LECTURE I
MEAN FIELD THEORIES

GENERAL IDEA

A system of N particles (objects) is in general described by a density function

$$F(W) = F(w_1, .., w_N, t)$$

with w_n the states of the objects. (particles: $w_n = (x_n, v_n)$ the positions and the velocities.)

- The evolution of F is, in general, described by a linear equation.
- This is, in general, too complex an object to handle.
- Goal: Reduce to an equation in w_1, t (nonlinear).

The BBGKY hierarchy

(Bogoliubov-Born-Green-Kirkwood-Yvon)

Identical particles:

$$F(\Pi W, t) = F(W, t), \ \forall \Pi \text{ permutations of } (w_1, .., w_N)$$

Projection on statistical independence:

$$PF(a, b) = f(a)g(b), \quad \int \psi(I - P)F \ dab = 0, \ \forall \psi = \psi(a), \psi(b)$$

$\Rightarrow$

$$f(a) = \int F(a, b) \ db, \quad g(b) = \int F(a, b) \ da$$

THE HIERARCHY

Use the product of the projections $P_N..P_1$ with

$$P_n F = f(w_1,..,w_n)g(w_{n+1},..,w_N)$$

$$P_1 F = f_1(w_1)g_1(w_2,..,w_N)$$

$$P_2 P_1 F = R(w_1,w_2)g_2(w_3,..,w_N)$$

$$\int \psi(w_1,w_2)Rg_2 \; dW = \int \psi(w_1,w_2)f_1(w_1)g_1(w_2,..,w_N) \; dW$$

$$\int \psi(w_3,..,w_N)Rg_2 \, dW = \int \psi(w_3,..,w_N)f_1(w_1)g_1(w_2,..,w_N) \, dW$$

$\Rightarrow$

$$g_1(w_2,..,w_N) = f_2(w_2)g_2(w_3,..,w_N)$$

$$P_2 P_1 F = f_1(w_1)f_2(w_2)g_2(w_3,..,w_N)$$

$\Rightarrow$

$$P_N..P_1 F = f_1(w_1)..f_N(w_N)$$

Decompose F:

$$F = \prod_{n=1}^{N} [P_n + (I - P_n)]F = \sum_{j_1=0}^{1} .. \sum_{j_N=0}^{1} [\prod_{n=1}^{N} P_n^{j_n}(I - P_n)^{1-j_n} F]$$

Identical particles: $P_n(I - P_k) = 0 \ \forall n, k$

$\Rightarrow$

$$F = \prod_{n=1}^{N} P_n F + \prod_{n=1}^{N} (I - P_n) F$$

Theorem:

Identical particles $\Rightarrow$ correlations vanish for $N \to \infty$.

$$\prod_{n=1}^{N} (I - P_n) F = O(\frac{1}{N})$$

weakly.

The linear $N-$ body equation:

$$\partial_t F + \mathcal{L}[F] = 0$$

This gives asymptotically for $N \to \infty$

$$\partial_t[\prod_{n=1}^{N} f(w_n,t)] + \mathcal{L}[\prod_{n=1}^{N} f(w_n,t)] = 0$$

Integrating out $w_2,..,w_N$:

$$\partial_t f(w_1,t) + L_f[f](w_1,t) = 0,$$

$$L_f[f](w_1,t) = \int \mathcal{L}[f(w_1,t)\prod_{n=2}^{N} f(w_n,t)]\ dw_2..w_N$$

The kinematic case (Poisson's equation)

$W = (X, V)$ with $X = (x_1, .., x_N)$ the positions and $V = (v_1, .., v_N)$ the velocities.

$$\mathcal{L}F = \nabla_X \cdot (VF) - \nabla_V \cdot (F \nabla_X \Phi) =$$

$$\sum_n \nabla_{x_n} \cdot (v_n F) - \nabla_{v_n} \cdot (F \nabla_{x_n} \Phi)$$

with $\Phi = \Phi(x_1, .., x_N)$ the many body potential

$$\Rightarrow$$

$$L_f[f] = \nabla_{x_1} \cdot (v_1 f) - \nabla_{v_1} \cdot (f E_f),$$

E_f: the mean field force:

$$E_f(x_1, v_1, t) = \int \prod_{n=2}^{N} f(x_n, v_n, t) \nabla_{x_1} \Phi(x_1, .., x_N) \; dx_2..x_N v_2..v_N$$

BINARY FORCES:

$$\Phi = \frac{1}{2N} \sum_{j,k,j \neq k} \phi(x_j - x_k) \Rightarrow$$

If the two - body interaction scales like $\frac{1}{N}$ then E_f can be written as $\nabla_x \phi_f[\rho]$

$$E_f = \frac{N-1}{N} \int f(x', v', t) \nabla_x \phi(x_1 - x') \, dx'v' = \nabla_{x_1} \phi_f(x_1, t)$$

with

$$\phi_f[\rho](x_1, t) = \int \phi(x_1 - x') \rho(x', t) \, dx', \quad \rho(x', t) = \int f(x', v', t) \, dv'$$

COULOMB FORCES AND POISSON'S EQUATION:

ϕ: Green's function of the Laplace operator or $\nabla\phi(x) = \frac{1}{|x|}$

$$\phi * \rho = \Delta^{-1}\rho \Rightarrow \Delta\phi_f[\rho] = \rho$$

Yields an effective one body Liouville equation + Poisson

$$\partial_t f + \nabla_x \cdot (vf) - \nabla_v \cdot (f\nabla_x\phi) = 0, \quad \Delta\phi_f = \rho = \int f \; dv$$

OTHER CASES:

- Molecules with a finite size:

$$\nabla\phi(x) = \frac{1}{|x - 2r|},$$

r: size of the particle

- Van der Waals potentials:
  change in the sign of $\nabla\phi(x)$ (different interaction for long and short range).

- piecewise definition of $\phi(x)$.

A NOTE ON MOLECULAR DYNAMICS

Suppose N is not so large

Start at $t = 0$ with an ensemble of particles

$$F(X, V, 0) = \prod_{n=1}^{N} \delta(x_n - y_n^0)\delta(v_n - q_n^0)$$

Solving the Newton equations

$$\frac{d}{dt}y_n = q_n, \quad \frac{d}{dt}q_n = -\nabla_{y_n}\Phi(y_1, .., y_N)$$

yields an exact solution of the many body problem

$$F(X, V, t) = \prod_{n=1}^{N} \delta(x_n - y_n(t))\delta(v_n - q_n(t))$$

Now we have to evaluate

$$\nabla_{y_n}\Phi(y_1, .., y_n) = \sum_{k \neq n} \nabla\phi(y_n - y_k), \quad n = 1 : N$$

$O(N^2)$ operations in each time step!

PARTICLE [3] MESH METHODS

Compute the $N-$ particle force $E(X) = \nabla_x \Phi$ approximately as

$$E = E^{near} + E^{far}$$

$$E_n^{near} = \sum_{|y_k - y_n| \le R} \nabla \phi(y_n - y_k), \qquad n = 1 : N$$

$$E_n^{far}(y_1, ..y_N) = \Delta^{-1} \nabla [\rho(y_n) - \rho_n^{near}(y_n)]$$

Algorithm:

Given N particles

Compute E^{near} with $O(N)$ operations.

Compute $\rho(y_n) - \rho^{near}(y_n),\ n = 1 : N$ on a mesh.

Solve the Poisson equation N times with the right hand side $\rho(y_n) - \rho^{near}(y_n),\ n = 1 : N$

Compute the forces $E_n = E_n^{near} + E_n^{far},\ n = 1 : N$ by interpolation and move the particles.

This requires that we solve the Poisson equation on a mesh exactly to give an $O(N)$ algorithm.

QUANTUM MECHANICS

Instead of $F(X,V,t)$ the behavior of the system is described by a wave function $\Psi(X,t)$, satisfying the $N-$ particle Schrödinger equation

$$i\hbar\partial_t\Psi = -\frac{\hbar^2}{2m}\Delta_X\Psi + \Phi(X)\Psi, \quad X = (x_1,..,x_N)$$

Same methodology:

$$\Psi(X,t) \to \prod_{n=1}^{N} \psi(x_n,t)$$

Gives an effective on - particle Schrödinger equation + Poisson.

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\Delta_x\psi + \phi_\rho(x)\psi,$$

$$\phi_\rho(x,t) = \int \rho(x-x',t)\phi(x')\ dx', \quad \rho(x',t) = |\psi(x,t)|^2$$

QUANTUM MOLECULAR DYNAMICS

Problem: The Schrödinger equation has no characteristics (Heisenberg - principle).

$$\psi(x,t) = \prod_{n=1}^{N} \delta(x_n - y_n(t))$$

is not a solution.

SOME REFERENCES

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