Assignment Sheet Nr. 6

Paul Monderkamp, Matr.Nr. 2321677

monderkamp@thphy.uni-duesseldorf.de

Contents

1 Exercise 8.1

1.1 a)

Since no particles are infinitesimaly close to one another, the radial distribution function should go to zero in the limit r -> 0.
What the computation of the radial distribution function via numerical methods basically consists of is counting the number of particles that are at a certain distance to one another and creating a histogram as a function of r.
However due to the fact that the number of particles in $[r, r + dr]$ scales with the corresponding area one normalizes with an isotropic distribution which is given by $area * (N/A_total)$.
Given for instance a square grid on which the particles reside: For small r the possible lie relatively far apart and one sees the distinctive peaks in the structure of g(r). For r to infinity however the possible r within [r , r + dr] get infinitely close to each other. This results in the physical phenomenon that the different bins in the histogram get similar. Due to the normalization to isotropic density, this results in the limit g(r) -> 1 for r to inf. In statistical physics this can be interpreted as particles' positions being uncorrolated for infinite distances.

1.2 b)

$ViewMD_functions.cpp"voublerdf(particle*p, intN, constdoubleBoxL, constintNbins)"//wherevou$
$double >$

1.3 c)

i) The code from which the function rdf(particle* p, int N, const double BoxL, const int Nbins) is called is located in the file "$distr_test.cpp$". View **random**$_conf_{gN}bins =$
$500.pngforthegraph.Arandomconfigurationcorrespondstoisotropicdistribution.Duetothenormaliz$
$p, intN, constdoubleBoxL, constintNbins)iscalledislocatedin"square_lattice.cpp".Theparticlesreside$
$7/6.Theanalyticalresultsforthepossibledistancesandthuspeaksing(r)canbefoundviaPythagoreant$

1.4 d)

The code that calls the function above for this exercise lies inside "nose$_hoover.cpp".Theradi$
$Hooverthermostatcanbeobservedin"g_nose_hoover.png".Thesamplingbeginsattau =$
$1.0; "ths_e n_equil.png" showsthediagramoftheenergiesanditcanbeobservedthatthesystemiswellequili$
$1.0;$

2 8.2

a)-c) For the function that is used to calculated the MSD, view "double MSD(particle* p0, particle* p, int N, const double BoxL)" inside "MD$_functions.cpp".Thetimeaverageisreplacedwithanensembleaverageovertheparticlesusingthee$
$[0, 0.05].Observingthegraphin"MSD.png"itisvisiblethatMSD(t)isofdegreeonebeyondthatpoint.$