Appendix B

Manual for TYSQ21 Matlab Package

B.1 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 code.)

TYSQ21 is the version 2.1 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

$$\beta V(r) = \begin{cases} \infty, & 0 < r < 1 \\ -c(r) = -K1\frac{e^{-Z1(r-1)}}{r} - K2\frac{e^{-Z2(r-1)}}{r}, & r > 1 \end{cases} \tag{B.1}$$

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

The Ornstein-Zernike equation is

$$h(\vec{r}) = c(\vec{r}) + \rho \int d\vec{r'} c(|\vec{r'}|) h(|\vec{r} - \vec{r'}|). \tag{B.2}$$

The closure form is

$$\begin{cases} h(r) = -1, & 0 < r < 1 \\ c(r) = K1\frac{e^{-Z1(r-1)}}{r} + K2\frac{e^{-Z2(r-1)}}{r}, & r > 1 \end{cases} \tag{B.3}$$

B.2 Installation

1. Obtain the compressed zip file, TYSQ21.zip

2. Extract the TYSQ21.zip to the directory where you want to install it. Let's assume the directory's name is '**HomeDir**'. You should find **TYSQ21** 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 flavor how to run this program. The second file is this manual.

B.3 Using the Package

1. Run your Matlab to have your Matlab command window.

2. Choose your working directory.

   Easy way (not recommended): run your own code under the directory **HomeDir/TYSQ21**. The problem of this method is that you can not choose a file which has the same name as that of some file under the directory **HomeDir/TYSQ21/private**.

   Neat way (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 know where your **TYSQ21** package is. The command you should use is 'addpath'.

Windows machine: type the following command in your Matlab command window: addpath HomeDir\TYSQ21 -begin

Linux or Unix machine: type the following command in your matlab command window: addpath HomeDir/TYSQ21 -begin

3. Now you are ready to use the package. The central function file is **CalTYSk.m** under the directory **HomeDir/TYSQ21**. 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 pari distribution function $g(r)$ with $Z1 = 10,\ Z2 = 2,\ K1 = 6,\ K2 = -1$, and volume fraction 20%. **CalTYSk.m** function always assumes that the hardcore diameter is one.

B.4 Q&A

1. Can $K1$ and $K2$ be zero?

   No. The codes assume that there must be two Yukawa terms. Therefore, if you want to make one or both of them zero, you can only do it by making them very small values.

2. Can I make $Z1$ and $Z2$ very large number?

   In principle, the answer is Yes. However, this is very subtle. In general, always try to make $Z1 > Z2$, when you want to try a very large number, such as $Z > 20$. This is because that $Z1$ and $Z2$ are treated in an asymmetric way in the computer codes. In order to make the calculation more accurate, $Z1 > Z2$ will be a nice trick. In general, when $Z < 20$, it dose not matter.

   When $Z > 25$, sometimes the intermediate results of this codes may run into the limit of the largest number that a computer can handle. Therefore, results may potentially become less reliable. Hence, the check of $g(r)$ becomes very important 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 cases that $Z1$ and $Z2$ have only very small differences.

B.5 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.