Blatt 1 - Hausaufgabe

Übung am 2. November 2018

Aufgabe 1: Morse potential

The Morse potential models the interatomic potential energy of a diatomic molecule. The potential is given by

$$\phi(r) = D_{\mathrm{e}} \left[1 - e^{-a(r-r_{\mathrm{e}})}\right]^2, \tag{1}$$

with r the distance between the two atoms of the diatomic molecule.

a) Sketch the potential.

b) Find the dimension and the physical interpretation of the parameters D_{e} and r_{e}.

c) Relate a to the force constant of the bond between the two atoms k. Hint: Taylor expand the potential to second order around its equilibrium position.

Aufgabe 2: External force field

Consider the following two-dimensional external force field

$$\mathbf{f}_{\mathrm{ext}}(x, y) = (\alpha \sin x + \beta \sin y)(\hat{\mathbf{e}}_x + \hat{\mathbf{e}}_y), \tag{2}$$

with α and β positive constants.

a) Find the conservative and non-conservative terms of $\mathbf{f}_{\mathrm{ext}}$, as well as the external potential corresponding to the conservative term.

b) Sketch the external force for the limiting cases: (i) $\alpha \to 0$, (ii) $\beta \to 0$, and (iii) $\alpha = \beta$.

c) Indicate in each case the equilibrium position(s) of a particle subject to the external field.

Variational Nonequilibrium Statistical Mechanics Wintersemester 2018/19 Lectures Prof. M. Schmidt Tutorials PD Dr. Daniel de las Heras	UNIVERSITÄT BAYREUTH

Blatt 1 - Präsenzübung

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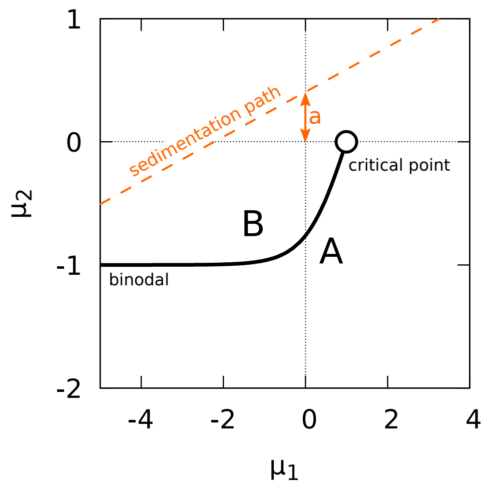
Aufgabe 3: Stacking diagrams

The figure shows the bulk phase diagram of a colloidal binary mixture in the plane of chemical potentials for a given temperature. The pure component 2 undergoes a first order $A - B$ phase transition. The binodal in the binary system is given by $\mu_{2,AB}(\mu_1) = \tanh(\mu_1 - \mu_1^c)$ if $\mu_1 < \mu_1^c$. The binodal ends at a critical point (empty circle) with coordinates $(\mu_1^c, \mu_2^c) = (1, 0)$.



The binary mixture is in equilibrium in a gravitational field. Assuming the height of the sample h is large enough ($h \to \infty$) and within a local density approximation, the sedimentation-diffusion-equilibrium can be described by the sedimentation path

$$\mu_2(\mu_1) = a + s\mu_1, \tag{1}$$

which in the $\mu_1 - \mu_2$ plane is a line with slope $s = m_2/m_1$ and $y-$intercept a. Here m_i is the buoyant mass of species i.

a) What are the possible stacking sequences that can be formed under gravity?

b) There exist three types of special sedimentation paths that define boundaries between two stacking sequences. That is, by infinitesimally varying s and/or a the stacking sequence changes. Find them.

c) Calculate and represent the stacking diagram of the mixture in the $s - a$ plane (assume $m_1 > 0$).

Further reading

[1] *The phase stacking diagram of colloidal mixtures under gravity*, D. de las Heras, and M. Schmidt, Soft Matter, **9**, 8636, (2013).
[2] *Sedimentation stacking diagram of binary colloidal mixtures and bulk phases in the plane of chemical potentials*, D. de las Heras, and M. Schmidt, J. Phys: Condens. Matter, **27**, 194115, (2015).
[3] *The role of sample height in the stacking diagram of colloidal mixtures under gravity*, T. Geigenfeind, and D. de las Heras, J. Phys: Condens. Matter, **29**, 064006, (2017).