Manual for TYSQ22 Matlab Package

Changes made in TYSQ22 compared with TYSQ21

Only one change:
One user found a case that the result may depend on the input Q range at very high volume fraction (about 0.58). It is found that this is due to the need to have a very accurate Fourier transformation to calculate g(r). Hence, in this package, we increased the number of points for the calculation of g(r).
In CalTYSk.m, this line was "

```
[rh,hc_r] = TInvFourier(kk,4*pi*ehk.*kk,0.8);
```

".
And it is now changed to "

```
[rh,hc_r] = TInvFourier(kk,4*pi*ehk.*kk,0.2);
```

"

Improvement of TYSQ21 over TYSQ01

For this version, the major revision is that the input value of Q could have zero value point compared with the previous version, TYSQ01.

Introduction

(Please cite the paper, Yun Liu, Wei-Ren Chen, Sow-Hsin Chen, "Cluster Formation in Two Yukawa Fluids", *Journal of Chemical Physics*, 122, 044507(2005), if you use the results produced by this package.)

TYSQ22 is the version 2.2 of the matlab package, TYSQ, written to calculate the structure factor of one component liquid systems interacting with a two-term Yukawa potential with the mean spherical approximation (MSA). The structure factor is generated by following Blum's paper (J. Stat. Phys., **16**, 399, 1977), in which the structure factor is solved from Ornstein-Zernike equation by Baxter's Q-method with MSA closure.

The potential *V(r)* is:

$$\beta V(r) = \begin{cases} \infty \quad \text{for } r < 1; \\ -c(r) = -K1\dfrac{e^{-Z1(r-1)}}{r} - K2\dfrac{e^{-Z2(r-1)}}{r} \quad \text{for } r > 1 \end{cases}$$

where $\beta = \dfrac{1}{k_B T}$.

The Ornstein-Zernike equation is

$$h(\vec{r}) = c(\vec{r}) + \rho \int d\vec{r}\,' c(|\vec{r}\,'|) h(|\vec{r} - \vec{r}\,'|) .$$

The closure form is

$$\begin{cases} h(r) = -1 \ \text{for } r < 1; \\ c(r) = K1\dfrac{e^{-Z1(r-1)}}{r} + K2\dfrac{e^{-Z2(r-1)}}{r} \ \text{for } \ r > 1. \end{cases}$$

Although much effort has been made to minimize the possible bugs in the code, I assume no responsibility for tis use and make no guarantees (expressed or implied) about it s quality and reliability. In other words, you use this code at your own risk.

If you have questions, please feel free to email me at yunliu@alum.mit.edu . I will try to answer your questions as best as I can.

Installation

1) Obtain the compressed zip file, TYSQ01.zip
2) Extract the TYSQ22.zip to the directory where you want to install it. Let's assume the directory name is '**HomeDir**'. You should find **TYSQ22** subdirectory under your directory **HomeDir**. There are also other two files under **HomeDir**: **TwoYukawaSample.m**, **Manual.pdf**. The first file is a sample file you can run to get a favor how to run this program. The second file is this manual file.

Using the package
0) Run your matlab to have your matlab command window.

1) Choose your working directory
Easy step (not recommended): run your own code under the directory **HomeDir/TYSQ22**. The problem of this method is that you can not choose a file which has a same name as that of some file under the directory **HomeDir/TYSQ22/private**.

Neat step (recommended): write your own program under different directory. Let's assume your working directory name is '**workDir**'. In this case, you have to let the matlab to find out where your **TYSQ22** package is. The command you should use is 'addpath'.
Windows machine: type this command in your matlab command window
addpath HomeDir\TYSQ01 –begin
Linux or Unix machine: : type this command in your matlab command window
addpath HomeDir/TYSQ01 –begin

2) Now you are ready to use the package. The central function file is **CalTYSk.m** under the directory **HomeDir/TYSQ22.** You can copy **TwoYukawaSample.m** from **HomeDir** directory to your **workDir**. Then type in command window **TwoYukawaSample**, and press enter key. It will take about 10 seconds to plot out a structure factor and its pair distribution function g(r) with Z1=10, Z2=2, K1=6, K2=-1, and volume fraction is 20%. **CalTYSk** function always assumes that the hardcore diameter is one!

Q&A

1. Can K1 and K2 zero?

The codes assume that there must be two Yukawa terms. Therefore, if you want to make them 0, you can only do it by making them very very small values. K1 and K2 can not be zero.

2. Can I make Z1 or Z2 very large number?

Always try to make Z1>Z2, when you want to have a very large Z number, such as Z>20, because in the codes, Z1 and Z2 are treated in an asymetric way.
In order to make the calculation more accurate, Z1>Z2 will be a nice trick.
In general, when Z<20, it dose not matter.

In general, when Z number becomes too large (>25), the intermediate results of this codes
may run into the limit of the number that a computer can handle. Therefore, results
may potentially become less reliable. Hence, the check of g(r) becomes very essential
in those situations.

So far, I did not find out any limitation of the value of K except that they can not be zero.

3. Can Z1 and Z2 be equal?

Z1 and Z2 should not be equal.
If they are equal, there is essentially only one Yukawa term.
Therefore, the algorithm designed for two term Yukawa potential will fail.
However, the codes can handle Z1 and Z2 when they only have
very small differences.