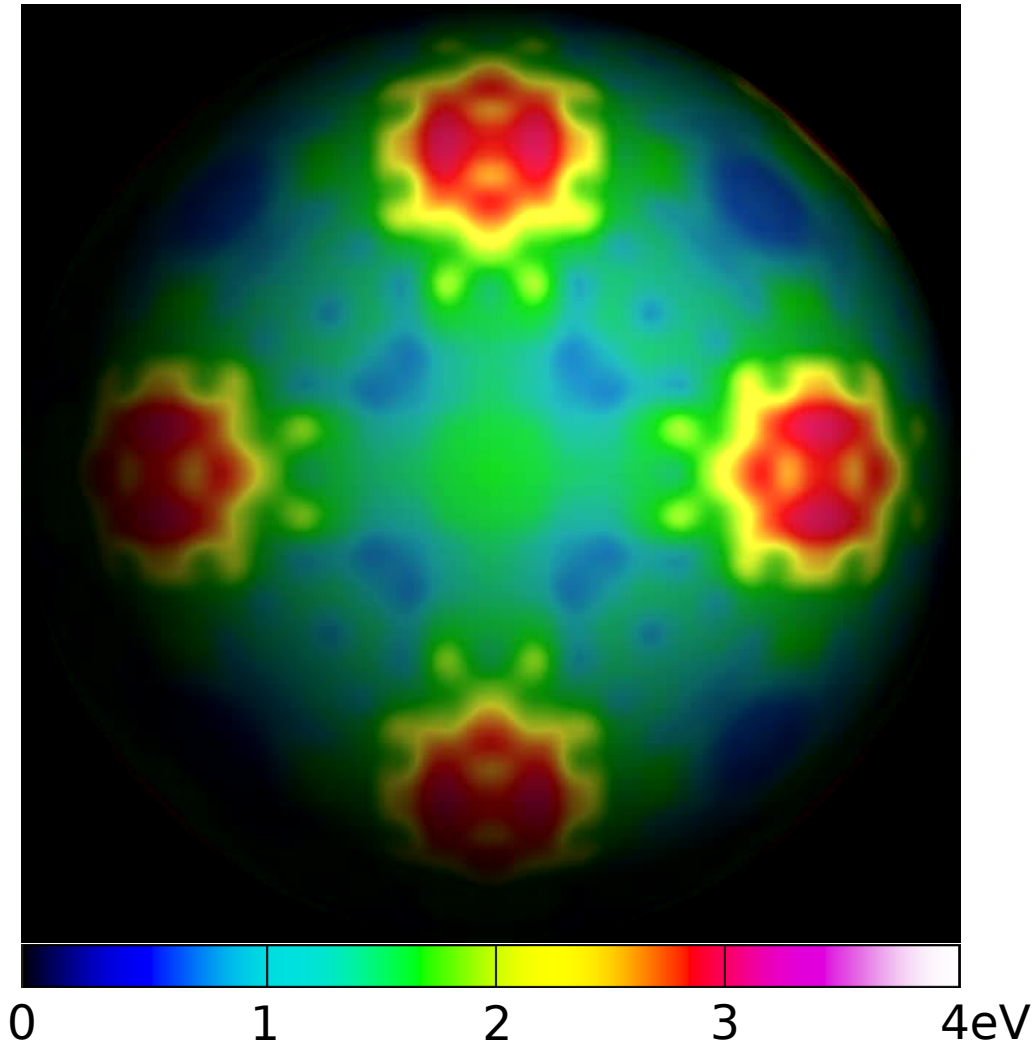
- Caro/Victoria, viscous, KE cutoff
- Viscous damping models work well
- KE cutoff model not so good
- Caro and Victoria density-dependent model best

Replacement Collision Sequences



- Caro/Victoria, viscous.
- Empty symbols show RCS's only.

Direction Dependence of Damping



Energy transfer 5 fs into a 2 keV cascade at 500 K.

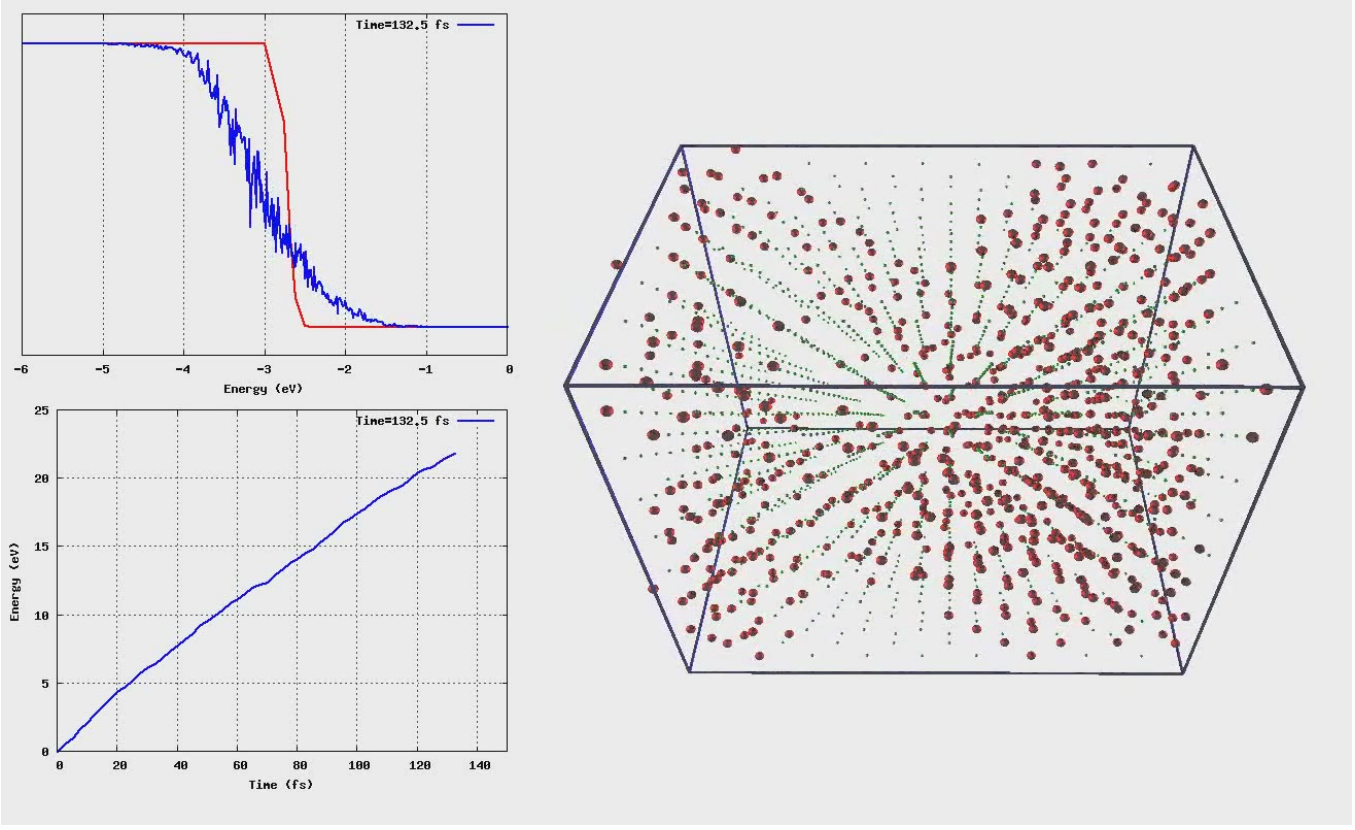
Validity of Damping Models

- Simple $\mathbf{F}_{\text{drag}} = -\beta\dot{\mathbf{R}}$ damping works surprisingly well when the energy transfer is averaged over the cascade.
- No evidence in support of low-energy cutoff.
- Replacement collision sequences have higher damping, suggesting that damping of individual ionic trajectories may be strongly direction and position dependent.

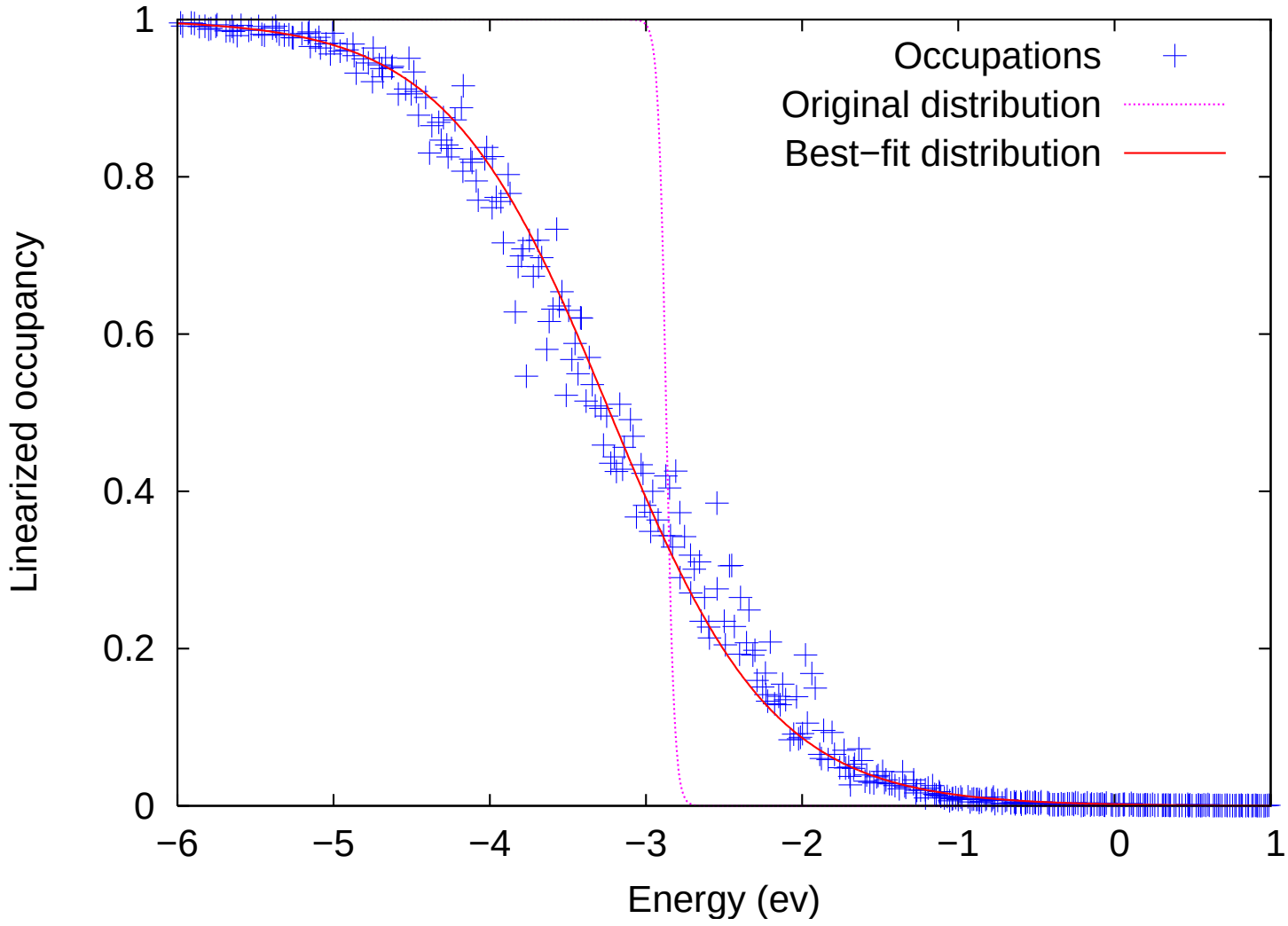
Outline

Electronic Heating

The final-state occupations of the instantaneous eigenstates look very like a Fermi-Dirac distribution.



Fermi-Dirac Fit



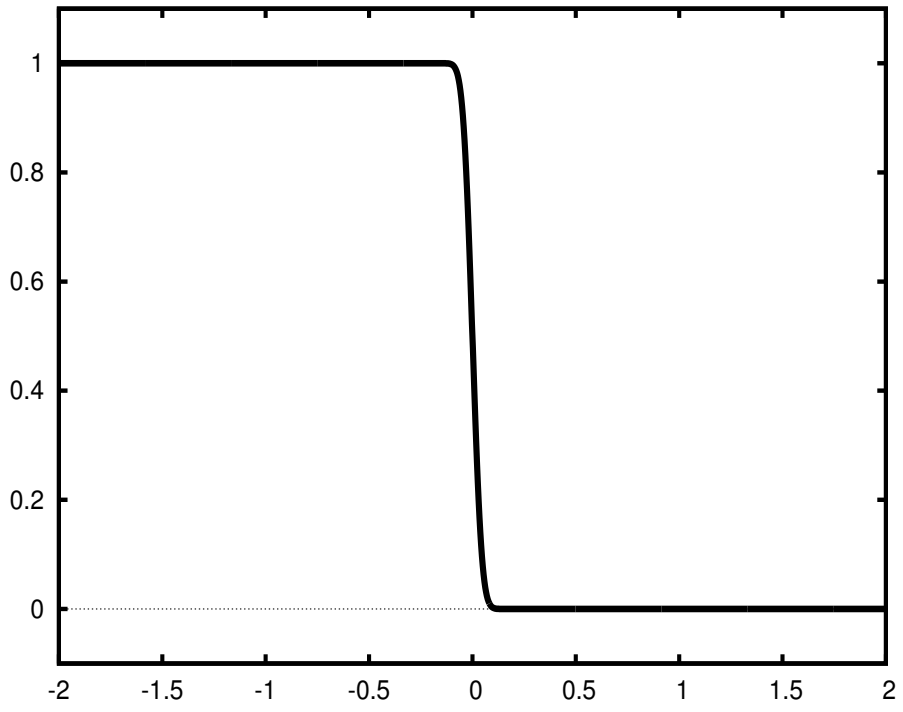
Why Fermi-Dirac?

- In the basis of instantaneous energy eigenfunctions, the electrons make transitions from state to state.
- The energies of these transitions depend on the frequency spectrum of the time-dependent potential of the moving ions.
- The frequency spectrum is not thermal.
- The electrons are non-interacting and cannot equilibrate with each other.
- So why do we see a Fermi-Dirac distribution?

Why Fermi-Dirac?

Explanation

The jumps in energy are small and more or less random, so the distribution of occupation numbers *diffuses*.



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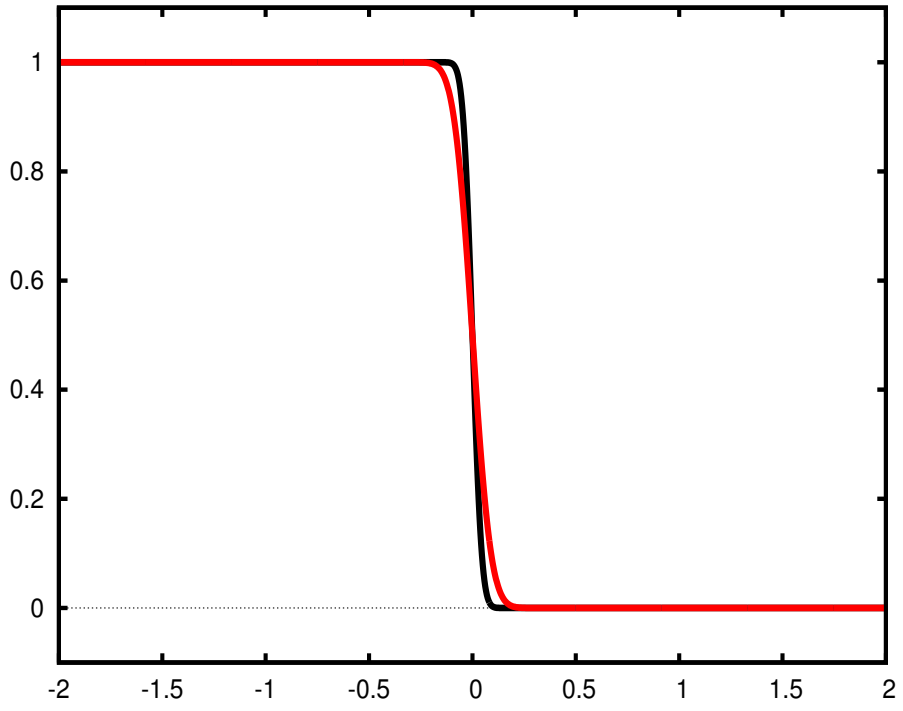

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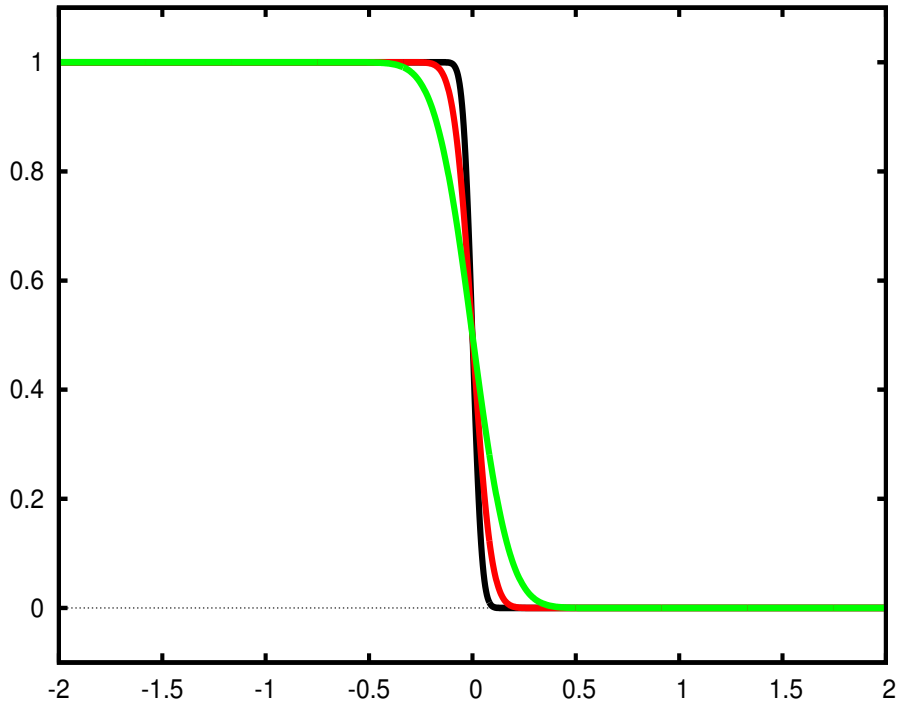

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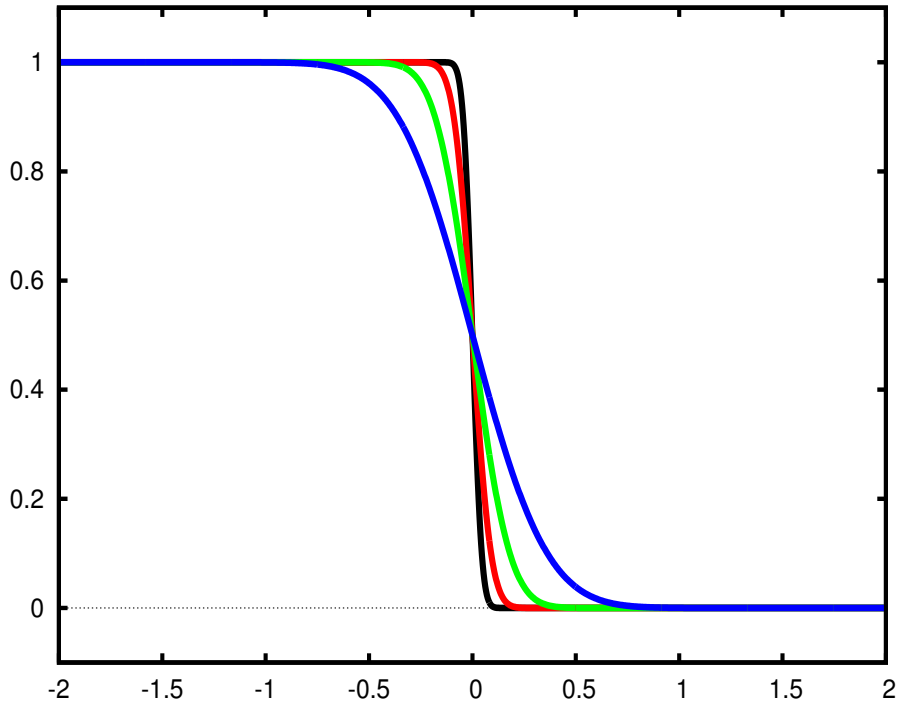

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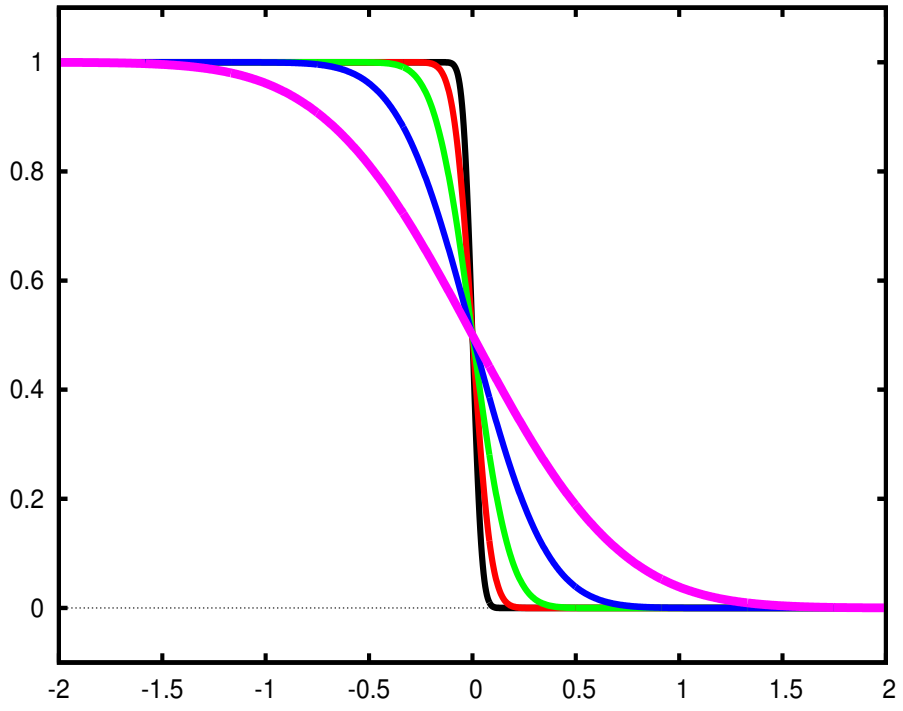

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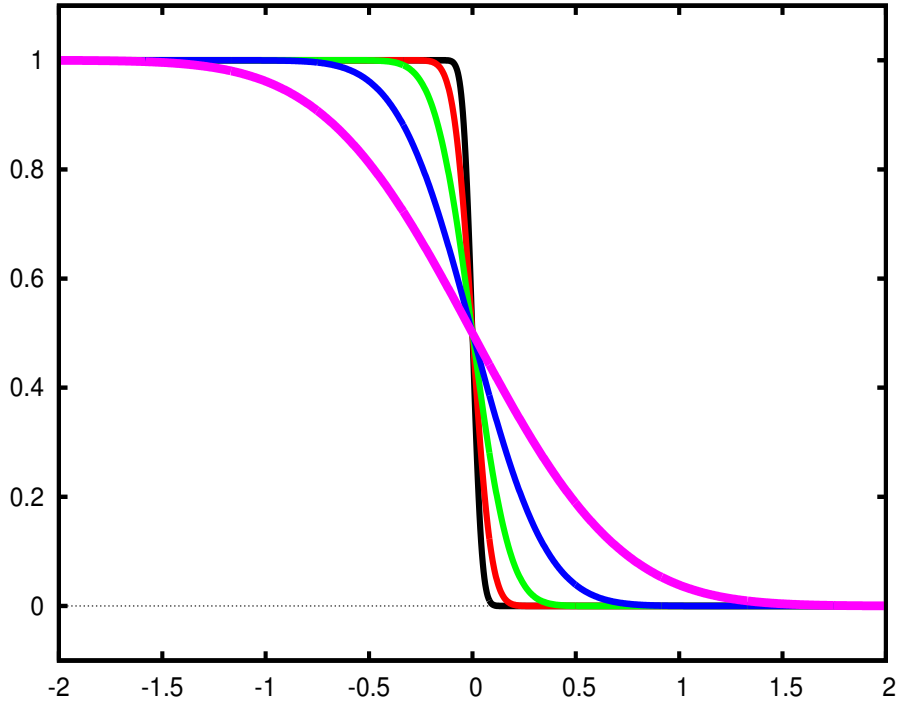
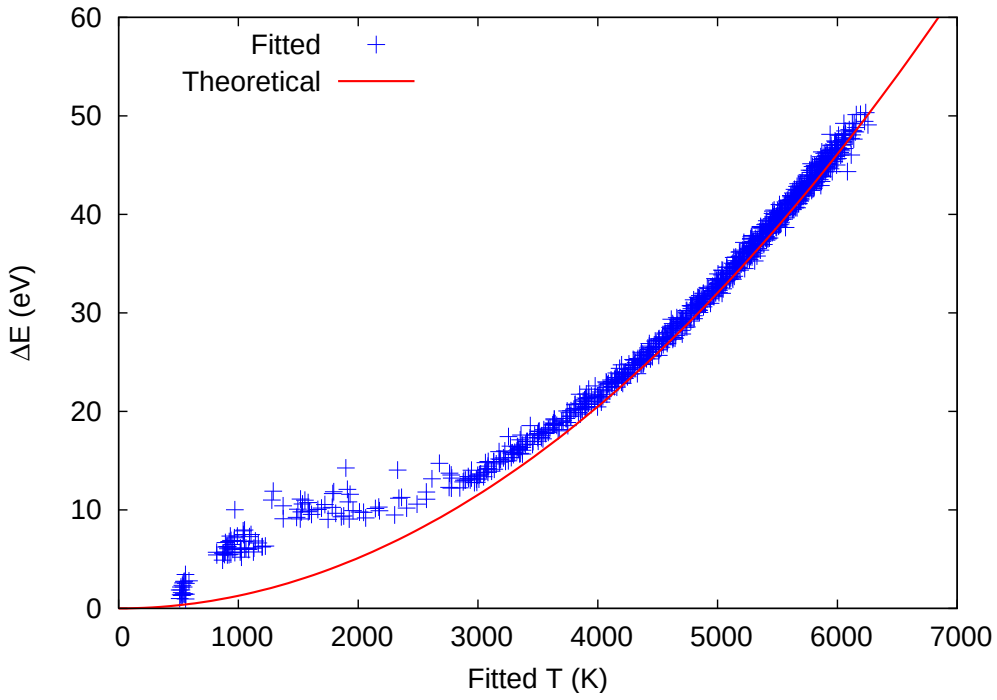


An error function looks very like a Fermi-Dirac distribution

From Temperature Back to Energy



- The fitted temperatures are consistent with the energy transferred to the electrons:

$$\Delta E = C_v T_e = \frac{\pi^2}{3} g(E_F) k_b^2 T_e \times T_e$$

- Can talk about an electronic temperature during the cascade.

Truly a Temperature?

- The one-electron Ehrenfest states evolve according to

$$i\frac{\partial \psi_i(t)}{\partial t} = \hat{H}(t)\psi_i(t)$$

- The instantaneous eigenfunctions of the Hamiltonian at time t may be obtained by solving

$$\hat{H}(t)u_i(t) = \epsilon_i(t)u_i(t)$$

  These also vary with time (because $\hat{H}$ does), but not in the same way as $\psi_i(t)$.
- Even if we start in an instantaneous eigenfunction, we do not remain in one.

The Ehrenfest-evolved states $\psi_i(t)$ are not the instantaneous energy eigenstates $u_i(t)$

Evolution of the Density Operator

- Under Ehrenfest evolution, the initial density operator

$$\hat{\rho}(t=0) = \sum_i |u_i(0)\rangle\, f_i\, \langle u_i(0)|$$

becomes

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- When re-expressed in the basis of instantaneous eigenstates $u_i(t)$, the Ehrenfest-evolved density matrix is not diagonal.

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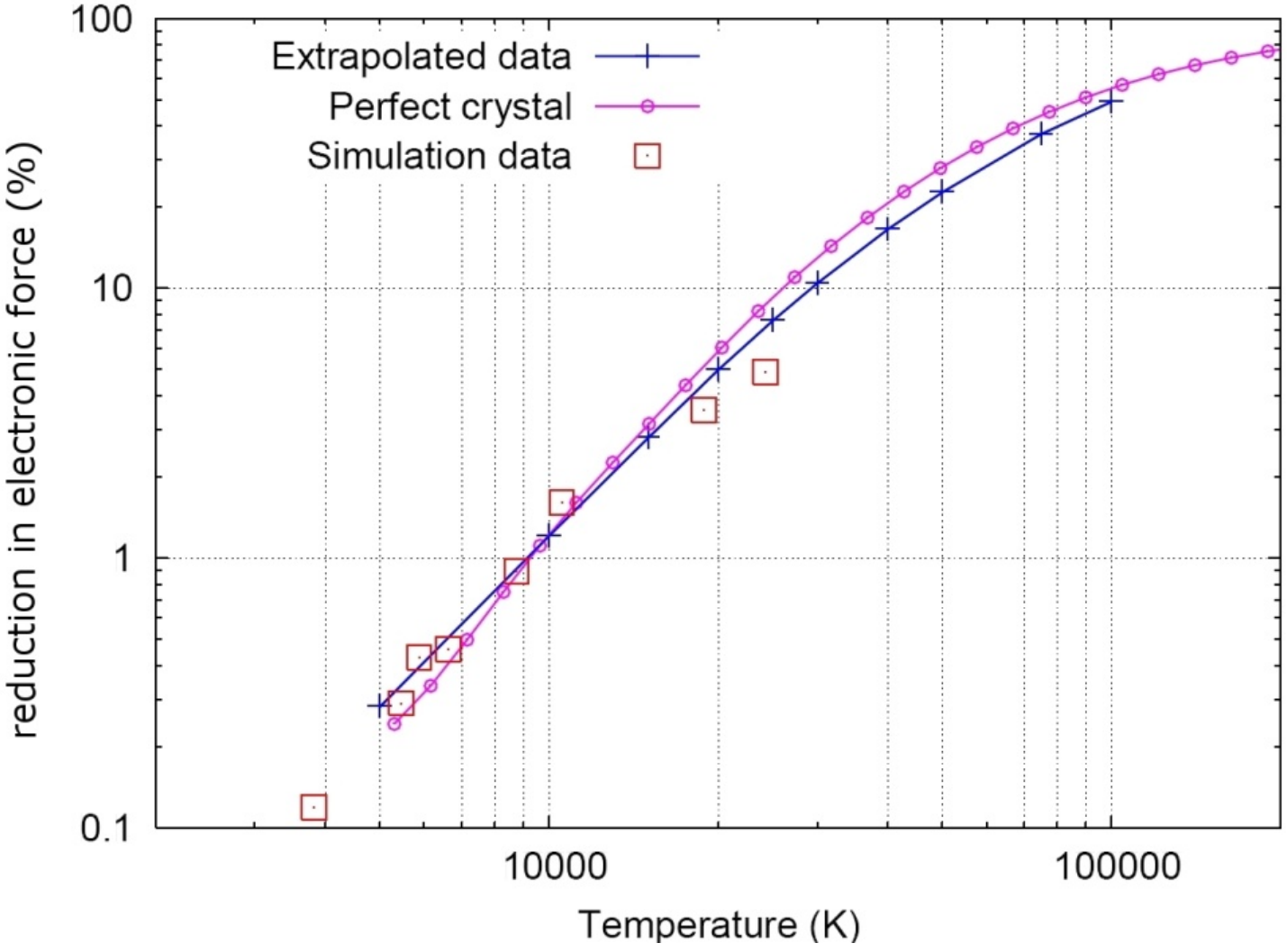
- Nevertheless, the occupations (diagonal elements) look thermal with a steadily rising temperature.
- Entropy is fixed, but temperature rises!
- If we forget off-diagonal density matrix elements, entropy rises correspondingly.

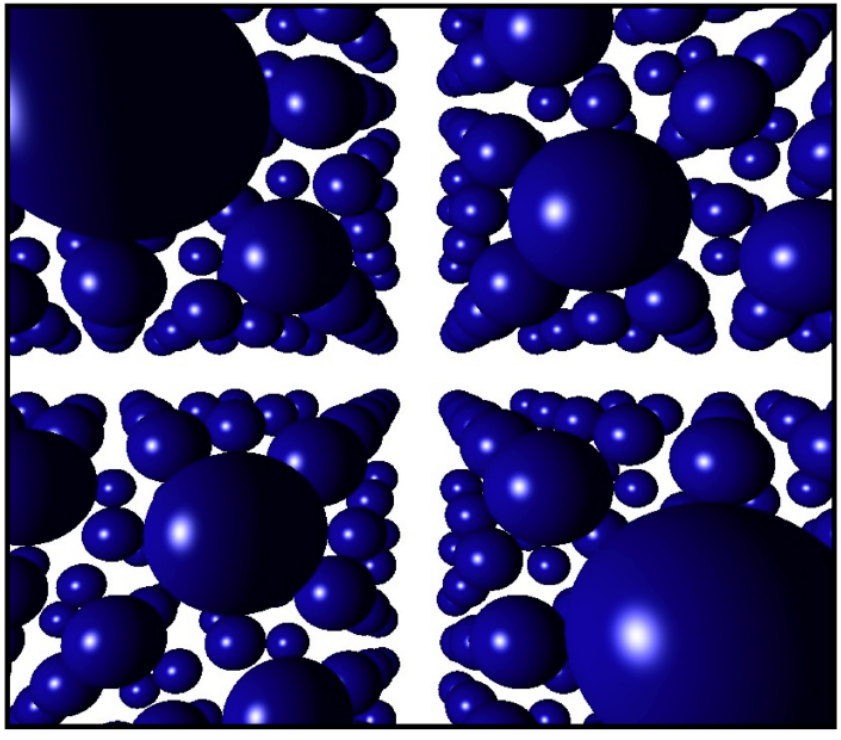
Electronic Excitations and Forces

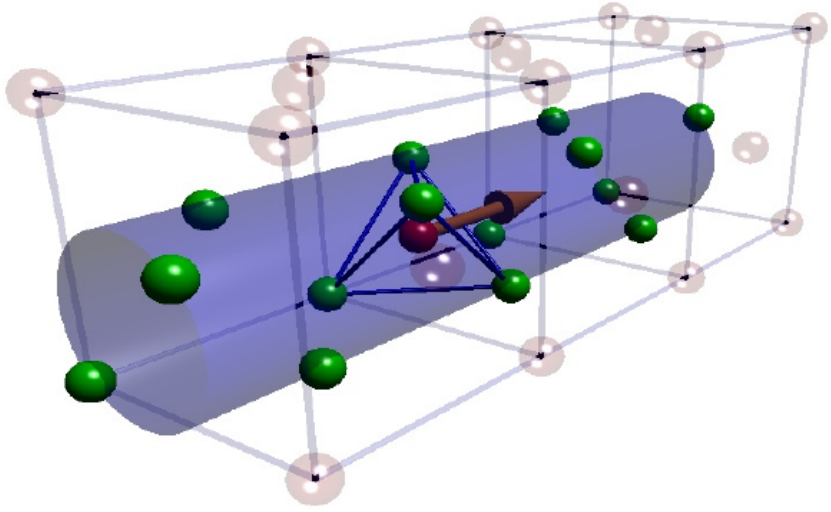
Heating the electrons weakens the bonds between atoms.



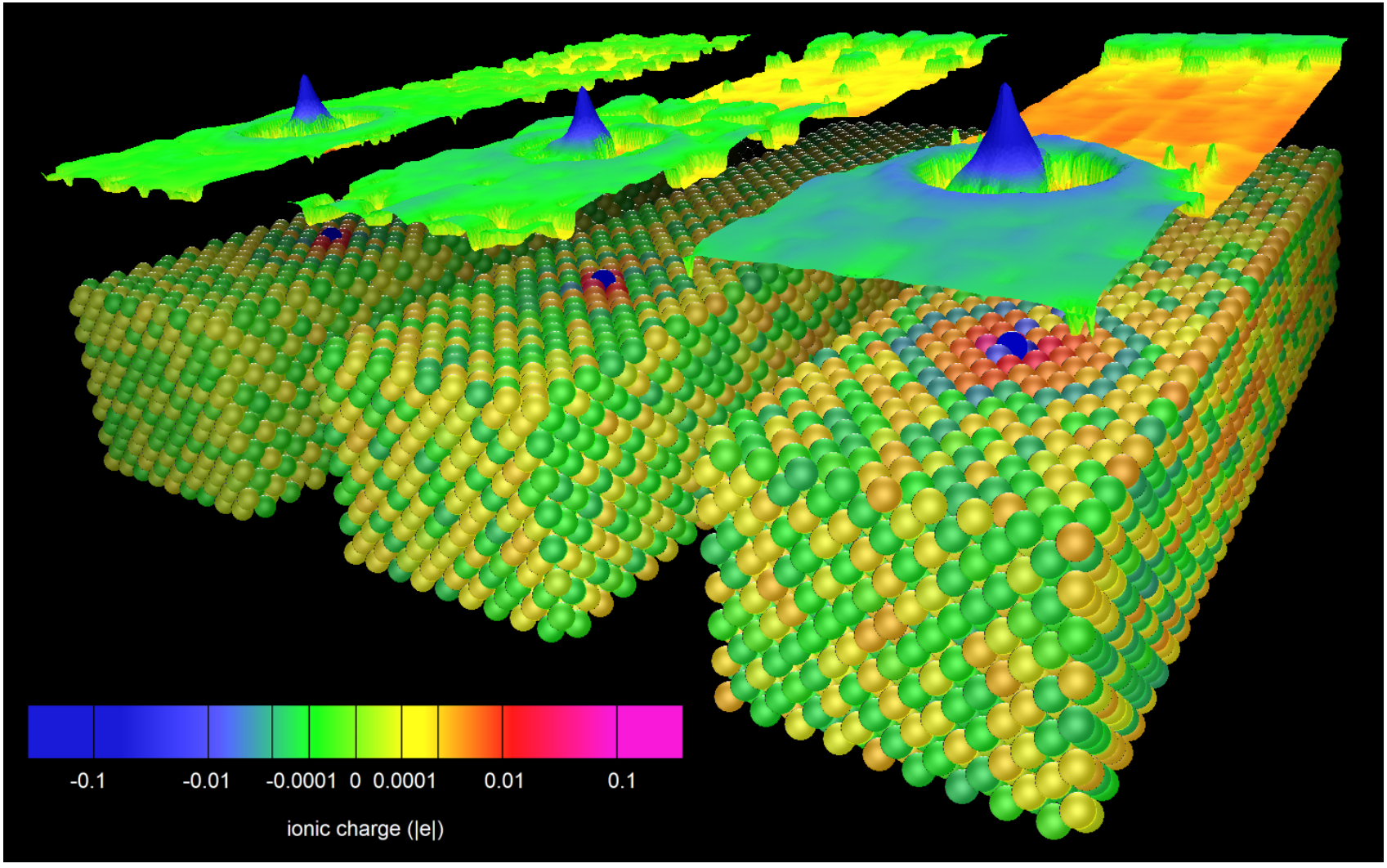
Outline

The ⟨100⟩ Channel in Cu



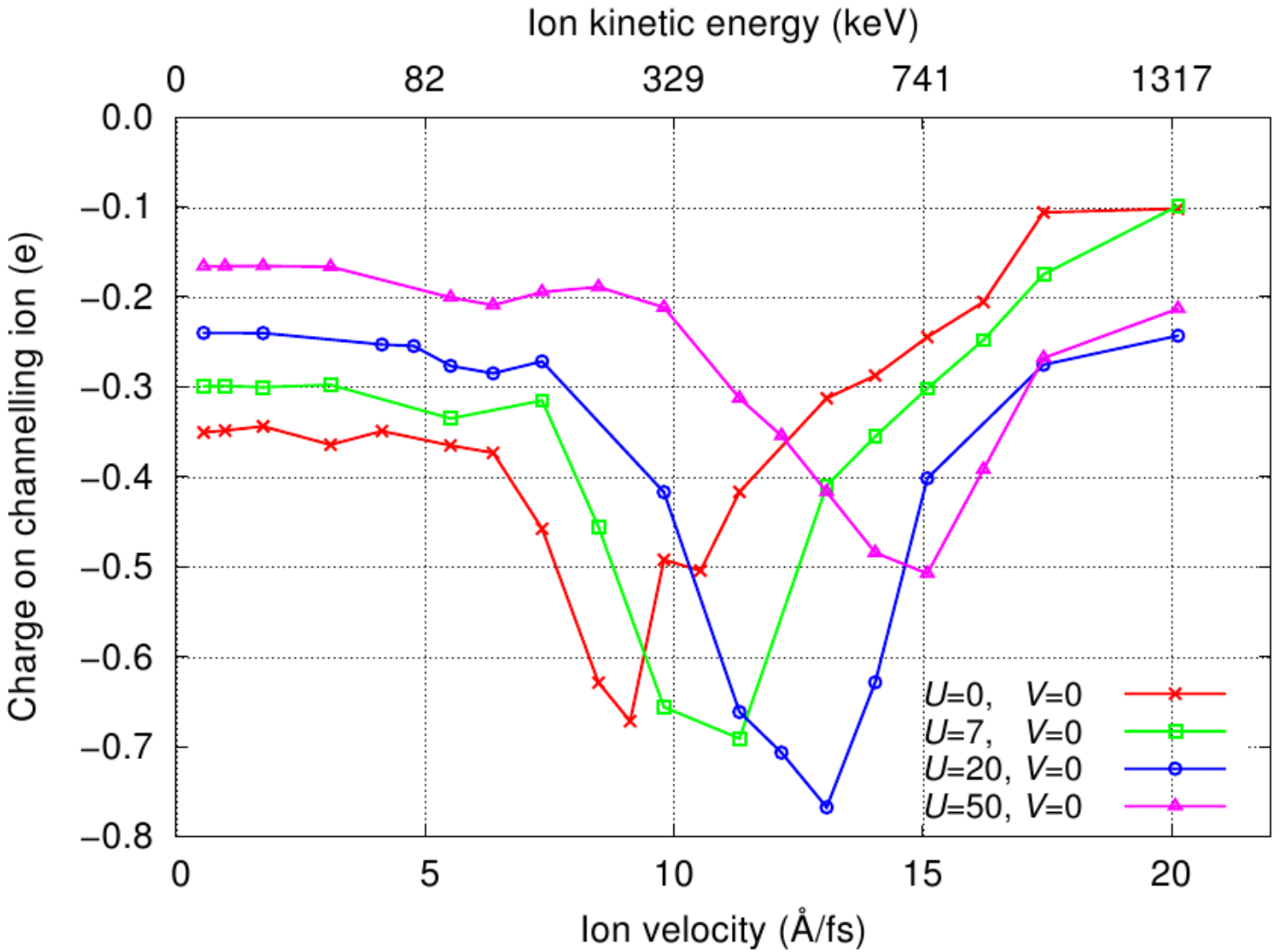


Screening Potential

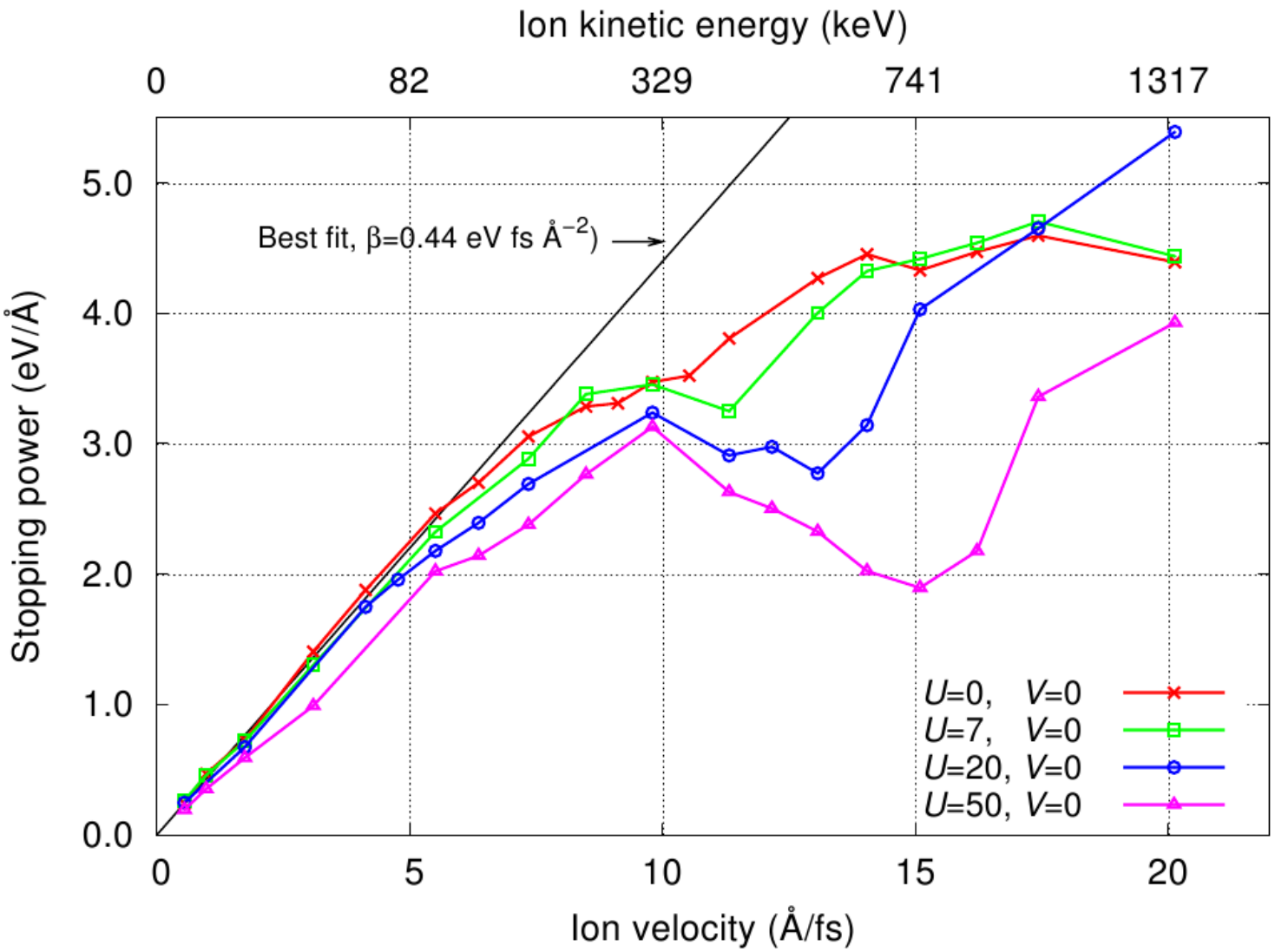


Hartree potential around an ion moving down a $\langle 100 \rangle$ channel at 0 keV, 10 keV, and 365 keV. Note the charge resonance at 365 keV.

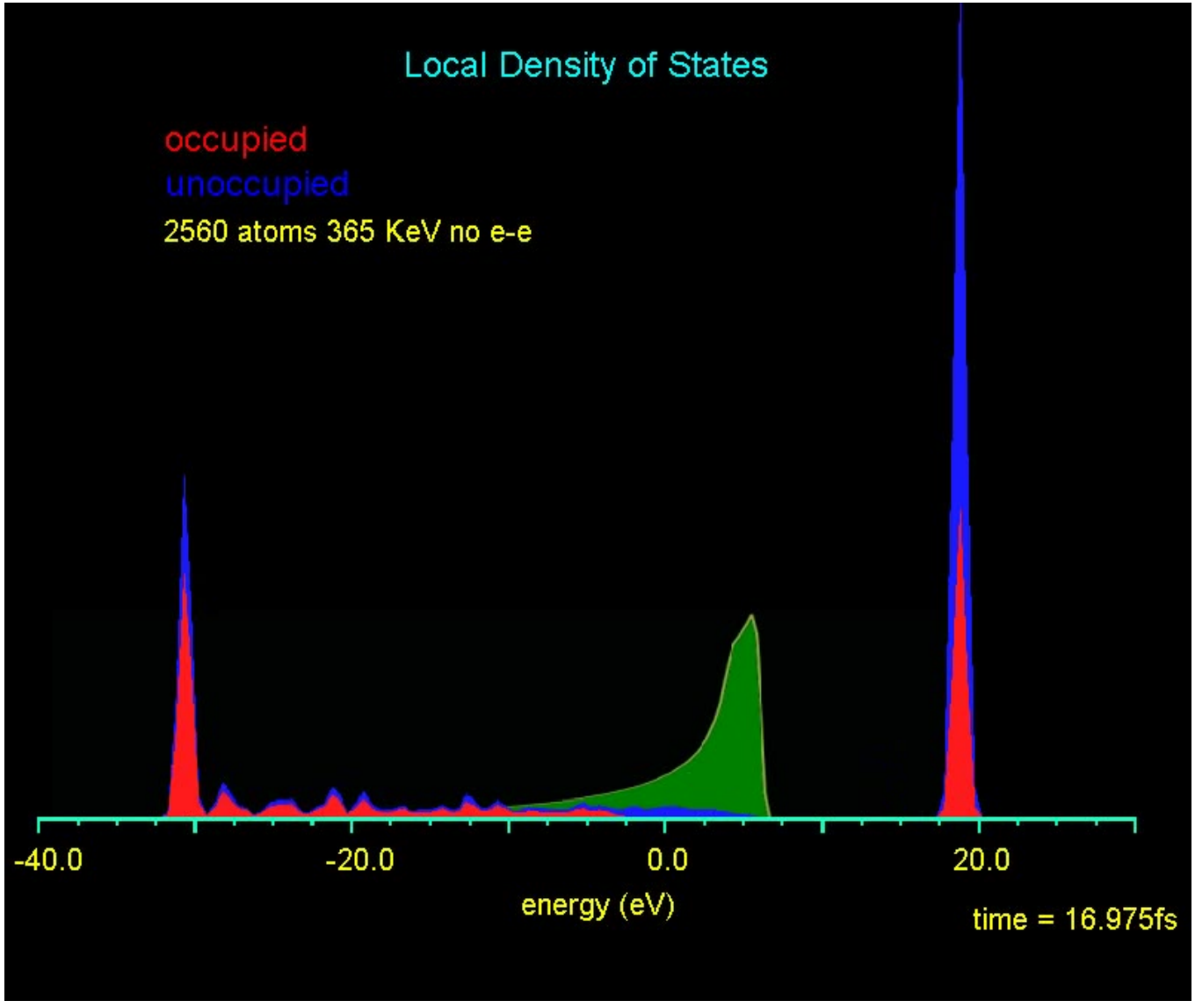
Charge Resonance



Stopping Power Resonance



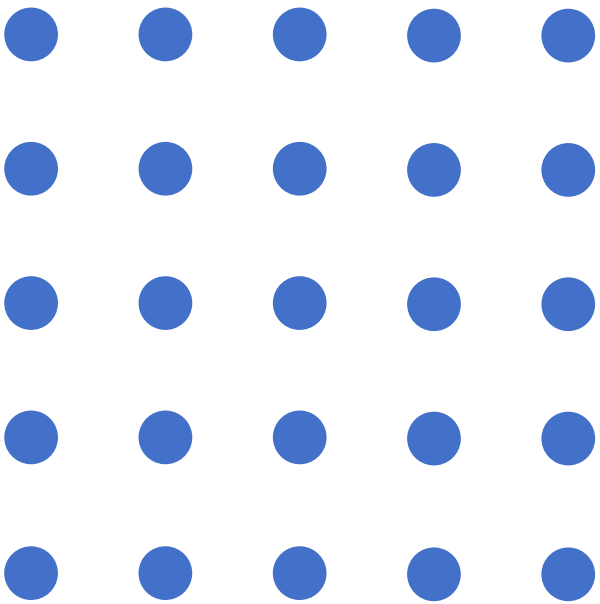
Resonant Excitation of Localized States



Outline

Electronic Friction as a Tensor

The drag coefficient β is really a position-, direction- and history-dependent tensor.



- Take a 2048-atom chunk of perfect crystal.

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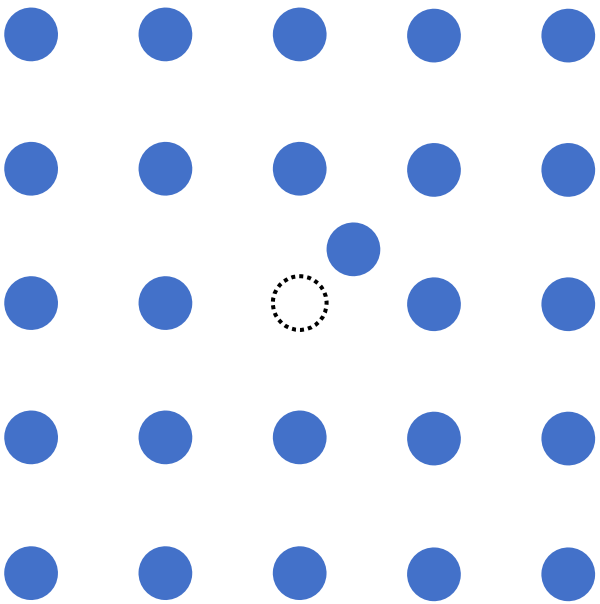

- Take a 2048-atom chunk of perfect crystal.
- Displace central atom.

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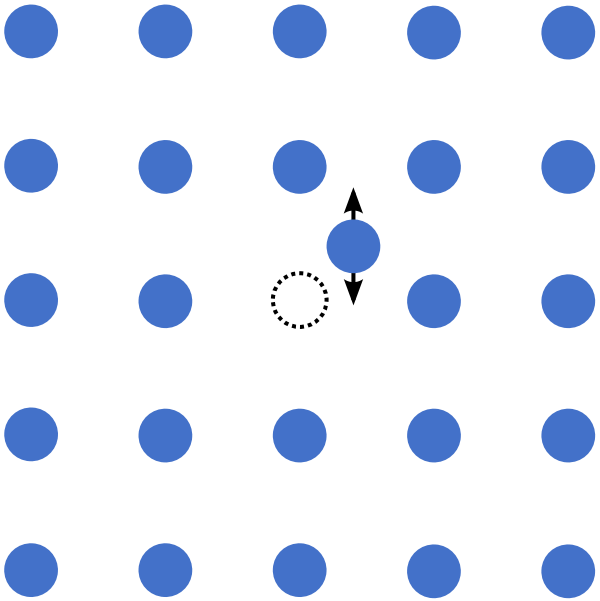

- Take a 2048-atom chunk of perfect crystal.
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- Vibrate with low amplitude at $\omega = 0.5\,\text{rad/fs}$.

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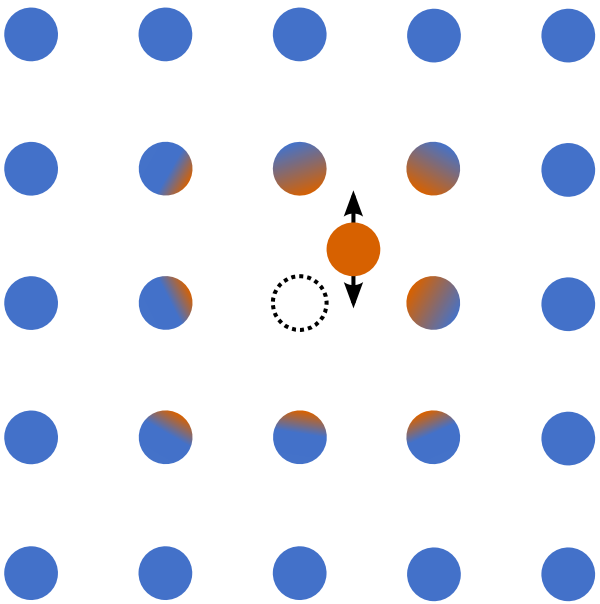
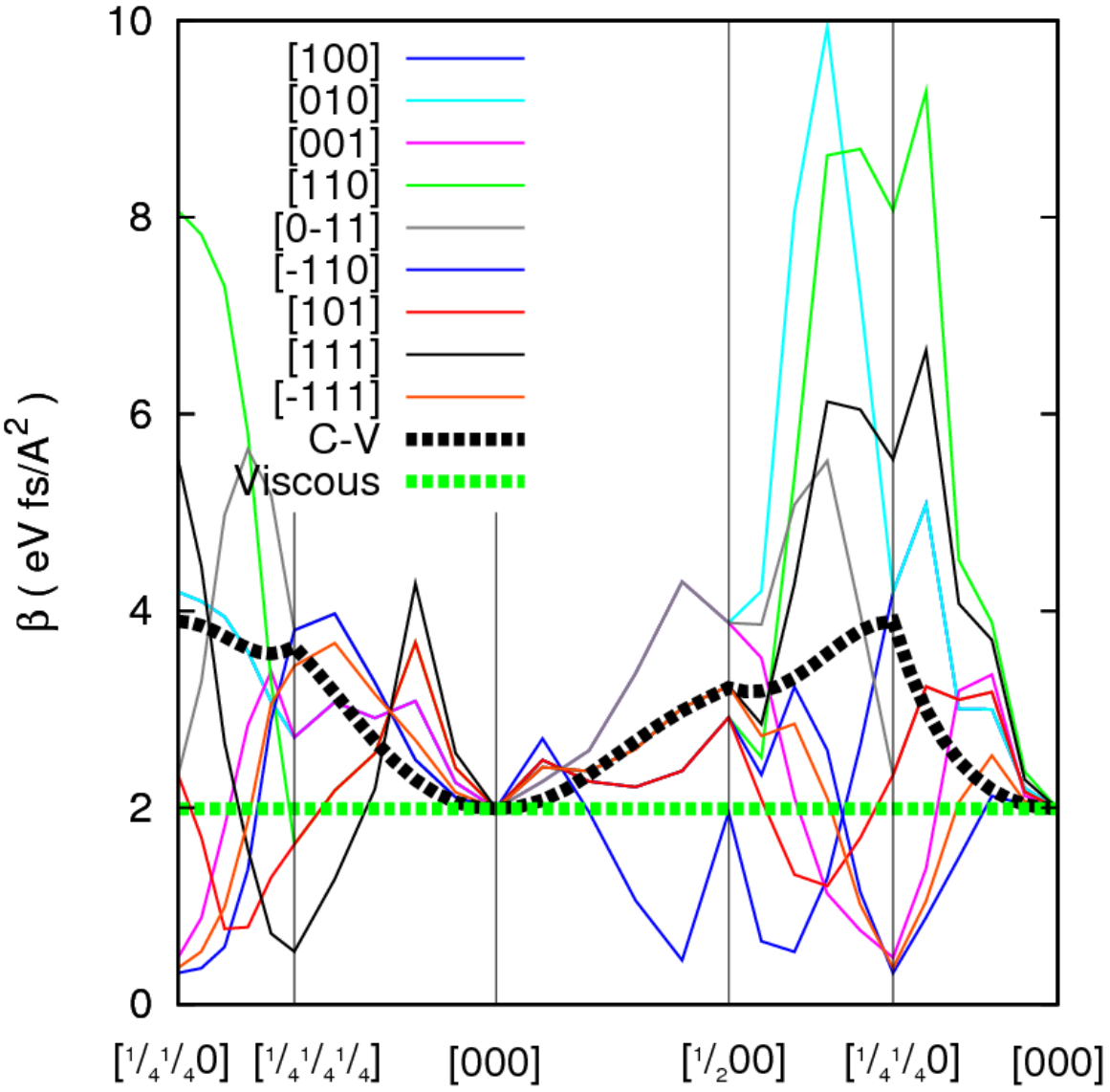


- Take a 2048-atom chunk of perfect crystal.
- Displace central atom.
- Vibrate with low amplitude at $\omega = 0.5\,\text{rad/fs}$.
- Measure energy transfer.

Directional Damping



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The Non-Adiabatic Force

$$\mathbf{F}_{\text{non-adi},a} = -\frac{2\hbar D_a}{D} \sum_{b \in \mathfrak{N}_a} D_a D_b \left[(\mathbf{v}_a - \mathbf{v}_b) \cdot \nabla_a H_{ba} \right] \nabla_a H_{ba}$$

Density of states per atom

Sum over neighbours

Local density of states on a

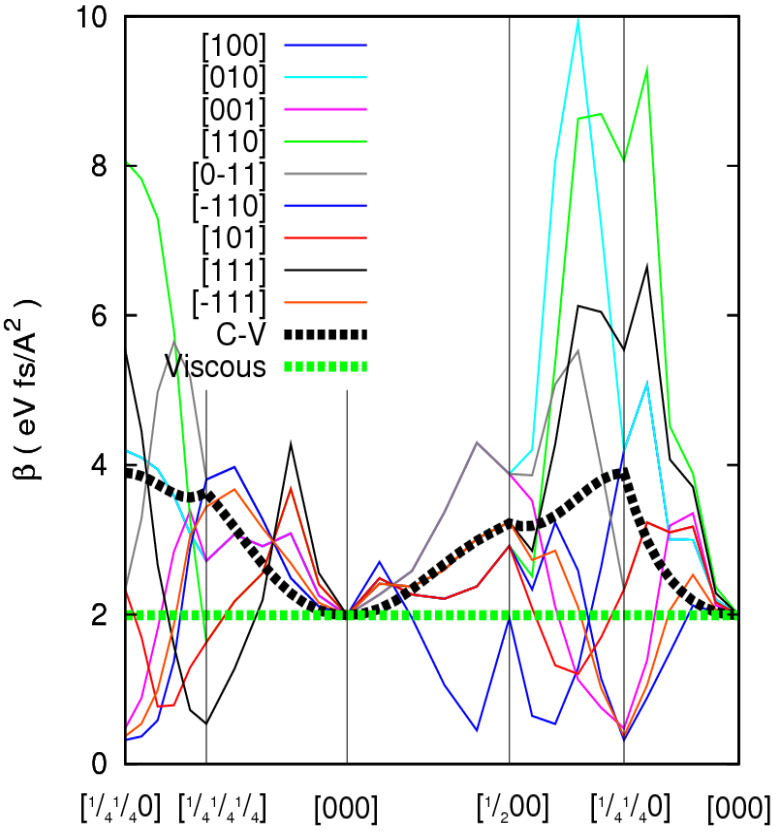
Relative velocity

Adiabatic force

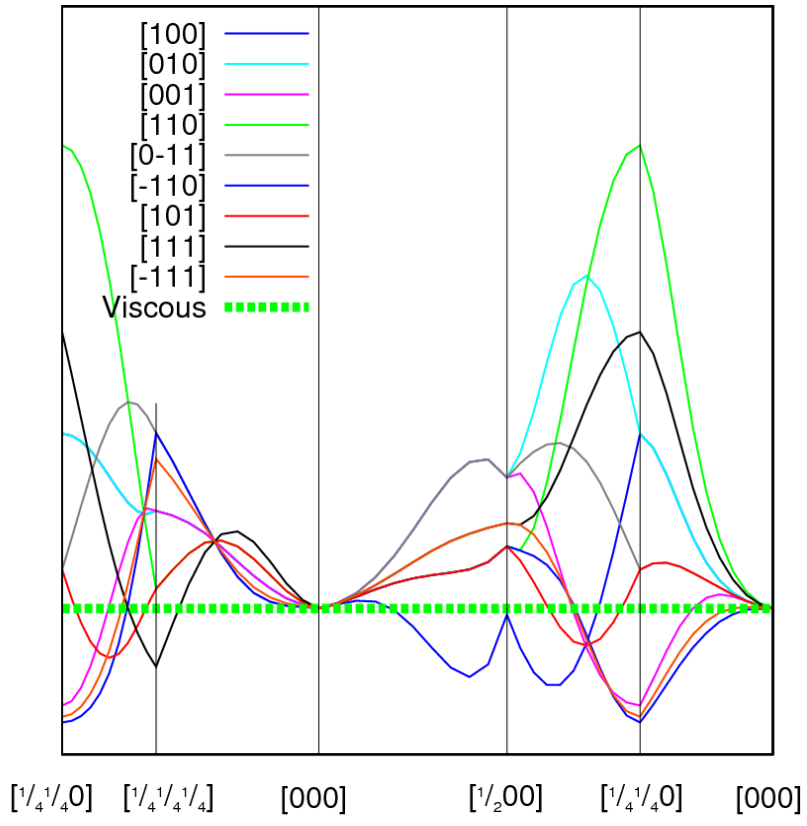
$$\mathbf{F}_{\text{non-adi},a} \approx -2\hbar\xi \sum_{b \in \mathcal{N}_a} \sqrt{\frac{\Phi_0}{\Phi_a^2 \Phi_b}} \left(\nabla_a H_{ab} \cdot \dot{\mathbf{r}}_{ab} \right) \nabla_a H_{ab}$$

- $\Phi_a = \sum_{b \in \mathcal{N}_a} (H_{ab})^2$ as in second-moment EAM.
- $\xi =$ adjustable parameter.
- Easy to evaluate and local.
- Easy to combine with EAM.

Directional Damping (again)

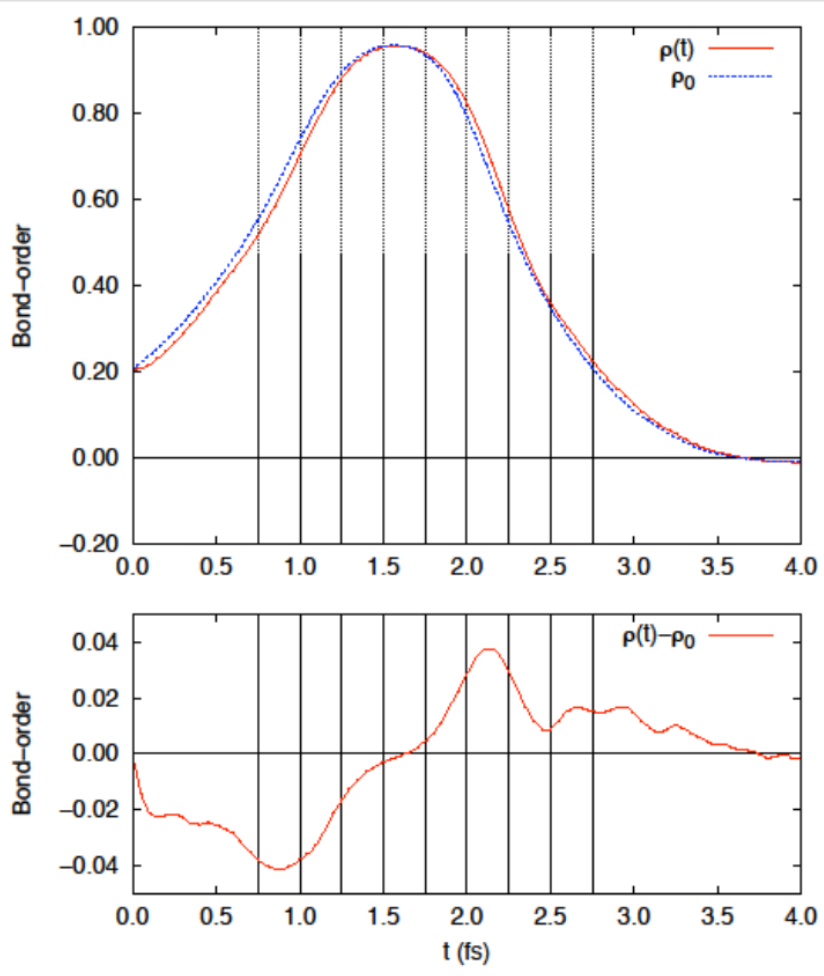


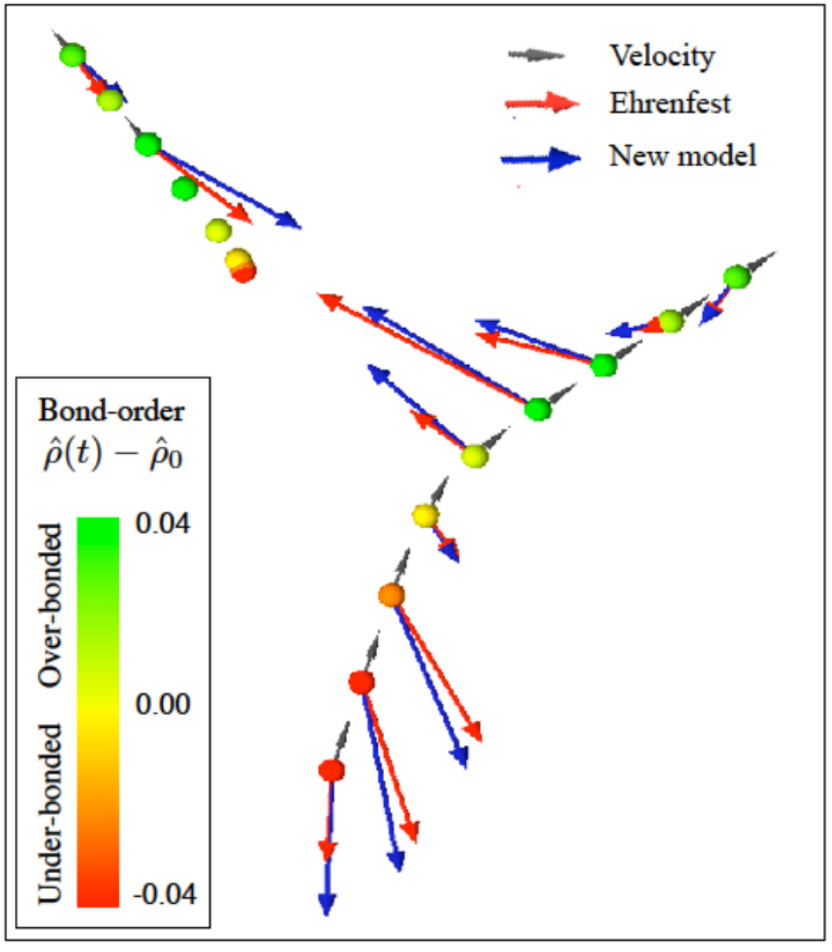
Simulation



Model

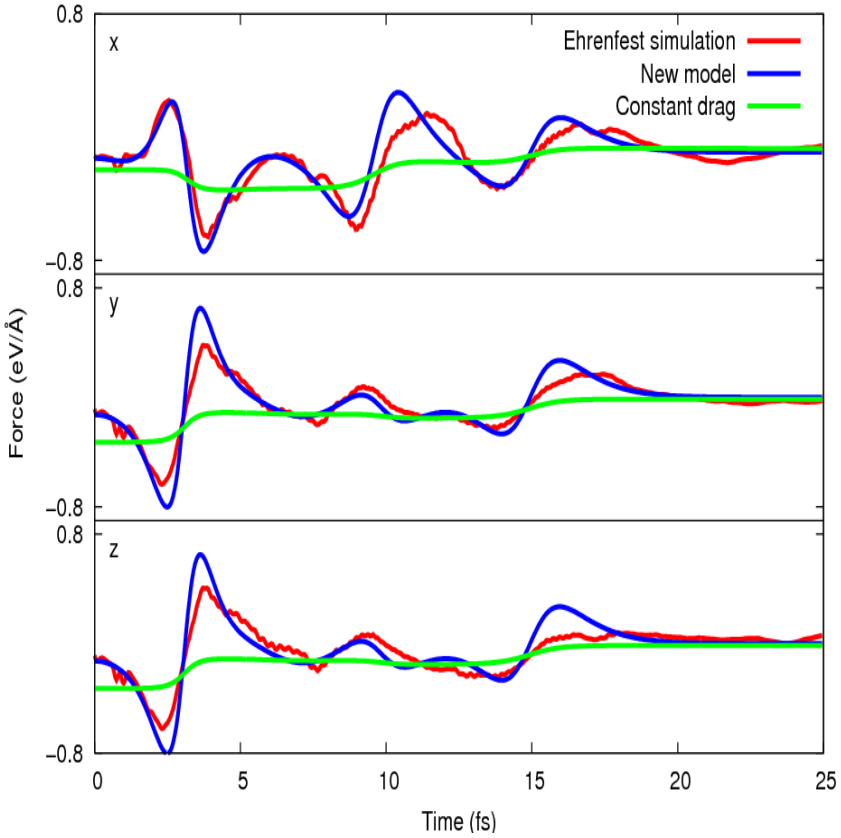
Oblique Collision (cont.)



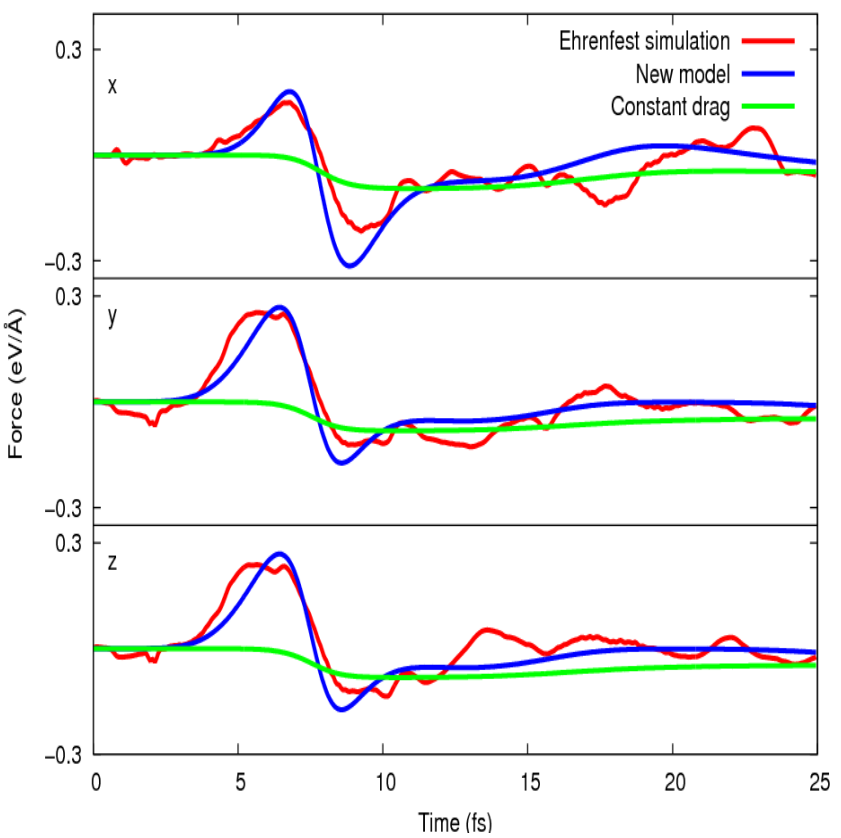


Resolved Forces

PKA



Later atom



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Summary

- MD is essential for understanding cascades, but it would be good to incorporate effects of electrons sensibly.
- Many small excitations heat the electrons.
- Viscous damping captures average energy transfer.
- But non-adiabatic force is really directional.
- Simple expression for non-adiabatic force captures its direction and magnitude.
- Can we also improve the description of electronic heat transport?
- See http://www.cmth.ph.ic.ac.uk/people/d.mason for more information.