Determining the Mobility of Charge Carriers in Organic Semiconductors

Masters' Thesis

Submitted in partial fulfillment of the requirements of
BITS F421T Thesis

By

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Declaration of Authorship

I, Pranay Venkatesh, declare that this Masters' Thesis titled, 'Determining the Mobility of Charge Carriers in Organic Semiconductors' and the work presented in it are my own. I confirm that:

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- Where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated.
- Where I have consulted the published work of others, this is always clearly attributed.
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- I have acknowledged all main sources of help.
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This is to certify that the thesis entitled, "*Determining the Mobility of Charge Carriers in Organic Semiconductors*" and submitted by Pranay Venkatesh ID No. 2019B2A11004P in partial fulfillment of the requirements of BITS F421T Thesis embodies the work done by him under my supervision.

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Abstract

Master of Science

Determining the Mobility of Charge Carriers in Organic Semiconductors

by Pranay Venkatesh

The Thesis Abstract is written here (and usually kept to just this page). The page is kept centered vertically so can expand into the blank space above the title too...

Acknowledgements

The acknowledgements and the people to thank go here, don't forget to include your project advisor...

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Abbreviations

LAH **L**ist **A**bbreviations **H**ere

Physical Constants

Speed of Light $c = 2.997\ 924\ 58 \times 10^8\ \mathrm{ms}^{-\mathrm{S}}$ (exact)

Dedicate this to someone, anyone.

Chapter 1

Introduction

1.1 Semiconductor Materials

1.2 Electronic Structure

The electronic structure is the solution of the quantum states of electrons in a given chemical system. Typically, this involves determining the energies and wavefunctions of the various states. This can be done by solving the Schrödinger equation for molecules.

1.3 Phonons

1.4 Path Integrals

Chapter 2

Organic Semiconductor Materials

2.1 Introduction

2.2 Rubrene

2.3 Y6

Chapter 3

Polarons

3.1 Introduction

3.2 Pekar's Polaron

3.3 Fröhlich Polaron

3.4 Holstein Polaron

Chapter 4

Path Integrals and Quantum Dynamics

4.1 Introduction

If we want to understand the electronic properties of materials, our limited understanding of analytically solvable quantum systems does not get us very far. There's only a limited number of systems with analytical solutions.

As in the case of classical mechanics, any realistic depiction of quantum systems would require understanding how the system couples with an environment, which influences it heavily. Open quantum system theory hence helps us with this problem since we can learn what happens to systems that interact with an environment and how that affects their dynamics. The easiest models of open quantum systems are called "system-bath" models where you have a (reasonably) solvable system coupled to a bath that represents the effects of an environment.

For studying electron-phonon systems, we need to construct models whereby we can understand what happens to the electrons when they interact with an ionic lattice as an environment. This chapter starts by covering the general theory of open quantum systems and the best ways to treat their evolution. We then move on to the path integral formulation and discuss how that helps us with the quantum dynamics of system-bath models. Once we have constructed these path integral equations, we move onto evaluating the path integrals using Monte Carlo simulations.

4.2 Dynamics of Open Quantum Systems

4.2.1 Liouville-von Neumann Equation

4.2.2 System-Bath Models and The Reduced Density Matrix

4.2.3 Quantum Master Equations

4.2.4 Adiabatic and Markov Approximations

4.3 Path Integral Treatment of Open Quantum Systems

4.4 Imaginary Time Path Integral Monte-Carlo

4.5 Real Time Path Integral Dynamics

4.5.1 Quasi-Adiabatic Propagator Path Integral (QuAPI)

4.5.2 Quantum-Classical Path Integral (QCPI)

4.5.3 Evaluating the Real-Time Path Integrals

4.6 Analytic Continuation Method

4.7 Determining Observables

4.7.1 Mobility

4.7.2 Polaron Radius

4.7.3 Self-Energy

Chapter 5

Modelling Real Materials

5.1 Introduction

5.2 Electronic Structure Data

5.3 Phonon Modes

5.4 Coupling Constants

5.5 Constructing Reference Hamiltonians

5.6 Modelling Dynamics

Appendix A

Feynman Variational Approach to the Polaron Problem