Recent experimental [1] and theoretical [2,3] work has shown that a classical one-component plasma in a 3D parabolic trap undergoes in the strong coupling limit a transition to a highly ordered crystalline state with a nested shell structure. In the case of pure Coulomb interaction a Mendeleev-type table was found including characteristic, occupation numbers, shell closures, and unusual stable “magic” configurations, see Ref. [2,3].

Here we extend this work to the more general case of a statically screened Coulomb interaction [4] to study interesting structural transitions in dependence on screening which cannot easily be controlled in the experiments. We present a detailed analysis of the shell configurations and energies of the ground and metastable states for a large range of screening parameter $\kappa$ and particle numbers $N \leq 60$. Interestingly some kind of anomalies in the shell filling occur: For example with increasing the particle number resilient shell filling behaviour is found.

We consider $N$ classical particles with equal charge $q$ in a 3D isotropic parabolic confinement trap with frequency $\omega_0$. Particles interact with screened Coulomb force. The Hamiltonian of the lowest energy states is given by

$$H = \sum_{i=1}^{N} \frac{m_i}{2} \omega_q^2 r_i^2 + \sum_{i=1}^{N} \sum_{j=i+1}^{N} \frac{q^2}{r_{ij}^3} e^{-\kappa r_{ij}}.$$  

Distance and energy are expressed in dimensionless units with using $r_0(\omega_0 q)^{-1}$ as the equilibrium position of a two-particle Coulomb system and $(4m_0q^2\omega_0^2)^{-1}$ as their energy. Note that the confinement potential is independent of the screening $\kappa$.

The stability of Yukawa balls can be analyzed by calculating the potential barriers. While in general – fluctuations depend not only on radial barriers but also on intershell barriers – a change in the configuration coincide with a radial transition. The following figures show the radial potential barriers for the cluster with $N=31$ particles. From the diagram of structural transitions one can see that the ground state configuration of $(4;27)$ changes to $(5;26)$ at a screening parameter above 1.5 and then to $(6;25)$ immediately after. The barriers are calculated by Monte Carlo simulations at a fixed Coulomb coupling constant $\Gamma=(2\omega_0^2/m_0q^2)^{1/3}$ which is the ratio of interaction energy to the temperature.

Structural transitions in screened 3D Coulomb crystals

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Abstract

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### Energy barriers

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### Intershell and intrashell-interparticle spacing

Intershell- and intrashell-interparticle spacing as a function of shell number for different number of particles $N$ and screening lengths.