

# PolaronMobility.jl: Implementation of the Feynman variational polaron model

Jarvist Moore Frost<sup>1, 2</sup>

<sup>1</sup> Department of Chemistry, University of Bath, UK. <sup>2</sup> Department of Materials, Imperial College London, UK.

DOI: [10.21105/joss.00566](https://doi.org/10.21105/joss.00566)

## Software

- [Review](#) ↗
- [Repository](#) ↗
- [Archive](#) ↗

Submitted: 29 October 2017

Published: 01 February 2018

## Licence

Authors of JOSS papers retain copyright and release the work under a Creative Commons Attribution 4.0 International License ([CC-BY](#)).

## Summary

An additional electron (i.e. a charge carrier) in a material applies a polarisation field. In a polar material (one where the ions of the lattice have different charge), this results in a large coupling into the lattice motion. Small distortions in the lattice can be described in terms of a harmonic restoring force, and thereby a harmonic quasi-particle of vibration termed a phonon. Electron-phonon coupling provides a scattering mechanism by which momentum (kinetic-energy) of an electron is dissipated. These scattering processes limit charge-carrier mobility in materials. Being able to predict charge-carrier mobility helps the computational design of new technological materials. Many new materials of potential utility and interest are polar. These include oxides used as battery anodes and transparent conductors for electronic displays; and chalcogenides and halides indicated for light emission (displays, lighting) and absorption (photovoltaic solar cells).

In a polar material the dielectric electron-phonon coupling dominates the electronic scattering. Unusually, this scattering process can be modelled without any empirical parameters, and so the temperature-dependent absolute-mobility of a polar material can be calculated.

This package is an implementation in the Julia programming language of solving the Feynman (Feynman 1955) variational path-integral solution to the Frohlich (Frohlich 1952) Hamiltonian specifying the polaron problem. The Frohlich Hamiltonian is very simple. Electrons are treated at the effective-mass (quadratic dispersion relationship) level, and the vibrational response of the material as a single effective-frequency harmonic mode. Finite-temperature (free) energies of Osaka (Osaka 1959) are used, as tabulated in the modern presentation of Hellwarth et al. (R. W. Hellwarth and Biaggio 1999). Hellwarth et al. also provides a rigorous method to calculate an effective frequency.

The physical system is specified by four parameters. 1) bare-band effective-mass; 2) high-frequency and 3) zero-frequency dielectric constants, and 4) an effective dielectric phonon frequency. These are most easily calculated by electronic structure calculations. Components 3 and 4 are dependent on the lattice response, and can be derived from calculation of the infrared (dielectric) properties of the harmonic phonons.

The Feynman polaron model integrates through the infinite quantum field of these (as specified) lattice vibrations. The method is variational, and consists of an optimisation of the finite-temperature (free) energies.

Having solved for the finite temperature polaron state, the codes can then calculate various parameters of interest for device physics. Most notably polaron mobilities in the original FHIP (Feynman et al. 1962) asymptotic limit, the Kadanoff (Kadanoff 1963) Boltzmann formulation and the most recent Hellwarth et al. (R. W. Hellwarth and Biaggio 1999)

explicit contour integral forms. The size and nature of the polaron state is also described, most of which was previously investigated by Schultz (Schultz 1959).

These codes were developed for and enabled a recent publication by Frost (Frost 2017), which provided calculated temperature-dependent mobilities and polaron configurations for the halide perovskite family of semiconductors.

In providing robust codes to calculate the polaron state, this work enables calculation of further parameters such as the nature of polaron scattering, frequency-dependent mobility and polaron optical absorption.

## References

- Feynman, R. P. 1955. “Slow Electrons in a Polar Crystal.” *Physical Review* 97 (3). American Physical Society (APS):660–65. <https://doi.org/10.1103/physrev.97.660>.
- Feynman, R. P., R. W. Hellwarth, C. K. Iddings, and P. M. Platzman. 1962. “Mobility of Slow Electrons in a Polar Crystal.” *Physical Review* 127 (4). American Physical Society (APS):1004–17. <https://doi.org/10.1103/physrev.127.1004>.
- Frohlich, H. 1952. “Interaction of Electrons with Lattice Vibrations.” *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* 215 (1122). The Royal Society:291–98. <https://doi.org/10.1098/rspa.1952.0212>.
- Frost, Jarvist Moore. 2017. <https://arxiv.org/abs/1704.05404>.
- Hellwarth, Robert W., and Ivan Biaggio. 1999. “Mobility of an Electron in a Multimode Polar Lattice.” *Physical Review B* 60 (1). American Physical Society (APS):299–307. <https://doi.org/10.1103/physrevb.60.299>.
- Kadanoff, Leo P. 1963. “Boltzmann Equation for Polarons.” *Physical Review* 130 (4). American Physical Society (APS):1364–9. <https://doi.org/10.1103/physrev.130.1364>.
- Osaka, Y. 1959. “Polaron State at a Finite Temperature.” *Progress of Theoretical Physics* 22 (3). Oxford University Press (OUP):437–46. <https://doi.org/10.1143/ptp.22.437>.
- Schultz, T. D. 1959. “Slow Electrons in Polar Crystals: Self-Energy, Mass, and Mobility.” *Physical Review* 116 (3). American Physical Society (APS):526–43. <https://doi.org/10.1103/physrev.116.526>.