

Dielectric Models as Preconditioners to Accelerate *Ab Initio* Calculations

Nick Woods

Cavendish Laboratory, Department of Physics, J J Thomson Avenue, Cambridge. CB3 0HE

Abstract

Preconditioners . . .

1. Introduction

2. Background Theory

2.1. *Density Functional Theory*

2.2. *Dielectrics*

2.3. *Preconditioning*

2.4. *Dielectric Model of Jellium and its use in CASTEP*

Study, into to linear response regime, good initial guess. analysis of M

3. Improved Dielectric Model

This follows the work of Levine and Louie (ref) who propose...

4. Results

5. Conclusions

Acknowledgements

Appendix A. Derivation of Newton's Method

Appendix B. Derivation of Broyden's Methods