Collective Coordinate Control of Density Distributions

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What are Collective Coordinates?

- If N identical point particles reside in a region Ω at positions $\boldsymbol{r}_1$ … $\boldsymbol{r}_N$, subject to periodic boundary conditions, the collective density variables $\rho(\boldsymbol{k})$ are defined thus:

$$\rho(\boldsymbol{k}) = \sum_{j=1}^{N} \exp(i\boldsymbol{k} \bullet \boldsymbol{r}_j)$$

- The applicable wave vectors have components:

$$k_\gamma = \frac{2\pi n_\gamma}{L_\gamma} \qquad (n_\gamma = 0, \underline{+}1, \underline{+}2, \ldots; \gamma = x, y, z)$$

- It is more convenient to work with the real quantities C(k)

$$\boldsymbol{C}(\boldsymbol{k}) = \sum_{j=1}^{N-1} \sum_{l=j+1}^{N} \cos[\boldsymbol{k} \bullet (\boldsymbol{r}_j - \boldsymbol{r}_l)]$$

$$-\frac{1}{2} N \le \boldsymbol{C}(\boldsymbol{k}) \le \frac{1}{2} N(N-1) \qquad (\boldsymbol{k} \neq 0)$$

Collective Coordinates in the Literature

- Description of independent plasma oscillations resulting from long-range Coulomb interactions between electrons in metals
- Derivation of self-consistent integral equations for pair correlation functions in classical fluids
- Obtaining corrections to the random phase approximations for the electron gas
- Illustrating that large-scale density variations in superfluid ^4He are long-wavelength phonons

Why Study Collective Coordinates?

- Improve understanding of the non-trivial mathematical properties of collective density variables
- Means of generating classical ground states for particle systems
  - These configurations have applications in diverse fields, .e.g., materials science and ecology
- Means of obtaining initial conditions for gravitational studies in astrophysics

Method of Approach

- Our approach involves constraining C(k) parameters that lie in the wave vector set Q to values that are consistent with the minimization of the objective function Φ

$$\Phi(\boldsymbol{r}_1 \ldots \boldsymbol{r}_N) = \sum_{\boldsymbol{k} \in \boldsymbol{Q}} \boldsymbol{V}(\boldsymbol{k}) \left[\boldsymbol{C}(\boldsymbol{k}) - \boldsymbol{C}_0(\boldsymbol{k}) \right]^2$$

$$\boldsymbol{Q} : 0 \le |\boldsymbol{k}| \le \boldsymbol{K}$$

$$\boldsymbol{C}_0(\boldsymbol{k}) = -\boldsymbol{N}/2 + \boldsymbol{D}|\boldsymbol{k}|^{\alpha}$$

- Two Investigated Problems:
  - Generating classical ground states (D = 0)
  - Tailoring the structure factor S(k) (D ≠ 0)

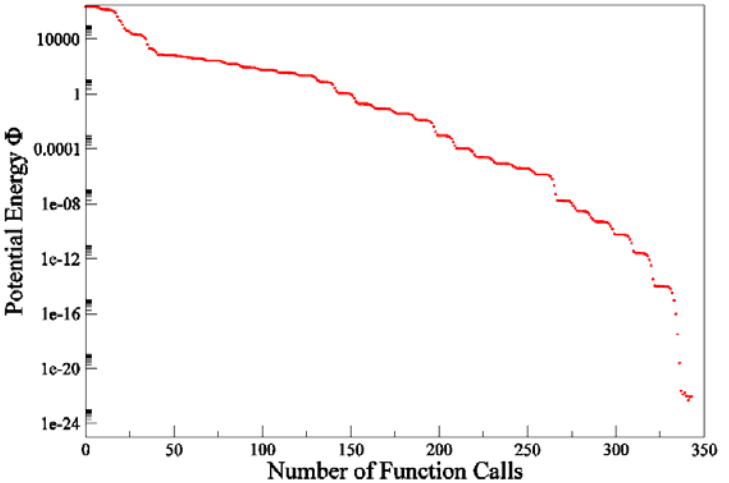
$$\boldsymbol{S}(\boldsymbol{k}) = 1 + \frac{2}{\boldsymbol{N}} \boldsymbol{C}(\boldsymbol{k})$$

- We utilize the MINOP optimization technique in order to achieve sets of $\boldsymbol{r}_1 \ldots \boldsymbol{r}_N$ for which Φ = 0.

The MINOP Algorithm†

- The algorithm minimizes a real-valued function of any number of variables based on user-provided first derivative and function information
- It applies a dogleg strategy which uses a gradient direction when one is far, a quasi-Newton direction when one is close, and a linear combination of the two when at intermediate distances from a solution

Tracking of the potential energy during an application of the **MINOP** algorithm to the structure factor tailoring problem.



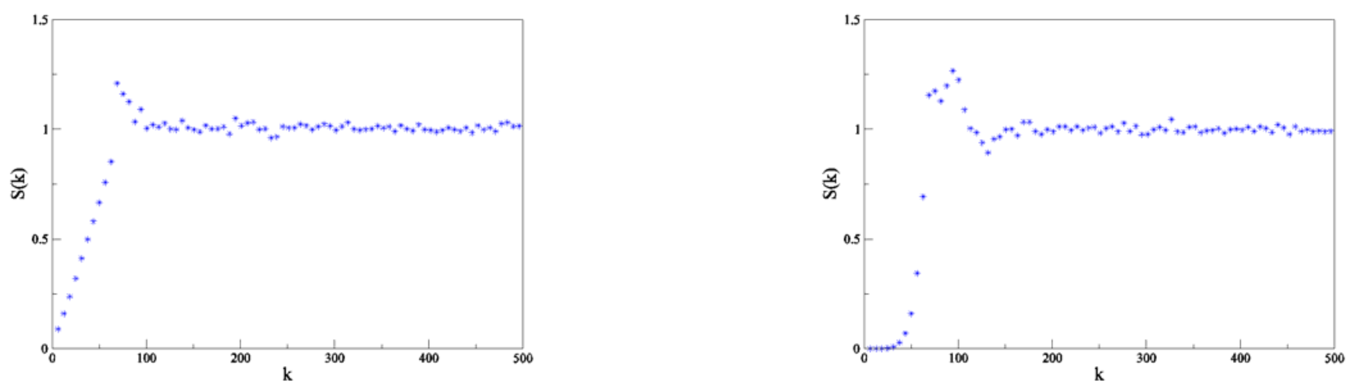
† J. E. Dennis and H. W. Mei, J. Optim. Theory Appl. **28**, 455 (1979).

Generating Classical Ground States

- As the number of constrained wave vectors is increased, the investigation distinguishes structural regimes as the number of wave vectors is increased
  - In one and two dimensions, three qualitatively distinct regimes are observed – disordered, intermediate, and crystalline regimes
  - In three dimensions, two distinct regimes emerge – disordered and crystalline regimes
- The choice of pair potential can lead to pair correlation functions that exhibit an effective hard core and thus, signal the formation of a hard-disk like equilibrium fluid
- Particle patterns that are hyperuniform in nature are generated. This supports the notion that structural glasses can be hyperuniform as the temperature $T \rightarrow 0$.

Tailoring the *S(k)* Behavior

- We generate multi-particle configurations for which $S(k) \propto |\mathbf{k}|^{\alpha}$, $|\mathbf{k}| \leq K$, and α = 1, 2, 4, 6, 8, and 10.
  - The case α = 1 is relevant for the Harrison-Zeldovich model of the early universe



Tailored *S(k)* behavior for the Harrison-Zeldovich spectrum (left panel) and the $\mathbf{k}^6$ spectrum (right panel).

- The corresponding real space particle patterns show decreasing clustering for increasing α

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