Week Five Phy-480

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September 2025

1. Structuring a Python Code for MD Simulations

Below you will find the Python code structured to carry out molecular dynamics simulations of a cloud of electrons in free space using the velocity Verlet algorithm.

1. **Initialization:**
   - Define constants
   - Initialize particle positions $\vec{r}_i(0)$ randomly in a region.
   - Initialize velocities $\vec{v}_i(0)$.
   - Initialize accelerations $\vec{a}_i(0)$.
2. **Force Calculation:**
   - Compute pairwise Coulomb forces between particles:

$$\vec{F}_{ij} = k_C \frac{e^2 \vec{r}_{ij}}{|\vec{r}_{ij}|^3}$$

   - Sum over j for each particle i.
3. **Time Integration (Velocity Verlet):**

$$\vec{r}_i(t+\delta t) = \vec{r}_i(t) + \delta t \vec{v}_i(t) + \frac{\delta t^2}{2m}\vec{F}_i(t),$$
$$\vec{v}_i(t+\delta t) = \vec{v}_i(t) + \frac{\delta t}{2m}\Big(\vec{F}_i(t) + \vec{F}_i(t+\delta t)\Big).$$

4. **Loop Over Timesteps:**
   - Update positions.
   - Recompute forces.
   - Update velocities.

- Save positions, velocities, and energies for analysis.

5. **Output and Analysis:**
   - Track kinetic, potential, and total energies.
   - Monitor conserved quantities and system behavior.

2. Mechanical Energy in an Electron Cloud

In an electron cloud in free space:

- There are no external forces on the system as a whole. By Newton's third law, internal forces cancel out in pairs. Which would mean that the **center of mass** of the system moves with constant velocity. If initially at rest, the center of mass must be fixed.
- The **total mechanical energy** of the system consists of the sum of kinetic and potential energies:

$$E_{\text{tot}} = \sum_i \frac{1}{2} m v_i^2 + \sum_{i<j} \frac{k_C e^2}{r_{ij}}.$$

- The total energy is conserved because there are no external forces.

Thus, the system's energy remains constant, and the COM motion is uniform.

3. Velocity Distribution and Temperature in Expanding Clouds

In an MD simulation of an expanding electron cloud in a micro-canonical ensemble:

- The system is far from equilibrium. Therefore, the **velocity distribution does not immediately follow Maxwell-Boltzmann statistics**.
- Over time, if collisions randomize velocities sufficiently, the distribution may relax toward a Maxwell-Boltzmann form, but during expansion, it typically deviates.
- The **concept of temperature** becomes less clear. Temperature is well-defined in equilibrium ensembles, but here, one can only assign an "effective temperature" based on average kinetic energy:

$$k_B T_{\text{eff}} \sim \frac{2}{3N} \sum_i \frac{1}{2} m v_i^2.$$

Thus, while temperature has limited meaning in far-from-equilibrium conditions, the velocity distribution can still provide insight into the system's dynamics.

4. Using MD Simulations to Characterize Expansion

MD simulations let us study the electron cloud expansion at the particle level. Key checks include:

- Tracking the average radius $\langle r \rangle$ and radial distribution over time.
- Monitoring energy conversion between potential and kinetic energy.
- Looking at radial velocities v_r to see if the expansion is isotropic.
- Comparing simulation forces with the analytic uniform-sphere model.

Together these show how the cloud spreads and whether it matches continuum expectations.

5. Comparison of Forces with Continuum Model

The continuum model predicts $E(r) \propto r$ inside the sphere and $E(r) \propto 1/r^2$ outside. In MD:

- Single particles feel noisy, fluctuating forces due to discreteness.
- Averaging over many particles gives results close to the continuum prediction.
- Deviations are strongest near the edge or with small particle numbers.

Thus the continuum model is accurate on large scales, but MD reveals small-scale differences.

6. Cooling and Maxwell-Boltzmann Statistics

The cloud's expansion is not cooling in the refrigeration sense:

- Energy shifts from potential to kinetic, driving bulk outward motion.
- Temperature can only be defined from velocity fluctuations, not true equilibrium.
- The velocity distribution is anisotropic, dominated by radial flow, and not Maxwell-Boltzmann.

So the system does not "cool" thermodynamically, but its fluctuations can resemble an effective non-equilibrium temperature.