

10.675 LECTURE 17

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1. TODAY

Running Car-Parrinello Code
MD/CP Eqs
MD trajectories
CP input, output, results

2. CAR-PARRINELLO

Initially, used to optimize the wave function and move nuclei at the same time.

Uses a variety of solver algorithms like velocity verlet

CP equations use a fictitious mass, that is the trick.

In MD, there is a period of time, called "equilibration time", where the system is in a non-physical state due to the initial input coordinate and velocity guesses put in by the user.

After that, the system is equilibrated and useful measurements can then be taken on the system.

$$B^{observable} = \frac{1}{t' - t} \int \beta(t) dt$$

