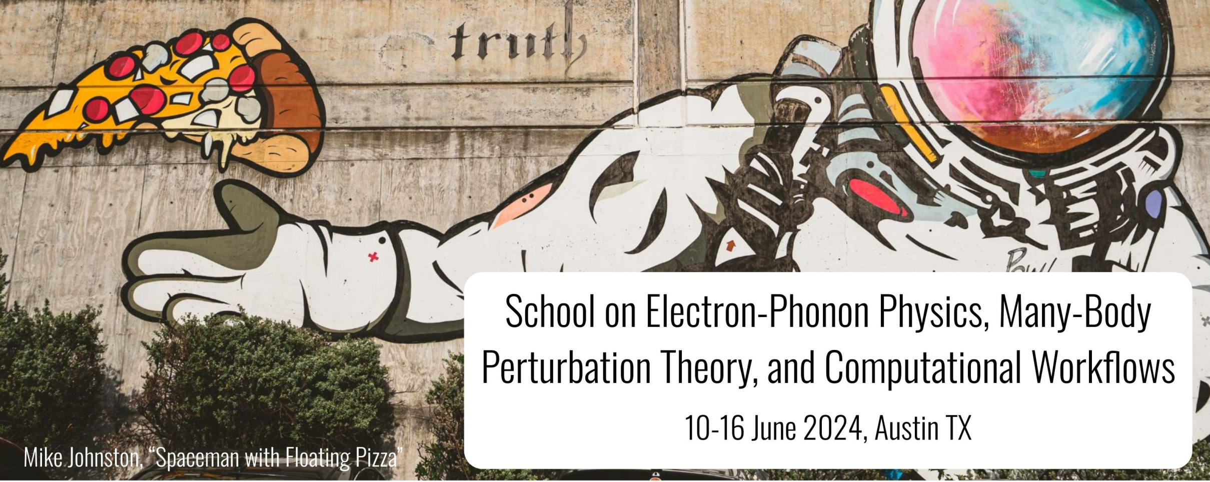

Mike Johnston, "Spaceman with Floating Pizza"

School on Electron-Phonon Physics, Many-Body Perturbation Theory, and Computational Workflows

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Hands-on Wed.6

Ionized-impurity and grain-boundary scatterings

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Contents

Theory for ionized-impurity scattering

- The development for this problem was published in [J. Leveillee, X. Zhang, E. Kioupakis, and F. Giustino, Phys. Rev. B **107**, 125207 (2023)].
- Infact, the real shape of the impuritiy potential depends the crystal structure, type of defect and its formation energy, which in principle requires sophisticated *ab initio* calculations for defect-containing supercells.
- The problem is simplified by considering the charged defects as point-charge system which is randomly distributed in host materials.

Scattering by a single point-charged defect

- From [C. Verdi and F. Giustino, Phys. Rev. Lett. **115**, 176401 (2015)], the Coulomb potential generated by a periodic point charge Q in Born-von Kármán supercell at τ is

$$\phi(\mathbf{r};\tau) = \frac{4\pi}{\Omega}\frac{Q}{4\pi\varepsilon_0}\frac{1}{N}\sum_{\mathbf{q}}\sum_{\mathbf{G}\neq-\mathbf{q}}\frac{\mathrm{e}^{i(\mathbf{q}+\mathbf{G})(\mathbf{r}-\tau)}}{(\mathbf{q}+\mathbf{G})\varepsilon(\mathbf{q}+\mathbf{G})}$$

- Considering an impurity with charge $Q = \pm Ze$, the potential energy feels by an electron at position $\mathbf{r}$ is

$$V(\mathbf{r};\tau) = \frac{-e^2}{4\pi\varepsilon_0}\frac{4\pi Z}{\Omega_{\mathrm{BvK}}}\sum_{\mathbf{q}}\sum_{\mathbf{G}\neq-\mathbf{q}}\frac{\mathrm{e}^{i(\mathbf{q}+\mathbf{G})(\mathbf{r}-\tau)}}{(\mathbf{q}+\mathbf{G})\varepsilon(\mathbf{q}+\mathbf{G})}$$

- The ionized-impurity scattering matrix between two states $|n\mathbf{k}\rangle$ and $|m\mathbf{k}+\mathbf{q}\rangle$

$$g_{mn}^{\mathrm{imp}}(\mathbf{k},\mathbf{q};\tau) = \frac{-e^2}{4\pi\varepsilon_0}\frac{4\pi Z}{\Omega_{\mathrm{BvK}}}\sum_{\mathbf{G}\neq-\mathbf{q}}\frac{\mathrm{e}^{i(\mathbf{q}+\mathbf{G})\tau}\langle u_{m\mathbf{k}+\mathbf{q}}|\mathrm{e}^{i\mathbf{G}\mathbf{r}}|u_{n\mathbf{k}}\rangle_{\mathrm{uc}}}{(\mathbf{q}+\mathbf{G})\varepsilon(\mathbf{q}+\mathbf{G})}$$

Scattering by multiple point-charged defects

- We consider a set of N_{imp} impurities at position $\tau_1, \tau_2, ..., \tau_{N_{\mathrm{imp}}}$, the scattering matrix

$$g_{mn}^{\mathrm{imp}}(\mathbf{k},\mathbf{q};\{\tau\}) = \frac{-e^2}{4\pi\varepsilon_0}\frac{4\pi Z}{\Omega_{\mathrm{BvK}}}\sum_{\mathbf{G}\neq-\mathbf{q}}\frac{\langle u_{m\mathbf{k}+\mathbf{q}}|\mathrm{e}^{i\mathbf{G}\mathbf{r}}|u_{n\mathbf{k}}\rangle_{\mathrm{uc}}}{(\mathbf{q}+\mathbf{G})\varepsilon(\mathbf{q}+\mathbf{G})}\sum_{I=1}^{N_{\mathrm{imp}}}\mathrm{e}^{-i(\mathbf{q}+\mathbf{G})\tau_I}$$

- The total scattering rate of state $|n\mathbf{k}\rangle$ in Born's approximation is

$$\frac{1}{\tau_{n\mathbf{k}}^{\mathrm{imp}}} = \sum_{m\mathbf{q}}\frac{2\pi}{\hbar}|g_{\mathrm{mn}}^{\mathrm{imp}}(\mathbf{k},\mathbf{q};\{\tau\})|^2\delta(\epsilon_{n\mathbf{k}}-\epsilon_{m\mathbf{k}+\mathbf{q}}) = \sum_{m\mathbf{q}}\Gamma_{n\mathbf{k}\to m\mathbf{k}+\mathbf{q}}^{\mathrm{imp}}$$

- Kohn-Luttinger ensemble average of scattering rate gives

$$\Gamma_{n\mathbf{k}\to m\mathbf{k}+\mathbf{q}}^{\mathrm{imp,ave}} = n_{\mathrm{ii}}\frac{2\pi}{\hbar}\left[\frac{e^2}{4\pi\varepsilon_0}\frac{4\pi Z}{\Omega}\right]^2\sum_{\mathbf{G}\neq-\mathbf{q}}\frac{|\langle u_{m\mathbf{k}+\mathbf{q}}|\mathrm{e}^{i\mathbf{G}\mathbf{r}}|u_{n\mathbf{k}}\rangle_{\mathrm{uc}}|^2}{|(\mathbf{q}+\mathbf{G})\varepsilon(\mathbf{q}+\mathbf{G})|^{\mathbf{2}}}\delta(\epsilon_{n\mathbf{k}}-\epsilon_{m\mathbf{k}+\mathbf{q}})$$

Scattering by grain-boundary

- Grain-boundary scattering can be calculated using the simplest possible model, whereby the relaxation time is given by

$$\tau_{n\mathbf{k}}^{\mathrm{gb}} = L/|\mathbf{v}_{n\mathbf{k}}|,$$

where, L is grain size and $\mathbf{v}_{n\mathbf{k}}$ is group velocity of carrier.

- **Exercise 1** and **Exercise 2** will show you how ionized-impurity and grain-boundary scatterings impact on carrier mobility, respectively. The system is chosen for this tutorial is cubic BN (c-BN), the same as in "Exercise 1 of Hands-on Wed.5"

References

- J. Leveillee, X. Zhang, E. Kioupakis, and F. Giustino, Phys. Rev. B **107**, 125207 (2023) [link]
- C. Verdi and F. Giustino, Phys. Rev. Lett. **115**, 176401 (2015) [link]
- N. Mingo and D. A. Broido, Nano Lett. 5, 1221 (2005) [link]