Liouvillian Dynamics for Materials Simulation

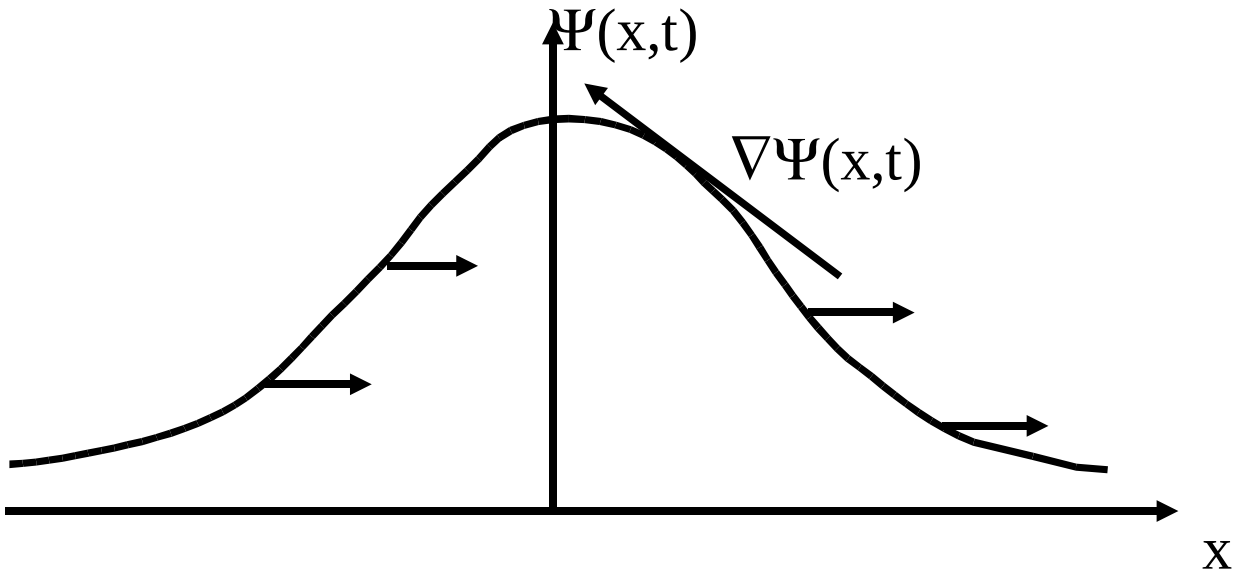
Roger Haydock, Department of Physics, University of Oregon(www.uoregon.edu)

Alternative Method for Simulating the Mechanical Properties of Materials
For Example Hardness

- Long Times − Green Functions for Linear Equations
- Rare Events −Analytic Integration over Distributions (moments)
- Correlated Motion of Many Atoms − Propagate only Disturbances

Liouville's Equation

For Functions on Phase Space (position and velocity)

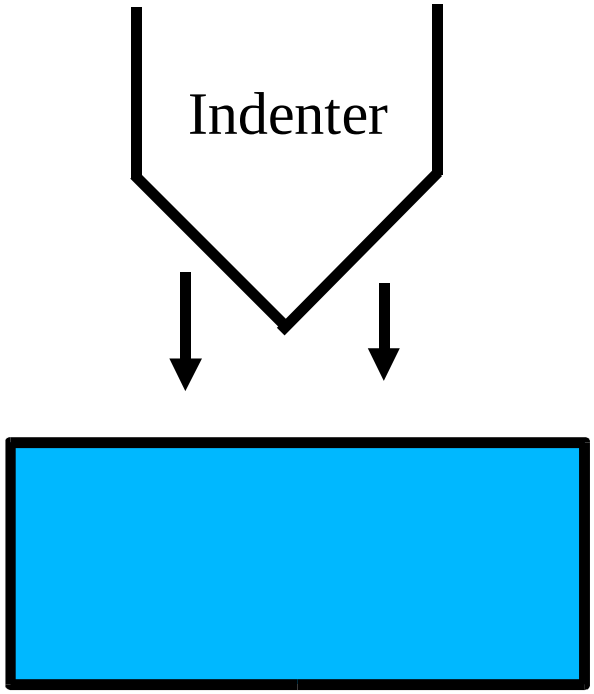


$$i\,\partial\Psi/\partial t = V_{elocity}\cdot(-i\nabla_X\Psi) + A_{cceleration}\cdot(-i\nabla_V\Psi)$$

Properties of Liouville's Equation

- Linear − a Classical Analogue of the Schrödinger Equation
- Liouvillian $L=V\cdot(-i\nabla_x) + A\cdot(-i\nabla_v)$ replaces the Hamiltonian
- Use Green Functions $(\omega - L)^{-1}$ to find long−time behavior
- Solve using moments $\langle L^n \rangle$ (Recursion)
- Many Atoms $\Rightarrow$ Function Space of High Dimension

Application to Correlated Motion in Materials



Represent local disturbances by operators

Operator u acts on phase space functions

modified $\Psi(X,V) = u\,\Psi(X,V)$

Evolve the Disturbance not the State

$$-i\,\partial u/\partial t = [L, u] = \Lambda\, u$$

The Liouvillian Commutator Equation is the Analogue of Heisenberg's Equation

- Green Functions for long times $(\omega - \Lambda)^{-1}$
- Moments include rare events $\langle\langle \Lambda^n \rangle\rangle$
- Motion of Disturbance rather than whole system reduces the problem of many atoms

Dynamical Basis Sets for Computation

Given N words of Memory, which is better?

1. Static −Perform Calculation in an N−Dimension Subspace storing N Components of a Vector

2. Dynamic − Perform Calculation in a 10^{18}−Dimensional Subspace storing the N/2 Indices for the N/2 largest Components of a Vector (64 bit word)

   Neglect of small Components leads to small errors in Tridiagonalization or Recursion

Liouvillian Commutator, Dynamic Basis, and Tridiagonalization

- Direct Calculation of Mechanical Properties
- Access to Long times
- Inclusion of Rare Events
- Many Correlated Atoms