CHEM 5914 Literature Review and Research Plan - COVER SHEET - Fall 2016

Student's Name	Kirk C Pearce
Review Title	Analytical Derivatives in Quantum Chemistry
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Date Submiteed	September 12, 2016
Response Deadline	N/A

X	**Outline.** Submit to the Research Director only. No specific response deadline.
	Preliminary Draft. Submit to Research Director only. Response needed by 10/14/16.
	First Draft. Submit to Advisory Committee. Responses needed by 11/16/16.
	Final Draft. Submit to Advisory Committee. Responses needed 12/14/16.

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Faculty Instructions are available on the CHEM Grad Program site in the Literature Review folder.

I. Introduction

A. Big picture of analytic derivatives

i. Usefulness in quantum chemical calculations

a. Properties of interest to all chemists

ii. Advantages of analytic versus. numerical differentiation

a. Numerical accuracy (obviously)

b. Increased computational efficiency

iii. Disadvantages

a. Computational cost with higher order derivatives

II. Electronic Structure Theory

A. Schrödinger Equation

B. Hartree-Fock Theory

i. Single Determinant Representation minimized with constraint that spin orbitals remain orthonormal

ii. Shortcomings - Mean field approximation (no electron correlation energy)

C. Møller-Plesset Perturbation Theory

i. Treat electron correlation as perturbation to the HF SCF solution

D. Coupled Cluster Theory

i. Exponential form of the wave function

ii. Size Consistency/Extensivity

III. Optical Response

A. Response Theory

i. Exact Response

ii. Linear Response

iii. Quadratic and Higher Order Response