[Thesis Title]

Thesis by
[Your Full Name]

In Partial Fulfillment of the Requirements for the
Degree of
[Name of Degree]

CALIFORNIA INSTITUTE OF TECHNOLOGY
Pasadena, California

[Year Degree Conferred]
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ABSTRACT

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TABLE OF CONTENTS

LIST OF ILLUSTRATIONS

Number *Page*

LIST OF TABLES

Number *Page*

Chapter 1

NOMENCLATURE

What follows is uses the restricted Hartree-Fock formalism with doubly occupied spatial orbitals.

Symbol	Description
i, j, k, l	Occupied orbitals
a, b, c, d	Virtual orbitals
p, q, r, s	General MO basis
$\mu, \nu, \lambda, \sigma$	AO basis
$(\mu\nu\|\lambda\sigma)$	Two-electron integrals

Chapter 2

G_0W_0

2.1 Interpretive procedure

The procedure that was used to compute the quasiparticle energies is given by the below equation:

$$\delta_{pq} F_{pq}^{HF}[\gamma^{DFT}] + \Sigma_p^{corr}(\varepsilon_p^{QP}) = \varepsilon_p^{QP} \tag{2.1}$$

We explain the notation starting from left to right. The first term corresponds to taking the diagonal δ_{pq} of the Hartree-Fock matrix F_{pq}^{HF} evaluated at a given electron density γ. These electron densities are obtained from a previous mean-field calculation, either γ_{DFT} or γ_{HF}. The second term evaluates the real part of the correlation self-energy for the ε_p^{QP} determined in the previous iteration. The right side of the equality gives the updated quasiparticle energy.

The Fock Matrix

In the basis of atomic orbitals, this is given by:

$$F_{\mu\nu}^{HF} = h_{\mu\nu} + \sum_{\lambda\sigma} P_{\lambda\sigma}(\mu\nu|\lambda\sigma) - \frac{1}{2}\sum_{\lambda\sigma} P_{\lambda\sigma}(\mu\lambda|\nu\sigma) \tag{2.2}$$

where $h_{\mu\nu}$ is the one-electron part of the Hamiltonian, $P_{\lambda\sigma}$ is the density matrix, and $(\mu\nu|\lambda\sigma)$ is one of the two-electron integrals. Cite Szabo. This is the simple form of the Hartree-Fock matrix that we want to use here and not the DFT Fock matrix. We transform this Fock matrix into the MO basis with:

$$F_{pq} = \sum_{\mu}\sum_{\nu} C_{\mu p}^{*} F_{\mu\nu} C_{\nu q} \tag{2.3}$$

where C is the matrix of MO coefficients. Another useful identity is for the density matrix in terms of the MO coefficients from the mean-field calculation:

$$P_{\mu\nu} = 2\sum_{i=1}^{N/2} C_{\mu i} C_{\nu i}^{*} \tag{2.4}$$

We note that the sum runs only over the $N/2$ occupied *spatial* orbitals.

Real Correlation-Solve Energy

This is the second term in 2.1. It is dynamic, as opposed to the previous Fock term that was discussed, as it is updated with a new quasiparticle energy in each

iteration. In the case of the G_0W_0 approximation, we are only interested in the diagonal element of Σ^{corr} corresponding to the orbital with index p. This function is evaluated at the QP energy ε_p^{QP} just obtained in the previous iteration. We will go into greater detail about the form of Σ^{corr} in the next chapter.

Chapter 3

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Chapter 4

THIS IS THE FOURTH CHAPTER

Chapter 5

THIS IS THE FIFTH CHAPTER

Chapter 6

THIS IS THE SIXTH CHAPTER

Chapter 7

THIS IS THE SEVENTH CHAPTER

Chapter 8

THIS IS THE EIGHTH CHAPTER

Appendix A

QUESTIONNAIRE

Appendix B

CONSENT FORM

POCKET MATERIAL: MAP OF CASE STUDY SOLAR SYSTEMS