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THE GRAND PARTITION FUNCTION  
OF CLASSICAL SYSTEMS IN THE GAUSSIAN  
EQUIVALENT REPRESENTATION  
OF FUNCTIONAL INTEGRALS

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# 1 Introduction

The idea of using of functional integrals in classical statistical mechanics was introduced more then 30 years ago [1,2,3]. This method has been used for lattice gases and spin systems. For continuum fluids the functional representation of grant partition function was introduced in [4]. This functional integral was calculated in frame of perturbation theory when the zeroth approximation is connected with the interaction on short distancies and is supposed to be known. The excess free energy is represented as a series over the interaction on large distances which is supposed to be weak. The main problem is to calculate the functional integral for the zeroth approximation. For this aim the Percus-Yevick (P-Y) approximation has been used. This P-Y equation allows to calculate correlation functions for the zeroth approximation. It turned out [5] that solutions of this equation is good when the density is not too high and becomes quite unsatisfactory for dense states. In this case the numerical experiments by Monte-Carlo or Molecular Dynamics are used.

Recently the method of calculation of functional integrals, called the Gaussian equivalent representation method, was worked out and applied to polaron problem [6,7]. In this paper we want to use this method for calculation of the grant partition function for dense fluids. We shall consider systems of classical particles for which the two-body potential is positive and its Fourier transform is a well-defined function. As examples we obtain the explicit expressions for exponential and Yukawa potentials. An instructive mathematical example is presented too.

We consider this paper as a preliminary version of our approach to

calculation of grand partition functions of the type:

$$\Xi_{\Lambda}(\beta, z) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int_{\Lambda} dx_1 \dots \int_{\Lambda} dx_n \exp \left\{ -\beta \sum_{i<j} V(x_i - x_j) \right\}.$$

## 2 The grand partition function in the Gaussian equivalent representation of functional integrals

Thermodynamics characteristics of a system of particles are determined by the grand partition function as a function of the temperature and chemical potential. This function is defined by

$$\Xi = \Xi_{\Lambda}(\beta, z) = \sum_{n=0}^{\infty} \frac{z^n}{n!} \int_{\Lambda} dx_1 \dots \int_{\Lambda} dx_n \exp \left\{ -\beta \sum_{i<j} V(x_i - x_j) \right\} \quad (1)$$

Here  $\beta = \frac{1}{kT}$ ,

$$z = \left( \frac{2\pi m}{\beta \hbar^2} \right)^{d/2} e^{\beta \mu}.$$

is activity,  $\mu$  is the chemical potential,  $\Lambda$  is a large region ( $\Lambda \subseteq \mathbb{R}^d$ ), real vectors  $x_j \in \mathbb{R}^d$ . A two-body positive potential  $V(x - y)$  is supposed to be positive and to have the Fourier transform

$$V(x) = \int \left( \frac{dp}{2\pi} \right)^d \tilde{V}(p) e^{ipx}. \quad (2)$$

where the function  $\tilde{V}(p)$  is positive too.

The problem is to find the free energy

$$F(\beta, z) = - \lim_{\Lambda \rightarrow \infty} \frac{1}{\Lambda} \ln \Xi_{\Lambda}(\beta, z). \quad (3)$$

According to these notation the pressure and the number density are defined like

$$\begin{aligned} P(\beta, z) &= -\frac{1}{\beta}F(\beta, z), \\ \rho(\beta, z) &= -z\frac{\partial F(\beta, z)}{\partial z}. \end{aligned} \quad (4)$$

The connection between the density and pressure determines the equation of state.

Our aim is to calculate this function by using the Gaussian equivalent representation method for computing of functional integrals [6]. Let us use the following well-known Gaussian functional representation

$$N_V \int \delta\phi \exp \left\{ -\frac{1}{2}(\phi V^{-1}\phi) + i\sqrt{\beta}(A\phi) \right\} = \exp \left\{ -\frac{\beta}{2}(AVA) \right\}, \quad (5)$$

where the following notation are introduced

$$\begin{aligned} (A\phi) &= \int_{\Lambda} dx A(x)\phi(x), \\ (AVA) &= \int_{\Lambda} \int_{\Lambda} dx dy A(x)V(x-y)A(y), \\ (\phi V^{-1}\phi) &= \int_{\Lambda} \int_{\Lambda} dx dy \phi(x)V^{-1}(x,y)\phi(y). \end{aligned}$$

The differential operator  $V^{-1}(x, y)$  satisfies the equation

$$\int_{\Lambda} dy V^{-1}(x, y)V(y - x') = \delta(x - x')$$

with appropriate boundary conditions which in the limiting case  $\Lambda \rightarrow \mathbb{R}^d$  are not important. The Gaussian measure is defined in the standard way

$$d\mu_V[\phi] = \frac{\delta\phi}{\sqrt{\det V}} \exp \left\{ -\frac{1}{2}(\phi V^{-1}\phi) \right\},$$

$$\int d\mu_V[\phi] = 1,$$

$$\frac{1}{\sqrt{\det V}} \xrightarrow{\Lambda \rightarrow \mathbb{R}^d} \exp \left\{ -\frac{\Lambda}{2} \int \left( \frac{dp}{2\pi} \right)^d \ln \bar{V}(p) \right\}.$$

Using the formula (5) for

$$A(x) = \sum_{j=1}^n \delta(x - x_j)$$

one can represent the grand partition function in the form

$$\Xi_\Lambda(\beta, z) = \int d\mu_V[\phi] \exp \left\{ z_1 \int_\Lambda dx e^{i\sqrt{\beta}\phi(x)} \right\} \quad (6)$$

where

$$z_1 = z \exp \left\{ \frac{\beta}{2} V(0) \right\}.$$

Our aim is to get the Gaussian equivalent representation of this functional integral (6) which is suitable for any parameters  $\beta$  and  $z$ . Let us perform the displacement of the functional variable

$$\phi(x) \rightarrow \phi(x) + ib(x)$$

and go over to the new Gaussian measure  $d\mu_D[\phi]$  where  $b(x)$  and  $D(x, y)$  are functions which should be determined. The functional integral (6) takes the form

$$\Xi_\Lambda(\beta, z) = \int d\mu_D[\phi] e^K, \quad (7)$$

$$K = \ln \sqrt{\frac{\det D}{\det V}} - \frac{1}{2}(\phi[V^{-1} - D^{-1}]\phi) - i(\phi V^{-1}b) + \frac{1}{2}(bV^{-1}b)$$

$$+ z_1 \int_\Lambda dx e^{\sqrt{\beta}(i\phi(x) - b(x))}$$

where

$$d\mu_D[\phi] = \frac{\delta\phi}{\sqrt{\det D}} \exp \left\{ -\frac{1}{2}(\phi D^{-1}\phi) \right\},$$

$$\int d\mu_D[\phi] = 1,$$

$$\int_{\Lambda} dy D^{-1}(x, y) D(y - x') = \delta(x - x')$$

and for  $\Lambda \rightarrow \mathbb{R}^d$

$$\frac{1}{\sqrt{\det D}} = \exp \left\{ -\frac{\Lambda}{2} \int \left( \frac{dp}{2\pi} \right)^d \ln \tilde{D}(p) \right\},$$

$$D(x - y) = \int d\mu_D[\phi] \phi(x) \phi(y).$$

We want to stress that in the limit  $\Lambda \rightarrow \mathbb{R}^d$  the function  $D(x, y)$  becomes translation invariant, i.e.  $D(x, y) = D(x - y)$ .

Now let us introduce the conception of the normal product according to the given Gaussian measure  $d\mu_D[\phi]$ , namely

$$: e^{i\sqrt{\beta}\phi(x)} := e^{i\sqrt{\beta}\phi(x)} e^{\frac{\beta}{2}D(0)}, \quad (8)$$

$$\phi(x)\phi(y) := \phi(x)\phi(y) + D(x - y),$$

in other words

$$\int d\mu_D[\phi] : e^{i\sqrt{\beta}\phi(x)} := 1. \quad (9)$$

The argument of the exponent in (7) can be rewritten in the form

$$\mathbf{K} = z_2 \int_{\Lambda} dx e^{-\sqrt{\beta}b(x)} : \left[ e^{i\sqrt{\beta}\phi(x)} - 1 - i\sqrt{\beta}\phi(x) + \frac{\beta}{2}\phi^2(x) \right] :$$

$$+ \left\{ \frac{1}{2} \ln \det \frac{D}{V} - \frac{1}{2}([V^{-1} - D^{-1}]D) + \frac{1}{2}(bV^{-1}b) + z_2 \int_{\Lambda} dx e^{-\sqrt{\beta}b(x)} \right\}$$

$$+i \left\{ z_2 \int_{\Lambda} dx e^{-\sqrt{\beta}b(x)} \sqrt{\beta} \phi(x) - (\phi V^{-1} b) \right\} \\ - \frac{1}{2} : \left\{ z_2 \int_{\Lambda} dx e^{-\sqrt{\beta}b(x)} \beta \phi^2(x) + (\phi [V^{-1} - D^{-1}] \phi) \right\} :$$

where

$$z_2 = z \exp \left\{ \frac{\beta}{2} [V(0) - D(0)] \right\}.$$

Our basic idea is that the main contribution into the functional integral (7) is concentrated in the quadratic Gaussian measure  $d\mu_D[\phi]$ . It means that the linear and quadratic terms over the integration variable  $\phi(x)$  should be absent in the integrand exponent. Thus we obtain two equations

$$z_2 \int_{\Lambda} dx e^{-\sqrt{\beta}b(x)} \sqrt{\beta} \phi(x) - (\phi V^{-1} b) = 0, \quad (10) \\ : \left\{ z_2 \int_{\Lambda} dx e^{-\sqrt{\beta}b(x)} \beta \phi^2(x) + (\phi [V^{-1} - D^{-1}] \phi) \right\} := 0,$$

which can be represented in an another form

$$\sqrt{\beta}b(x) = \beta z_2 \int_{\Lambda} dy V(x-y) e^{-\sqrt{\beta}b(y)}, \quad (11) \\ D(x, x') = V(x-x') - \beta z_2 \int_{\Lambda} dy V(x-y) e^{-\sqrt{\beta}b(y)} D(y, x').$$

In the limit  $\Lambda \rightarrow \mathbb{R}^d$  the functions  $b(x)$  and  $D(x, y)$  become translation invariant, i.e.

$$b(x) = b = \text{const}, \quad D(x, y) = D(x-y).$$

These equations after some simple transformations and substitution  $c = \sqrt{\beta}b$  can be rewritten for  $\Lambda \rightarrow \mathbb{R}^d$

$$\tilde{D}(p) = \tilde{V}(0) \cdot \frac{v(p)}{1 + cv(p)}, \quad v(p) = \frac{\tilde{V}(p)}{\tilde{V}(0)},$$

$$c = \beta z \tilde{V}(0) \exp \{-c + \beta R(c)\}, \quad (12)$$

$$\beta R(c) = \frac{\beta}{2}[V(0) - D(0)] = \frac{\beta \tilde{V}(0)}{2} \int \left(\frac{dp}{2\pi}\right)^d \frac{cv^2(p)}{1 + cv(p)}.$$

This equations determine the parameter  $c = \sqrt{\beta b}$  and the modified "potential" function  $D(x - y)$ . As a result we get the Gaussian equivalent representation for the initial functional integral (3):

$$\Xi_{\Lambda}(\beta, z) = e^{-\Lambda F_0} \int d\mu_D[\phi] e^{W[\phi]}. \quad (13)$$

Here the following notation are introduced

$$W[\phi] = \frac{c}{\beta \tilde{V}(0)} \int_{\Lambda} dx : e^{i\sqrt{\beta}\phi(x)} :, \quad (14)$$

where

$$\begin{aligned} : e^{i\sqrt{\beta}\phi(x)} : &= : \left[ e^{i\sqrt{\beta}\phi(x)} - 1 - i\sqrt{\beta}\phi(x) + \frac{\beta}{2}\phi^2(x) \right] : \\ &= e^{i\sqrt{\beta}\phi(x) + \frac{\beta}{2}D(0)} - 1 - i\sqrt{\beta}\phi(x) + \frac{\beta}{2}[\phi^2(x) - D(0)], \\ -F_0(\beta) &= \frac{1}{2} \int \left(\frac{dp}{2\pi}\right)^d \left[ \ln \frac{\tilde{D}(p)}{\tilde{V}(p)} - \frac{\tilde{D}(p)}{\tilde{V}(p)} + 1 \right] + \frac{2c + c^2}{2\beta \tilde{V}(0)} \quad (15) \\ &= -\frac{1}{2} \int \left(\frac{dp}{2\pi}\right)^d \left[ \ln(1 + cv(p)) - \frac{cv(p)}{1 + cv(p)} \right] + \frac{2c + c^2}{2\beta \tilde{V}(0)} \end{aligned}$$

and the parameter  $c$  is determined by the equation (12).

We would like to stress that in the Gaussian equivalent representation (13) the effective coupling constant is

$$G_{\text{eff}} = \frac{c}{\beta \tilde{V}(0)} \quad (16)$$

If the potential has the form

$$V(x) = gf \left( \frac{x}{r_0} \right) = gf(s), \quad s = \frac{x}{r_0},$$



where  $f(s)$  is a dimensionless function and parameters  $g$  and  $r_0$  define the energy and space scale of this potential. Then the dimensionless coupling constant is

$$G_{\text{eff}} = \frac{c}{\beta g \tilde{f}(0)}, \quad \tilde{f}(0) = \int d^d s f(s). \quad (17)$$

### 3 The modified perturbation theory and the accuracy

Using the representation (13) we can calculate the highest perturbation corrections to  $F_0$ :

$$F = - \lim_{\Lambda \rightarrow \infty} \frac{1}{\Lambda} \ln \Xi_{\Lambda}(\beta, z) = F_0 + F_1 + F_2 + F_3 + \dots \quad (18)$$

where

$$\begin{aligned} F_1 &= - \int d\mu_D[\phi] W[\phi] \equiv 0, \\ F_2 &= -\frac{1}{2} \lim_{\Lambda \rightarrow \infty} \frac{1}{\Lambda} \int d\mu_D[\phi] W[\phi] W[\phi] \end{aligned} \quad (19)$$

and so on. The explicit form for the second correction is

$$F_2 = -\frac{1}{2} \left( \frac{c}{\beta \tilde{V}(0)} \right)^2 \int d^d x \left[ e^{-\beta D(x)} - 1 + \beta D(x) - \frac{1}{2} \beta^2 D^2(x) \right] \quad (20)$$

The accuracy of the zeroth approximation can be evaluated as

$$F = F_0 \left( 1 + O \left( \frac{F_2}{F_0} \right) \right) \quad (21)$$

## 4 The exponential potential

In this section we apply the Gaussian equivalent representation to the exponential potential in the space  $\mathbb{R}^3$ :

$$V(r) = \frac{g}{8\pi} e^{-ar}. \quad (22)$$

Let us introduce the following dimensionless variables and parameters:

$$\gamma = g\beta, \quad s = ar, \quad \tilde{\mu} = \frac{\mu}{g}, \quad \tilde{z} = \lambda c^{\gamma\tilde{\mu}} \gamma^{-3/2},$$

$$\lambda = \frac{1}{a^3} \left( \frac{2\pi mg}{h^2} \right)^{3/2}.$$

Then for the exponential potential one can get

$$\begin{aligned} \beta V(r) &= \frac{\gamma}{8\pi} e^{-s}, & \beta \tilde{V}(p) &= \gamma v(p), \\ v(p) &= \frac{1}{(p^2 + 1)^2}, & \beta \tilde{V}(0) &= \gamma, \\ \beta R(c) &= \frac{\beta}{2} [V(0) - D(0)] = \frac{\gamma}{2} \int \left( \frac{dp}{2\pi} \right)^3 \frac{cv^2(p)}{1 + cv(p)} \\ &= \frac{\gamma}{16\pi} \left[ 1 - \sqrt{\frac{2}{1 + \sqrt{1 + c}}} \right]. \end{aligned}$$

For function  $D$  we obtain

$$\begin{aligned} \tilde{D}(p) &= \frac{1}{(p^2 + a^2)^2 + ca^4}, & D(s) &= \frac{1}{4\pi} \Delta(s, c), \\ \Delta(s, c) &= \exp \left( -s \sqrt{\frac{1 + \sqrt{1 + c}}{2}} \right) \cdot \frac{\sin \left( s \sqrt{\frac{c}{2(1 + \sqrt{1 + c})}} \right)}{s\sqrt{c}}. \end{aligned}$$

The basic equation looks like

$$c = \frac{\lambda}{\sqrt{\gamma}} \exp \left\{ -c + \gamma\tilde{\mu} + \frac{\gamma}{16\pi} \left[ 1 - \sqrt{\frac{2}{1 + \sqrt{1 + c}}} \right] \right\}. \quad (23)$$

The free energy in the zeroth and second approximation is defined as

$$F_0(\beta) = \frac{a^3}{6\pi} \cdot \left[ 1 - \frac{1+c+(1-\frac{c}{4})\sqrt{1+c}}{\sqrt{2(1+c)(1+\sqrt{1+c})}} - \frac{3\pi}{\gamma}(2c+c^2) \right], \quad (24)$$

$$F_2(\beta) = -\frac{a^3}{6\pi} \cdot \left( \frac{2c}{\gamma} \right)^2 \int_0^\infty ds s^2 \exp_2 \left\{ -\frac{\gamma}{4\pi\sqrt{c}} \Delta(s, c) \right\}, \quad (25)$$

$$\exp_2(u) = e^u - 1 - u - \frac{u^2}{2}.$$

The numerical calculations are done for  $\lambda = \tilde{\mu} = 1$  and for the function

$$F_j(\beta) = -\frac{a^3}{6\pi} S_j(\gamma) \text{ and are given in the table 1.}$$

**Table 1**

$\gamma$	$S_0(\gamma)$	$S_2(\gamma) * 10^7$	$c$
.1	1.75	-6.8	1.13
.5	12.74	-8.1	.93
1.0	28.26	-7.9	1.00
2.0	55.71	-7.4	1.35
5.0	107.03	-5.8	3.09
10.0	162.81	-3.4	6.96
20.0	261.87	-1.0	15.89
50.0	549.87	-0.0	44.73
100.0	1024.00	-0.0	94.28
1000.0	9428.00	-0.0	1005.00

## 5 The Yukawa potential

In this section we apply the Gaussian equivalent representation to the Yukawa potential in the space  $\mathbb{R}^3$ .

$$V(r) = \frac{g}{4\pi} \frac{e^{-ar}}{r}, \quad \tilde{V}(p) = \frac{g}{p^2 + a^2}. \quad (26)$$

For function  $D$  we obtain

$$\tilde{D}(p) = \frac{g}{p^2 + a^2(1+c)}, \quad D(r) = \frac{g}{4\pi} \frac{e^{-ar\sqrt{1+c}}}{r}. \quad (27)$$

Let us introduce the following dimensionless variables and parameters:

$$\gamma = \frac{ga\beta}{4\pi}, \quad \nu = \frac{4\pi\mu}{ga},$$

$$z = \lambda \frac{e^{\tau\nu}}{\gamma^{3/2}}, \quad \lambda = \left(\frac{mga}{2h^2}\right)^{3/2}.$$

Then for the Yukawa potential one can get

$$\beta R(c) = \frac{\beta}{2}[V(0) - D(0)] = \gamma [\sqrt{1+c} - 1].$$

The basic equation (12) looks like

$$c + \ln c - \gamma [\sqrt{1+c} - 1] = \gamma\nu - \frac{1}{2} \ln \gamma + \ln \left(\frac{4\pi\lambda}{a^3}\right) \quad (28)$$

or

$$\ln c + \left(\sqrt{1+c} - \frac{\gamma}{2}\right)^2 = \left(1 - \frac{\gamma}{2}\right)^2 + \gamma\nu - \frac{1}{2} \ln \gamma + \ln \left(\frac{4\pi\lambda}{a^3}\right).$$

Let us introduce the functions

$$\mathbf{F}_j(\beta) = -\frac{a^3}{4\pi} \cdot \mathbf{S}_j(\beta). \quad (29)$$

The free energy in the zeroth and second approximation is defined as

$$S_0(\beta) = -\frac{1}{3} \left( 1 - \left( 1 - \frac{c}{2} \right) \sqrt{1+c} \right) + \frac{2c+c^2}{2\gamma}, \quad (30)$$

$$S_2(\beta) = \frac{1}{2\gamma^2} \cdot \frac{c^2}{(1+c)^{3/2}} \int_0^\infty ds s^2 \exp_2 \{-E(s)\},$$

$$\exp_2(u) = e^u - 1 - u - \frac{u^2}{2}, \quad E(s) = \gamma \sqrt{1+c} \cdot \frac{e^{-s}}{s}.$$

In the limit  $\beta \rightarrow \infty$  ( $\gamma \rightarrow \infty$ ) we have  $c \rightarrow \gamma^2$  and the free energy in the zeroth and second approximation look like

$$S_0(\beta) \rightarrow \frac{2}{3} \gamma^3 \left( 1 + O\left(\frac{1}{\gamma}\right) \right), \quad (31)$$

$$S_2(\beta) = \left( -\frac{\gamma^3}{8} \right) \left( 1 + O\left(\frac{1}{\gamma}\right) \right), \quad (32)$$

so that in this limit

$$\frac{S_2(\beta)}{S_0(\beta)} = -\frac{3}{16} \left( 1 + O\left(\frac{1}{\gamma}\right) \right) \approx 20\%. \quad (33)$$

Practically this asymptotic behavior begins from  $\gamma \geq 10$ .

The numerical calculations are done for

$$\frac{4\pi\lambda}{a^3} = \nu = 1$$

and are given in the table 2.

**Table 2**

$\gamma$	$S_0(\gamma)$	$S_2(\gamma)$	$c$
.01	330.04	-.088	1.756
.10	18.331	-.022	1.154
.50	3.222	-.038	1.029
.80	2.380	-.055	1.147
1.00	2.222	-.072	1.268
1.50	2.405	-.141	1.700
2.00	3.249	-.284	2.475
5.00	48.960	-8.489	18.206
10.00	548.216	-101.857	89.470
20.00	5003.087	-938.135	385.123
50.00	82210.432	-15420.111	2481.731

## 6 The mathematical example

In this section we would like to demonstrate the efficiency of our method on a simple mathematical example and we hope that this investigation helps us to clarify the basic idea of our method. Let us consider the function

$$J(\beta) = \sum_{n=0}^{\infty} \frac{z^n}{n!} e^{-\frac{\beta}{2}n^2} = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} \exp \left\{ -\frac{x^2}{2} + ze^{i\sqrt{\beta}x} \right\}. \quad (34)$$

where  $z = z_0 e^{\beta}$ . Let us apply the Gaussian equivalent representation to this integral. Let us perform all transformations leading to the Gaussian equivalent representation, namely, we do the displacement  $x \rightarrow x + ib$  and introduce a new parameter  $\omega$ , defining the Gaussian measure. We

get

$$\begin{aligned}
 J(\beta) &= \int d\sigma_\omega e^{K(x,\beta,b,\omega)}, \tag{35} \\
 d\sigma_\omega &= \frac{dx}{\sqrt{2\pi\omega}} \exp\left\{-\frac{x^2}{2\omega}\right\}, \\
 K(x,\beta,b,\omega) &= \frac{1}{2} \ln \omega - \frac{x^2}{2}\left(1 - \frac{1}{\omega}\right) - ibx + \frac{b^2}{2} + ze^{-\sqrt{\beta}b} e^{i\sqrt{\beta}x}.
 \end{aligned}$$

The conception of the normal product with respect to the measure  $d\sigma_\omega$  means that

$$\begin{aligned}
 e^{i\sqrt{\beta}x} &:= e^{i\sqrt{\beta}x} : e^{-\frac{\beta}{2}\omega}, & x^2 &:= x^2 : +\omega, \\
 \int d\sigma_\omega : e^{i\sqrt{\beta}x} &:= 1, & \int d\sigma_\omega : x^n &:= 0 \quad \forall n, \\
 : e^{i\sqrt{\beta}x} &:=: e_2^{i\sqrt{\beta}x} + 1 + i\sqrt{\beta}x - \frac{\beta x^2}{2} :, \\
 e_2^s &= e^s - 1 - s^2 - \frac{s^2}{2}, \\
 : e_2^{i\sqrt{\beta}x} &:= e^{i\sqrt{\beta}x + \frac{\beta\omega}{2}} - 1 - i\sqrt{\beta}x + \frac{\beta}{2}(x^2 - \omega).
 \end{aligned}$$

Let us substitute these representations into  $K(x,\beta,b,\omega)$  and require the coefficients in front of the linear  $x$  and quadratic  $x^2$  terms to be equal zero. As a result one can obtain

$$\begin{aligned}
 J(\beta) &= e^{S_0(\beta)} \int d\sigma_\omega \exp\left\{\frac{c}{\beta} : e_2^{i\sqrt{\beta}x} : \right\}, \tag{36} \\
 S_0(\beta) &= \frac{1}{2} \ln \omega - \frac{\omega}{2}\left(1 - \frac{1}{\omega}\right) + \frac{c^2}{2\beta} + ze^{-c-\frac{\beta}{2}\omega},
 \end{aligned}$$

where  $c = \sqrt{\beta}b$  and parameters  $c$  and  $\omega$  satisfies the equations

$$\begin{aligned}
 c &= \beta ze^{-c-\frac{\beta}{2}\omega} = \beta z_0 e^{\beta-c-\frac{\beta}{2}\omega}, \tag{37} \\
 \frac{1-\omega}{\omega} &= \beta ze^{-c-\frac{\beta}{2}\omega}.
 \end{aligned}$$

These equations lead to

$$\omega = \frac{1}{1+c}.$$

Finally the function  $c = c(\beta)$  is defined by the equation

$$\beta - c - \frac{\beta}{2(1+c)} - \ln \frac{c}{\beta} + \ln z_0 = 0. \quad (38)$$

The "free energy" in the zeroth and second approximations looks like

$$\begin{aligned} \ln J(\beta) &= S(\beta) = S_0(\beta) + S_2(\beta) + S_3(\beta) + \dots, & (39) \\ S_0(\beta) &= -\frac{1}{2} \ln(1+c(\beta)) + \frac{c(\beta)}{2(1+c(\beta))} + \frac{1}{\beta} \left[ \frac{c^2(\beta)}{2} + c(\beta) \right], \\ S_1(\beta) &= \frac{c(\beta)}{\beta} \int d\sigma_\omega : e_2^{i\sqrt{\beta}x} := 0, \\ S_2(\beta) &= \frac{1}{2} \left( \frac{c(\beta)}{\beta} \right)^2 \int d\sigma_\omega \left( : e_2^{i\sqrt{\beta}x} : \right)^2 \\ &= \frac{1}{2} \left( \frac{c(\beta)}{\beta} \right)^2 \left[ e^{-\beta\omega(\beta)} - 1 + \beta\omega(\beta) - \frac{\beta^2\omega^2(\beta)}{2} \right], \end{aligned}$$

where  $\omega(\beta) = \frac{1}{1+c(\beta)}$ .

The numerical calculations are done for  $z_0 = 1$  and are given in the table 3.



**Table 3**

$\beta$	$S(\beta)$	$S_0(\beta)$	$S_2(\beta)$
.1	1.003	1.002	-.0006
.5	1.054	1.057	-.003
.8	1.113	1.120	-.006
1.0	1.159	1.170	-.008
1.5	1.291	1.311	-.015
2.0	1.441	1.470	-.021
5.0	2.616	2.619	-.041
10.0	5.010	4.811	-.052
15.0	7.501	7.121	-.056
20.0	10.000	9.483	-.059
30.0	15.000	14.287	-.061
50.0	25.000	24.036	-.063
100.0	50.000	48.694	-.064
1000.0	500.000	497.546	-.066

## 7 Appendix

Here we list the integrals arising in our calculations with the exponential potential:

$$\int_0^\infty \frac{dq}{(q^2 + 1)^2 + c} = \frac{\pi}{2} \cdot \frac{1}{\sqrt{2(1+c)(1+\sqrt{1+c})}},$$

$$\int_0^\infty \frac{dq}{[(q^2 + 1)^2 + c]^2} = \frac{\pi}{4} \cdot \frac{2 + 3\sqrt{1+c}}{[2(1+c)(1+\sqrt{1+c})]^{3/2}},$$

$$\int_0^\infty \frac{dq}{(q^2 + 1)[(q^2 + 1)^2 + c]} = \frac{\pi}{2c} \cdot \left[ 1 - \sqrt{\frac{1+\sqrt{1+c}}{2(1+c)}} \right],$$

$$\int_0^{\infty} \frac{dq}{(q^2+1)[(q^2+1)^2+c]^2} = \frac{\pi}{2c^2} \cdot \left\{ 1 - \sqrt{\frac{1+\sqrt{1+c}}{2(1+c)}} \cdot \frac{4+6c+(4+5c)\sqrt{1+c}}{4(1+c)(1+\sqrt{1+c})} \right\}.$$

$$\int_0^{\infty} \frac{dq q^2}{(q^2+1)[(q^2+1)^2+c]^2} = \frac{\pi}{4c} \cdot \left\{ 1 - \sqrt{\frac{2}{1+\sqrt{1+c}}} \right\}.$$

$$\int_0^{\infty} \frac{dq q^4}{(q^2+1)[(q^2+1)^2+c]^2} = \frac{\pi}{2c^2} \cdot \left\{ 1 - \frac{1+c+(1-\frac{c}{4})\sqrt{1+c}}{\sqrt{2(1+c)(1+\sqrt{1+c})}} \right\}.$$

$$\begin{aligned} \frac{1}{2} \int \left( \frac{dp}{2\pi} \right)^3 \left[ \ln \left( 1 + \frac{c}{(q^2+1)^2} \right) - \frac{c}{(q^2+1)^2+c} \right] \\ = \frac{a^3}{6\pi} \cdot \left\{ 1 - \frac{1+c+(1-\frac{c}{4})\sqrt{1+c}}{\sqrt{2(1+c)(1+\sqrt{1+c})}} \right\}. \end{aligned}$$

$$\int_0^{\infty} \frac{dq q^2}{(q^2+1)(q^2+1+c)} = \frac{\pi}{2c} \cdot [\sqrt{1+c} - 1].$$

$$\int_0^{\infty} \frac{dq q^4}{(q^2+1)(q^2+1+c)^2} = \frac{\pi}{2c^2} \cdot \left[ 1 - \left( 1 - \frac{c}{2} \right) \sqrt{1+c} \right].$$

$$\int_0^{\infty} dq q^2 \left[ \ln \left( 1 + \frac{c}{q^2+1} \right) - \frac{c}{q^2+1+c} \right] = \frac{\pi}{3} \cdot \left[ 1 - \left( 1 - \frac{c}{2} \right) \sqrt{1+c} \right].$$

## References

1. S.F.Edwards.*Phil.Mag.***4** (1959) 1171
2. A.J.F.Siegert.*Stat.Phys.***3**, Brandeis Summer Institute, (1962)
3. J.Glimm, A.Jaffe.*Quantum Physics. A Functional Integral Point of View*, Springer-Verlag, N.-Y. Heidelberg Berlin, (1981).
4. R.G.Storer.*Aust.J.Phys.***72** (1969) 747
5. L.Verlet.*Phys.Rev.***A5** (1972) 939
6. G.V.Efimov, G.Ganbold.*Phys.Stat.Sol.* **B168** (1991) 165
7. M.Dineykhon, G.V.Efimov, G.Ganbold, S.N.Nedelko "Oscillator Representation in Quantum Physics", *Lectures Notes in Physics*, Springer-Verlag, **m26** (1995)

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