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September 30, 1992

Dr. Donald H. Liebenberg
Office of Naval Research
Department of the Navy
Arlington, VA 22217-5000

Dear Don,

I am pleased to provide a "close-out" report for the ONR Grant N00014-89-J-1379.

Thank you very much for you interest and support.

Sincerely,

Original Signed by
Robert E. Wyatt
W. T. Doherty Professor of Chemistry and
Director, Institute for Theoretical
Chemistry

REW/me

Enclosures
cc: ONR- Austin
NRL
DTIC

1. Title: Quantum Dynamics of Shock Waves in Molecular Crystals

2. Objective: This research has focused upon theoretical studies of shock wave transport in model molecular lattices via both classical and quantal techniques. In the *previous grant period*, the cluster model was developed and applied to model harmonic and cubic anharmonic molecular lattices. During *this grant period*, the cluster method has been extended to three more complex and physically significant situations. These are: (1) shock wave propagation in a linear chain of Morse oscillators; (2) shock wave propagation in a linear NCCN lattice with Morse interaction potentials; (3) shock wave propagation in a 2D model CH_3NO_2 lattice.

3. Summary of Progress: During this grant period, the semiclassical cluster model was applied to three lattice models of increasing complexity.

In the first study, which has been published in *J. Phys. Condens. Matter*, a lattice of diatomic molecules was considered. All interatomic interactions were described by Morse potentials. The molecular vibrational energies were found to differ quantitatively from the classical results.

In the second study, which has been published in *J. Phys. Chem. Solids*, a linear lattice of tetratomic molecules (NCCN) was considered. This was the first study in which both classical and quantum feedback between the cluster molecule and the surrounding lattice were considered. When the classical and quantum results were compared, the internal mode energies of the NCCN molecules showed quantitative differences.

In the third and possibly most interesting of the three studies (now about 60% complete), the first semiclassical results on shock wave propagation in a 2D lattice are being developed. The 2D lattice is the same model for CH_3NO_2 that was studied using classical dynamics by Oran, Boris, and coworkers at NRL. The classical dynamics simulations have been completed for one shock wave propagation. The results are displayed as a series of "snapshots" showing the particles in the lattice.

The computer codes required to perform the quantum mechanical studies have been completed and preliminary results have been compared with those from the classical simulations. In the future, it is planned to conduct convergence studies, complete the quantum results for several different shock waves, and perform detailed comparisons with the classical results. The result should be a quite detailed comparison which will help answer the question: "How important are quantum effects during shock wave propagation through molecular solids?"

4. Papers published in refereed journals:

a. T.-G. Wei and R. E. Wyatt, "Semiclassical Dynamics of Shock Wave Propagation and Energy Redistribution Among Vibrational Modes in a Morse Molecular Lattice," *J. Phys. Chem. Solids* **53**, 871(1992).

b. T.-G. Wei and R. E. Wyatt, "Semiclassical Dynamics of Shock Wave Propaagation in Molecular Crystals: Application to the Morse Lattice," *J. Phys.: Condens. Matter* **2**, 9787(1990).

c. T.-G. Wei and R. E. Wyatt, "Classical and Semiclassical Dynamics of Shock Wave Propagation in a 2-D Molecular Lattice," manuscript in preparation.

5. Technical Reports or non-refereed papers:
none

6. Books or book chapters:
none

7. Patents:
none

8. Invited Presentations:
none

9. Honors/Awards to P.I.:
Fellow, American Physical Society, 1988
Fellow, American Association for the Advancement of Science, 1987

10. Graduate students supported:
T.-G. Wei

11. Post docs supported:
none

12. Summary of significant results:
The research described above has led to the following developments:

a. Application of the semiclassical cluster model to more complex systems than were treated during the previous funding period.

b. The first comparisons between quantum and classical methods for cluster-lattice feedback.

c. The first classical-semiclassical comparisons of molecular energy transfer in a 2D model lattice.