Polarons: A Successful Application of Path Integration

Linus Aliani
University of Birmingham

Introduction

Polarons posed historically one of the first problems which was successfully explained by path integral methods in the 1950s, demonstrating the technique's versatility and easy applicability outside of QED. They since reemerged in research after 30 years of relative obscurity.

Polarons are now for example being investigated because of their application as charge carriers in PV-cells[5] while the theory is also being "recycled" in other areas of consensed matter physcis like the physics of electron-ripplon interaction[1].

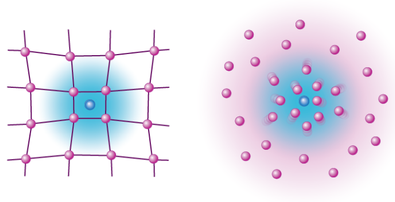

Fig. 1: A schematic sketch of the formation of polarons: The left hand side shows the electron in the middle locally distorting the lattice sites. The right hand side shows the virtual phonons produced by the electron-lattice interaction. They swarm towards the electron leading to what is called "dressing"-effect in which the electron "drags" the phonons with itself.

Gaussian Integrals

The principle idea is using the more natural representation of paths in terms of their deviation from the optimal path as shown in the figure. This is more natural because it makes use of path integrals solving boundary value problems implying that the deviation will go to zero at both ends.

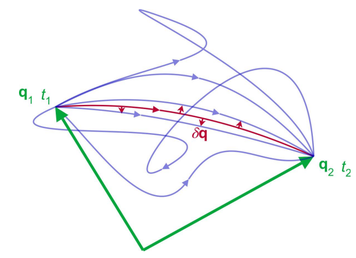

Fig. 2: Diagram for paths taken between points q1 and q2. Blue paths represent generic deviating paths. The red path is the optimal path given by the classical principle of least action with red arrows indicating the deviations from it.

If $S = S(x, \dot{x}, x^2, \dot{x}^2)$ then the path can be represented as: $x = X_{classic} + q_{deviation}$. X and X^2 dependent terms are constants of the path integral. Terms linear in y and $\dot{y}$ vanish by definition while y^2 and $\dot{y}^2$ terms give a path-independent constant[3]

Introduction and Lagrangian

If an electron moves though a polar crystal lattice it distorts it periodically resulting in local polarisation and phonons leading to electron-phonon interaction. The resulting Lagrangian is very much simplified but shows the most important features of polarons.

$$S = \int_0^t \frac{\dot{\mathbf{r}}^2}{2} + \sum_{\mathbf{k}} [\dot{\mathbf{q}}^2 + \mathbf{q}^2] + \sqrt{8}\pi\alpha \sum_k \frac{q_k}{k} e^{i\mathbf{k}\cdot\mathbf{r}} dt \tag{1}$$

1. term represents the free electrons kinetic energy
2. term represents the energy of the lattice vibrations
3. term represents the coupling of electron to the electric field with a coupling constant α introduced by Fröhlich in 1950.[4]

This is then put to action in the path integral:

$$K(x_a, t_a; x_b, t_b) = \int e^{i\frac{S}{\hbar}} \mathcal{D}x(t) \tag{2}$$

Representing the scattering amplitude for a free polaron going from space-time coordinate $(x_a x_a, t_a)$ to (x_b, t_b).

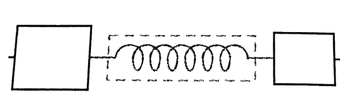

Fig. 3: The simplified model used by Feynman for the trial-action: The electron is physically coupled up with its virtual phonons resulting in a parabolic potential. This only works for low energy polarons in which the electron never leaves the bottom of the potential by much which limits the use to slow polarons.

Simplified Lagrangian and Variational Principle

The simplified action of the path integral is now:

$$S = \int -\frac{\dot{\mathbf{r}}^2}{2} dt + \frac{\alpha}{\sqrt{8}} \int\int \frac{e^{-|t-s|}}{|\mathbf{r}(t) - \mathbf{r}(s)|} dt ds \tag{3}$$

Which still is not easy to integrate but already portrays nicely what is expected of the polaron-photon coupling term.
It decays quickly in time and space. The electron is only being effected by phonons in its near vicinity which have been produced a short time ago. This is a mathematical representation of the dressing-effect.

The Variational Principle

Since the action is still difficult to sum over, a trial action is used. The idea is similar to that of the classical analog used in Fermat's principle for example. But since path integrals as sums over possible paths are like quantum physics "very statistical" One tries to minimize:

$$\langle S - S' \rangle = \delta \tag{4}$$

Where S' is an easier to integrate trial action and the average is the average over all paths. In the low temperature limit this approach then also yields an upper limit for the polarons ground state energy.

Trial action and results

The best working trial action was chosen by Feynman as seen in the above block. Resulting (this example is for small $\alpha < 3$)in:

$$E = -\alpha - \alpha^2/81 \tag{5}$$

The RHS of the above equation changes its dependence on α with different choices of α. Overall the ground state always depends on the coupling strength leading to an increased effective mass and reduced mobility[2]

References

[1] A. O. Badrutdinov, D. G. Rees, J. Y. Lin, A. V. Smorodin, and D. Konstantinov. Unidirectional charge transport via ripplonic polarons in a three-terminal microchannel device. *Phys. Rev. Lett.*, 124:126803, Mar 2020.

[2] R. P. Feynman. Slow electrons in a polar crystal. *Phys. Rev.*, 97:660–665, Feb 1955.

[3] Richard P. Feynman. An operator calculus having applications in quantum electrodynamics. *Phys. Rev.*, 84:108–128, Oct 1951.

[4] H. Fröhlich, H. Pelzer, and S. Zienau. Xx. properties of slow electrons in polar materials. *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science*, 41(314):221–242, 1950.

[5] Hui Zhang and Nam-Gyu Park. Polarons in perovskite solar cells: effects on photovoltaic performance and stability. *Journal of Physics: Energy*, 5(2):024002, feb 2023.

Fig1: Frédéric Chevy, "Bose Polarons that strongly interact", Physics, 9, 86,(2016)) Fig2: Link: https://fisicatabu.com/caida-libre-respuestas-de-veinte-siglos-de-fisica/ (last seen:04.05.23) Fig3: Link: ://www.doubtnut.com/question-answer-physics/as-shown-in-the-figure-two-equal-masses-each-of-2kg-are-suspended-