Phase transitions in mesoscopic dust clusters

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Motivation and Contents

Contents

➢ Model
➢ Structure transitions by change of
  ➢ Screening
  ➢ Temperature
➢ Radial potential barriers as
  ➢ Indicator for stability against change of screening
  ➢ Measurement for radial melting

Motivation

➢ Explanation of non-ground state configuration in experiments
➢ Screening effects
➢ Temperature effects
Model\textsuperscript{[1]}

\[ H = \sum_{i=1}^{N} \frac{P_i^2}{2m_i} + \sum_{i=1}^{N} \frac{m_i \omega_0^2}{2} r_i^2 - \sum_{i=1}^{N} \sum_{j=i+1}^{N} q^2 \frac{1}{r_i - r_j} \exp(-\kappa |r_i - r_j|) \]

kinetic energy

external confinement (screening independant)

interaction energy

with 2-particle equilibrium distance and energy

\[ r_0 = \left( \frac{2q^2}{m \omega_0^2} \right)^{1/3} \]

\[ E_0 = \left( 4m \omega_0^2 q^4 \right)^{1/3} \]

\[ H = \sum_{i=1}^{N} r_i^2 + \sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{1}{r_{ij}} e^{-\kappa r_{ij}} \]

Structure transitions by screening

\[ \kappa(12;0) = 4.05, \kappa(2,9;1) = 19.5, \kappa(5,6;1) = 4.75 \]

Structure transitions by screening

Ground states$^3$ by Molecular Dynamics simulations

The numbers in the brackets denote the particles on the inner shell(s)

Monte Carlo method

Replacement of the time-averaging in Molecular dynamics by the averaging over ensembles

Condition: ergodicity which is given by a adequate displacement algorithm

statististical description in the canonical ensemble \((N,V,T)\)

Monte-Carlo method

\[
\langle A \rangle = \sum_{x \in \Omega} P(x) A(x)
\]

Metropolis function\(^{[4]}\)

\[
P(r_i \rightarrow r_j) = \begin{cases} 
\exp(-\beta (V(r_i) - V(r_j))) & \text{for } \Delta V > 0 \\
1 & \text{otherwise}
\end{cases}
\]

\[
\Rightarrow \quad \langle A \rangle = \frac{1}{N} \sum_{i=1}^{N} A(x_i)
\]

Typically \(\sim 10^8\) MC steps (while 1 MC step is the random displacement of \(N\) particles)

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Temperature effect

Relative distance fluctuations

$$u_r^2 = \frac{\sigma_r^2}{r_0^2} = \frac{2}{N(N-1)} \sum_{i=1}^{N} \sum_{j=i+1}^{N} \sqrt{\langle r_{ij}^2 \rangle} / \langle r_{ij} \rangle^2 - 1$$

Intrashell fluctuations

$$u_{\varphi,0}^2 = \frac{2}{N_{s}(N_{s}-1)} \sum_{i=1}^{N_{s}} \sum_{j=i+1}^{N_{s}} \sqrt{\langle r_{ij}^2 \rangle} / \langle r_{ij} \rangle^2 - 1$$

Radial fluctuations

$$u_{rad}^2 = \frac{\sigma_{rad}^2}{r_0^2} = \frac{1}{N} \sum_{i=1}^{N} \sqrt{\langle r_i^2 \rangle} / \langle r_i \rangle^2 - 1$$

Critical temperatures

0.000259

0.000243

0.000346

Metastable configurations (N=31) are expected for temperatures $k_B T > 0.000346$

Structure transitions by temperature

Configurations\(^{[5]}\) for N=18, \(\kappa = 0.33\)

Ground state configuration (17;1) stays dominant in a wide range of temperature

Compared to the structure transitions by screening:

Poster P 16.35
D. Block et al.
Experimente zu metastabilen Konfigurationen von Yukawa-Balls

Minima of the total energy

N=12, $\kappa = 4.040$

$\Delta E = 0.00394$
Potential barrier height does not depend on the temperature

$$\Gamma = \frac{1}{k_B T}$$
Example: N=31

\( \kappa = 1.585 \)

\( \kappa = 1.635 \)

Potential barrier height can predict stability against increase/decrease of screening
Example: $N=40$, $\kappa=0.0$

Radial melting occurs at $\sim 10\%$ of the radial potential barrier height.
Summary

➢ Structure transitions with increase of screening parameter $\kappa$
➢ Structure transitions with increase of temperature $k_B T$
➢ Radial potential barriers as indicator for stability against change of
  ➢ Screening
  ➢ Temperature
➢ Radial potential barriers as measurement for the radial melting temperature

Outlook

➢ Calculation of Intrashell potential barriers
➢ Calculation of Rotational (rotation of two shell against each other) potential barriers
Thank you!

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Noch einbauen:
Experiment Configurations of Melzer paper (Kaeding) as comparison to
Dietmars Poster