Electronic structure Periodic boundary conditions TCM 1993-6

Mike Payne's 60th Birthday – Celebratory symposium

Guy Makov, Ben-Gurion University

Beginnings 1993

Iterative minimization techniques for *ab initio* total-energy calculations: molecular dynamics and conjugate gradients

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This article describes recent technical developments that have made the total-energy pseudopotential the most powerful *ab initio* quantum-mechanical modeling method presently available. In addition to presenting technical details of the pseudopotential method, the article aims to heighten awareness of the capabilities of the method in order to stimulate its application to as wide a range of problems in as many scientific disciplines as possible.

CONTENTS

- The "agenda":

Expanding application of Total Energy methods

Condensed matter

Materials Science

Chemistry

Biochemistry

….

Cluster project

- Obtain the relaxed cluster structures of (Nb)n
- Calculate the IP as a function of size
- Relaxation of ionic positions

Cluster project

- Obtain the relaxed cluster structures of (Nb)n
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- Relaxation of ionic positions

- Computational resources
  - Cray
  - Workstations
- Convergence of supercells

The energy and elastic dipole tensor of defects in ionic crystals calculated by the supercell method

M Leslie† and M J Gillan‡

JPhysC (1985)

- "However, what we want is not this energy Earray in a periodic array of defects, but the energy E of a defect in an otherwise perfect infinite crystal."
- "It seems likely that the dominant correction will be due to the Coulomb interaction between the defects."
- "If the repeating unit is large, we can treat this by a macroscopic approximation, … the Coulomb energy of a periodic array of point charges Q with a neutralising background immersed in a structureless dielectric."

$$\Delta E = \Delta E_{\text{array}} + \tfrac{1}{2}\alpha Q^2/\varepsilon_0 L\,.$$

Problem formulation

$$\phi(\mathbf{r}) = \int_{\text{sample}} d^3r' \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$
$$= \sum_l \int_{\text{cell}} d^3r' \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'+\boldsymbol{l}|} \ , \qquad (2)$$

Electrostatics only

Fixed density – isolated defect

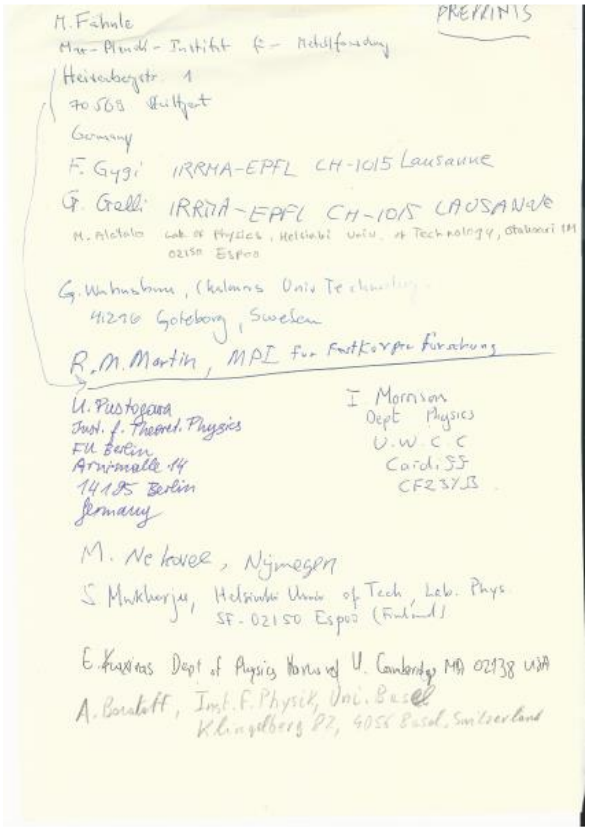
PHYSICAL REVIEW B VOLUME 51, NUMBER 7 15 FEBRUARY 1995-I

Periodic boundary conditions in *ab initio* calculations

G. Makov and M. C. Payne

- Results for atoms/molecules/clusters
  - Neutral systems converge as $O(L^{-5})$
  - Charged or dipolar can converge as rapidly
- Results for condensed matter – e.g. charged point defects
  - Could converge as $O(L^{-5})$ with effective quantities – dielectric constant, quadrupole moment

Publication



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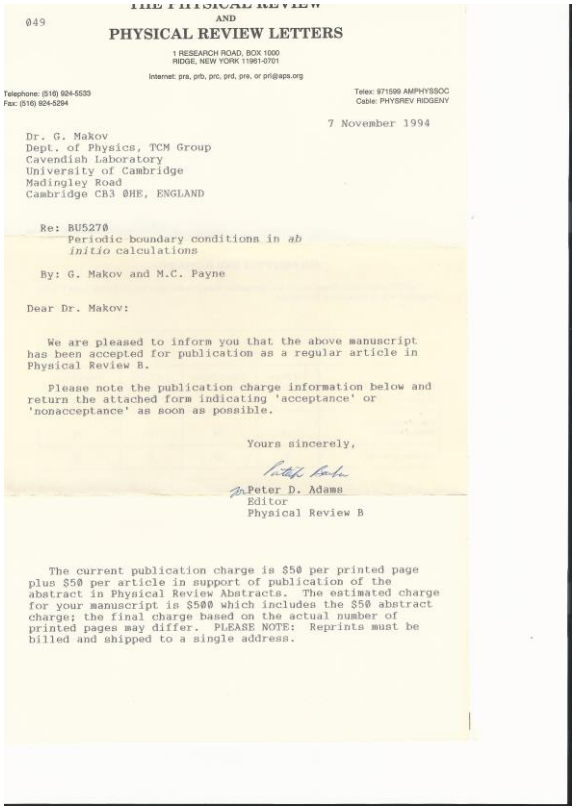

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PHYSICAL REVIEW LETTERS

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7 November 1994

Dr. G. Makov
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Re: BU5270
Periodic boundary conditions in *ab initio* calculations

By: G. Makov and M.C. Payne

Dear Dr. Makov:

We are pleased to inform you that the above manuscript has been accepted for publication as a regular article in Physical Review B.

Please note the publication charge information below and return the attached form indicating 'acceptance' or 'nonacceptance' as soon as possible.

Yours sincerely,

Peter D. Adams
Editor
Physical Review B

The current publication charge is $50 per printed page plus $50 per article in support of publication of the abstract in Physical Review Abstracts. The estimated charge for your manuscript is $500 which includes the $50 abstract charge; the final charge based on the actual number of printed pages may differ. PLEASE NOTE: Reprints must be billed and shipped to a single address.

Impacts

- First citation (1995)
- 1996
  - Resta – Theory of polarization in PBC
  - Car – Application to molecules, clusters, defects
  - Payne – PBC, Applications
  - Needs – PBC for QMC
- Improvements, testing, exceptions, application, citation,…

PHYSICAL REVIEW B VOLUME 53, NUMBER 23 15 JUNE 1996-I

Periodic boundary conditions in *ab initio* calculations. II. Brillouin-zone sampling for aperiodic systems

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- How to sample k-points to accelerate convergence of aperiodic systems due to defect band dispersion?

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Periodic boundary conditions in *ab initio* calculations. II. Brillouin-zone sampling for aperiodic systems

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- How to sample k-points to accelerate convergence of aperiodic systems due to defect band dispersion?

REVIEWS OF MODERN PHYSICS, VOLUME 86, JANUARY–MARCH 2014

First-principles calculations for point defects in solids

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TCM memories


Happy
Birthday
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