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Equations of State for Simple Liquids from the Gaussian Equivalent Representation Method

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Abstract Within the framework of Gaussian equivalent representation method a new procedure of obtaining equations of state for simple liquids is discussed in some technical details. The developed approach permits one to compute partition and distribution functions for simple liquids with arbitrary form of the central two-body potential of inter-molecular interaction. The proposed approach might become of great use for computing thermodynamic and structural quantities of simple particle and polymer systems. We believe that this technique can also provide an interesting possibility to reduce the sign problem of other methods of computer simulation based on a functional integral approach.

Keywords Self-consistent-field methods · Macromolecular and polymer solutions · Polymer melts · Swelling

1 Introduction

The calculation of partition and distribution functions is a basic problem of statistical physics [1]. All thermodynamics characteristics of statistical systems are determined by these functions. As is well known, the calculation of those quantities is a formidable problem [2–4].

In this paper we develop a functional integration method for systematic approximate calculations of classical partition functions of two-body potentials with positive and negative Fourier transforms over the entire density and temperature range.

The Gaussian equivalent representation method has been recently introduced by Efimov and Ganbold in the context of quantum-field theory and statistical physics to compute integrals over Gaussian measure [5–7]. The GER approach has already been proven to be very effective for computing thermodynamic properties and structural quantities of simple classical many-particle systems interacting with purely repulsive potentials like the Gauss-core

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or the Yukawa potential, possessing positive Fourier coefficients [8–10] as well as for calculating the thermodynamics properties of flexible polymer systems [11, 12]. Moreover, it has successfully been employed to reduce the numerical sign problem in conjunction with Monte Carlo simulation [13, 14]. In the meantime, the real liquid description demands of considering the potentials having both attraction and repulsion parts [15, 16]. In the present work the author extends the approach for systems, where the particles interact through potentials with positive and negative Fourier coefficients. This increases the range of applicability of this method for computational simulations [19–22].

2 The Equations of State in the Theory of Simple Liquids

The simple fluid of the particle density $n = N/V$ is thought of as a dense cloud of N particles occupying the volume V and interacting via two-body potential of the form $V(\mathbf{x}-\mathbf{x}')$ [17, 18]. Thermodynamics of such a system is described by the partition function

$$Z_V = \int_V \frac{d\mathbf{x}_1}{|V|} \cdots \int_V \frac{d\mathbf{x}_N}{|V|} \exp\left[-\beta \sum_{i<j}^{N} V(\mathbf{x}_i - \mathbf{x}_j)\right]. \tag{1}$$

For given two-body potential $V(\mathbf{x}-\mathbf{x}')$ the free energy of the system can be computed and can be written in the form

$$E(n,\beta) = -\frac{1}{\beta} \lim_{|V|\to\infty} \ln Z_V. \tag{2}$$

For systems of particles interacting via the two-body potentials having attraction V_1 and repulsion V_2 parts the total potential can conveniently be represented in the matrix form

$$V^{-1} = \begin{pmatrix} V_1^{-1} & 0 \\ 0 & V_2^{-1} \end{pmatrix}. \tag{3}$$

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

$$\int d\mathbf{y} V^{-1}(\mathbf{x}-\mathbf{y}) V(\mathbf{y}-\mathbf{x}') = \delta(\mathbf{x}-\mathbf{x}'), \quad \text{or } V^{-1}V = I \tag{4}$$

and has a form

$$V^{-1}(\mathbf{x}-\mathbf{y}) = \frac{1}{\widetilde{V}(-\Delta)} \delta(\mathbf{x}-\mathbf{y}) = \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}(\mathbf{x}-\mathbf{y})}}{\widetilde{V}(\mathbf{k})} \tag{5}$$

where $\widetilde{V}(\mathbf{k}) = \int d\mathbf{x} V(\mathbf{x}) e^{i\mathbf{kx}}$ is the Fourier-image of the potential. The identity

$$\int \frac{D\phi}{C_V} e^{-\frac{1}{2}(\phi V^{-1}\phi) + i(b\phi)} = e^{-\frac{1}{2}(bVb)} \tag{6}$$

with

$$b(\mathbf{x}) = \sqrt{\beta} \sum_{j=1}^{N} \delta(\mathbf{x}-\mathbf{x_j})$$

permits one to represent Boltzmann factor as

$$e^{-\beta\sum_{i<j}^{N}V(\mathbf{x_i}-\mathbf{x_j})} = e^{N\frac{\beta}{2}V(0)-\frac{\beta}{2}\sum_{i,j}^{N}V(\mathbf{x_i}-\mathbf{x_j})} = \int\frac{D\phi}{C_V}e^{-\frac{1}{2}(\phi V^{-1}\phi)+i(b\phi)+N\frac{\beta}{2}V(0)}$$
$$= \int\frac{D\phi}{C_V}e^{-\frac{1}{2}(\phi V^{-1}\phi)}\prod_{j=1}^{N}e^{i\sqrt{\beta}\phi(\mathbf{x_j})+\frac{\beta}{2}V(0)}$$
$$= \int\frac{D\phi}{C_A}e^{-\frac{1}{2}(\phi V^{-1}\phi)}\prod_{j=1}^{N}\vdots e^{i\sqrt{\beta}\phi(\mathbf{x_j})}\vdots_V \tag{7}$$

where the following notation is utilized

$$(b\phi) = \int_V d\mathbf{x}b(\mathbf{x})\phi(\mathbf{x}), \tag{8}$$

$$(bVb) = \int_V\int_V d\mathbf{x}d\mathbf{y}b(\mathbf{x})V(\mathbf{x}-\mathbf{y})b(\mathbf{y}), \tag{9}$$

$$(\phi V^{-1}\phi) = \int_V\int_V d\mathbf{x}d\mathbf{y}\phi(\mathbf{x})V^{-1}(\mathbf{x}-\mathbf{y})\phi(\mathbf{y}). \tag{10}$$

Let us consider the partition function in the form of functional integral

$$Z_V = \int_V\frac{d\mathbf{x_1}}{|V|}\cdots\int\frac{d\mathbf{x_N}}{|V|}e^{-\beta\sum_{i<j}^{N}V_1(\mathbf{x_i}-\mathbf{x_j})}e^{\beta\sum_{i<j}^{N}V_2(\mathbf{x_i}-\mathbf{x_j})}$$
$$= \frac{1}{|V|^N}\int\frac{D\phi}{\sqrt{\det V_1}}\int\frac{D\psi}{\sqrt{\det V_2}}e^{-\frac{1}{2}(\phi V_1^{-1}\phi)}e^{-\frac{1}{2}(\psi V_2^{-1}\psi)}\left[\int_V d\mathbf{x}\vdots e^{i\sqrt{\beta}\phi(\mathbf{x})}e^{\sqrt{\beta}\psi(\mathbf{x})}\vdots_V\right]^N$$
$$= \frac{1}{|V|^N}\int\frac{D\Phi}{\sqrt{\det V}}e^{-\frac{1}{2}(\Phi V^{-1}\Phi)}\left[\int_V d\mathbf{x}\vdots e^{i\sqrt{\beta}\Phi(\mathbf{x})J}\vdots_V\right]^N = \frac{N!}{2\pi i}\frac{1}{|V|^N}\oint\frac{dz}{z^{N+1}}I_V(z) \tag{11}$$

where

$$\Phi(x) = (\phi(x),\psi(x)),\qquad J = \begin{pmatrix}1\\-i\end{pmatrix},$$
$$I_V(z) = \int\frac{D\Phi}{\sqrt{\det V}}e^{-\frac{1}{2}(\Phi V^{-1}\Phi)+z\int_V d\mathbf{x}\vdots e^{i\sqrt{\beta}\Phi J}\vdots_V}. \tag{12}$$

Following the line of argument of the GER, the integral $I_V(z)$ is written as follows

$$I_V(z) = \sqrt{\frac{\det D}{\det V}}\int\frac{D\Phi}{\sqrt{\det V}}e^{-\frac{1}{2}(\Phi D^{-1}\Phi)-\frac{1}{2}(\Phi[V^{-1}-D^{-1}]\Phi)-(\Phi V^{-1}\Phi_0)} \tag{13}$$
$$\times\, e^{z\int_V d\mathbf{x}i\sqrt{\beta}(\Phi(\mathbf{x})+\Phi_0)J+\frac{1}{2}(V_1(0)-V_2(0))} = e^{W_0(z)}\int\frac{D\Phi}{\sqrt{\det D}}e^{-\frac{1}{2}(\Phi D^{-1}\Phi)}e^{W_I[\Phi]}, \tag{14}$$

where

$$(JVJ) = \int d\mathbf{x}\int d\mathbf{y}J\delta(\mathbf{x}-\mathbf{x}')V(\mathbf{x}-\mathbf{y})J\delta(\mathbf{x}'-\mathbf{y}) = V_1(0)-V_2(0). \tag{15}$$

As a result, we obtain two equations

$$\text{Equation I}: \quad \frac{1}{2}\int d\mathbf{x}\int d\mathbf{y}(\Phi(\mathbf{x})[V^{-1}(\mathbf{x}-\mathbf{y})-D^{-1}(\mathbf{x}-\mathbf{y})]|\Phi(\mathbf{y})) + \frac{1}{2}\int d\mathbf{x}\int d\mathbf{y}[-\beta(\Phi J)^2]e^{i\sqrt{\beta}(\Phi_0 J)+\frac{\beta}{2}[J(V-D)J]}=0 \tag{16}$$

or, more specifically this equation reads

$$\int \frac{d\mathbf{k}}{(2\pi)^3}\frac{e^{i\mathbf{k}(\mathbf{x}-\mathbf{y})}}{\widetilde{V}(\mathbf{k})}-\int \frac{d\mathbf{k}}{(2\pi)^3}\frac{e^{i\mathbf{k}(\mathbf{x}-\mathbf{y})}}{\widetilde{D}(\mathbf{k})}=-z\beta(J)^2e^{i\sqrt{\beta}(\Phi_0 J)+\frac{\beta}{2}[J(V-D)J]}$$

$$\Longrightarrow \quad \frac{1}{\widetilde{V}(\mathbf{k})}-\frac{1}{\widetilde{D}(\mathbf{k})}=-z\beta(J)^2e^{i\sqrt{\beta}(\Phi_0 J)+\frac{\beta}{2}[J(V-D)J]}, \tag{17}$$

$$\text{Equation II:} \quad -(\Phi V^{-1}\Phi_0)+iz\sqrt{\beta}\int d\mathbf{x}(\Phi(\mathbf{x})J)e^{i\sqrt{\beta}(\Phi_0 J)+\frac{\beta}{2}[J(V-D)J]} \tag{18}$$

or

$$\Phi_{0i}=iz\sqrt{\beta}\int d\mathbf{x}(\Phi J)e^{i\sqrt{\beta}(\Phi_0 J)+\frac{\beta}{2}[J(V-D)J]}, \quad i=1,2. \tag{19}$$

Assume $\Phi_{0i}=ic_i/\beta$, where

$$c_i=z\beta\widetilde{V}_{ij}(0)J_je^{-c_iJ_i+\frac{\beta}{2}[J(V-D)J]}. \tag{20}$$

Making use of (20) in (17), we obtain

$$\left(\frac{1}{\tilde{V}(k)}-\frac{1}{\tilde{D}(k)}\right)_{11}=-\frac{c_1}{\tilde{V}_1(0)}, \qquad \left(\frac{1}{\tilde{V}(k)}-\frac{1}{\tilde{D}(k)}\right)_{22}=\frac{c_1}{\tilde{V}_1(0)}, \tag{21}$$

$$\left(\frac{1}{\tilde{V}(k)}-\frac{1}{\tilde{D}(k)}\right)_{12}=\left(\frac{1}{\tilde{V}(k)}-\frac{1}{\tilde{D}(k)}\right)_{21}=-\frac{c_2}{\tilde{V}_2(0)}. \tag{22}$$

This can be combined in the matrix

$$\frac{1}{\tilde{D}(k)}=\begin{pmatrix} \frac{1}{\tilde{V}_1(k)}+\frac{c_1}{\tilde{V}_1(0)} & \frac{c_2}{\tilde{V}_2(0)} \\ \frac{c_2}{\tilde{V}_2(0)} & \frac{1}{\tilde{V}_2(k)}-\frac{c_1}{\tilde{V}_1(0)} \end{pmatrix}=\tilde{D}^{-1}(k). \tag{23}$$

Thus, we obtain for $\tilde{D}(k)$

$$\tilde{D}(k)=\frac{1}{\Delta}\begin{pmatrix} \frac{1}{\tilde{V}_2(k)}-\frac{c_1}{\tilde{V}_1(0)} & -\frac{c_2}{\tilde{V}_2(0)} \\ -\frac{c_2}{\tilde{V}_2(0)} & \frac{1}{\tilde{V}_1(k)}+\frac{c_1}{\tilde{V}_1(0)} \end{pmatrix}, \tag{24}$$

where

$$\Delta=\det\left(\frac{1}{\tilde{D}(k)}\right)=\left(\frac{1}{\tilde{V}_1(k)}+\frac{c_1}{\tilde{V}_1(k)}\right)\left(\frac{1}{\tilde{V}_2(k)}-\frac{c_1}{\tilde{V}_1(0)}\right)-\left(\frac{c_2}{\tilde{V}_2(0)}\right)^2.$$

At large N we can use Stirling's formula

$$\frac{N!}{|V|^N} \quad \Longrightarrow \quad e^{|V|(n\ln n-n)}=e^{|V|f_n}, \quad \text{where } f_n=n\ln n-n. \tag{25}$$

It is convenient to introduce function

$$|V|R(c) = |V|f_n + W_0 - N\ln z \tag{26}$$

where

$$W_0 = \frac{1}{2}\ln\frac{\det D}{\det V} - \frac{1}{2}\mathrm{Tr}[D(V^{-1} - D^{-1})] - \frac{1}{2}(\Phi_0 V^{-1}\Phi_0) + z\int_V d\mathbf{x} e^{-cJ+\frac{\beta}{2}(J[V-D]J)}$$
$$= \frac{1}{2}|V|\int \frac{d\mathbf{k}}{(2\pi)^3}\left[\ln\frac{\Delta^{-1}(\mathbf{k})}{\tilde{V}_1(\mathbf{k})\tilde{V}_2(\mathbf{k})} + \mathrm{Tr}(1 - \tilde{D}(\mathbf{k})\tilde{V}^{-1}(\mathbf{k}))\right]$$
$$- \frac{\Phi_{01}^2}{2\tilde{V}_1(0)} - \frac{\Phi_{02}^2}{2\tilde{V}_2(0)} + \frac{c_1}{\beta\tilde{V}_1(0)} \tag{27}$$

and

$$\ln z = \ln\frac{c_1}{\beta\tilde{V}_1(0)} + cJ - \frac{\beta}{2}(J[V-D]J). \tag{28}$$

After some algebra we obtain the partition function in the form:

$$Z_V = \frac{1}{2\pi i}\oint\frac{dz}{z}e^{|V|R(c(z))}\int\frac{D\phi}{\sqrt{\det D}}e^{-\frac{1}{2}(\Phi D^{-1}\Phi)}e^{W_I[\Phi]}, \tag{29}$$

where

$$W_I[\Phi] = \frac{c(z)}{b}\int_V d\mathbf{x} :e_2^{i\sqrt{\beta}\Phi(\mathbf{x})}:_D. \tag{30}$$

The partition function integral has been derived in a similar form in Sect. III of reference [23] for potential models with positive Fourier coefficients (see (29)–(31)). As a point of interest, we consider the lowest approximation partition function having the form

$$Z_V^0 = \frac{1}{2\pi i}\oint\frac{dz}{z}e^{|V|R(c(z))}. \tag{31}$$

In the case $V \longrightarrow \infty$ integral (31) could be done using the steepest descent method

$$Z_V^0 = \frac{1}{2\pi i}\oint\frac{dz}{z}e^{|V|R(c(z))} \quad\Longrightarrow\quad \frac{1}{2\pi i}\oint\frac{dc}{c}e^{|V|R(c_m)} \quad\Longrightarrow\quad e^{|V|R(c_m)}. \tag{32}$$

The point of global maximum c_m is defined by the equation

$$\frac{d}{dc}R(c) = I_1(c) + I_2(c) + I_3(c) + N. \tag{33}$$

The explicit form of functions $I_1(c),\ I_2(c),\ I_3(c),\ N$ reads

$$I_1(c) = \int_0^\infty \frac{dk}{(2\pi)^2}k^2\left[\frac{1}{\Delta(k)\tilde{V}_1(0)(\frac{1}{\tilde{V}_1(k)} - \frac{1}{\tilde{V}_2(k)})}\right],$$

$$I_2(c) = \int_0^\infty \frac{dk}{(2\pi)^2} \frac{k^2}{\tilde{V}_1(0)\Delta^2(k)} \left(\frac{1}{\tilde{V}_2(k)} - \frac{1}{\tilde{V}_1(k)} \right)$$
$$\times \left[\frac{1}{\tilde{V}_1(k)\tilde{V}_2(k)} \left(2 + \frac{c}{\tilde{V}_1(0)} \left(\tilde{V}_1(k) - \tilde{V}_2(k) \right) \right) + 1 \right],$$
$$I_3(c) = \int_0^\infty \frac{dk}{(2\pi)^2} \frac{\beta k^2}{2} \frac{n}{\Delta^2(k)\tilde{V}_1(0)} \left(\frac{1}{\tilde{V}_2(k)} - \frac{1}{\tilde{V}_1(k)} \right)^2,$$
$$N(c) = \frac{1}{\beta V_1(0)} - \frac{n}{c} - n \left(1 - \frac{\tilde{V}_2(0)}{\tilde{V}_1(0)} \right) - \frac{c}{\tilde{V}_1^2(0)\beta} \left(1 - \frac{\tilde{V}_2(0)}{\tilde{V}_1(0)} \right).$$

The final expression for $R(c)$ is given by

$$R(c) = M_1(c) + M_2(c) + P(c) \tag{34}$$

where

$$M_1(c) = \int_0^\infty \frac{dk}{(2\pi)^2} k^2 n\beta \left(\tilde{V}_1(k) - \tilde{V}_2(k) \right) \left[\frac{1}{\Delta(k)\tilde{V}_1(k)\tilde{V}_2(k)} - 1 \right],$$
$$M_2(c) = \int_0^\infty \frac{dk}{(2\pi)^2} k^2 \Bigg[\ln \frac{1}{\Delta(k)\tilde{V}_1(k)\tilde{V}_2(k)} + 2$$
$$- \frac{1}{\Delta(k)\tilde{V}_1(k)\tilde{V}_2(k)} \left[2 + \frac{c}{\tilde{V}_1(0)} \left(\tilde{V}_1(k) - \tilde{V}_2(k) \right) \right] \Bigg],$$
$$P(c) = n \left(\ln n - 1 - \ln \frac{c}{\beta \tilde{V}_1(0)} \right) + \left(1 - \frac{\tilde{V}_2(0)}{\tilde{V}_1(0)} \right) \left(\frac{c^2}{2\beta \tilde{V}_1(0)} - nc \right) + \frac{c}{\beta \tilde{V}_1(0)}.$$

All other thermodynamic functions may be found from $E(n, \beta)$ by the Maxwell relations in thermodynamics

$$P = -\left(\frac{\partial E}{\partial V} \right)_T = \frac{1}{\beta} \left(\frac{\partial \ln Z(n, \beta)}{\partial V} \right)_T, \qquad S = -\left(\frac{\partial E}{\partial T} \right)_V. \tag{35}$$

In particular, from above it follows

$$R(n, \beta) = P(n, \beta). \tag{36}$$

where P is pressure of system.

3 Summary

The developed procedure of computing the equation of state can be summarized as follows. First, we solve (33), and, second, the obtained roots are inserted in (34) which is the equation of state. Thus, the developed procedure permits one to get the equation of state for simple liquids, composed of particles interacting via two-body potential with attractive and repulsive counterparts and having bound states. The application of this procedure to the simple liquid models with specific potentials is the subject of forthcoming article.

We hope that the techniques presented in this Letter can also be useful for other fields of computer simulation, where the sign problem does occur. We can contribute in this way to establish the auxiliary field methodology as a standard tool for computation and this technique can also provide an interesting possibility to reduce the sign problem of other methods of computer simulation based on a functional integral approach.

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Appendix A: Normal Form of Functional

Let us introduce normal form of functional with respect to Gauss measure. Consider the equality:

$$\int \frac{D\phi}{C_A} e^{-\frac{1}{2}(\phi D^{-1}\phi)+i(b\phi)} = e^{-\frac{1}{2}(bDb)} \tag{37}$$

and identity:

$$\int \frac{D\phi}{C_A} e^{-\frac{1}{2}(\phi D^{-1}\phi)} e^{i(b\phi)+\frac{1}{2}(bDb)} \equiv 1. \tag{38}$$

The normal form of functional with respect to Gauss measure with Green function D will understand multiplication

$$\vdots e^{i(b\phi)} \vdots_D \equiv e^{i(b\phi)+\frac{1}{2}(bDb)}. \tag{39}$$

This definition is identity and valid with any b, therefore expanding both hands of (39) with respect to b we obtain

$$\begin{aligned}
\vdots \phi(x) \vdots_D &= \phi(x), \\
\vdots \phi(x_1)\phi(x_2) \vdots_D &= \phi(x_1)\phi(x_2) - D(x_1, x_2), \\
\vdots \phi(x_1)\phi(x_2)\phi(x_3) \vdots_D &= \phi(x_1)\phi(x_2)\phi(x_3) - D(x_1, x_2)\phi(x_3) \\
&\quad - D(x_2, x_3)\phi(x_1) - D(x_3, x_1)\phi(x_2), \\
&\dots
\end{aligned}$$

We can use the functional in normal form as:

$$\begin{aligned}
\int d\sigma_{\phi,D} \vdots e^{i(b\phi)} \vdots_D &\equiv 1, \\
\int d\sigma_{\phi,D} \vdots \phi(x_1 \dots\dots \phi(x_n)) \vdots_D &\equiv 0.
\end{aligned} \tag{40}$$

In particular:

$$\vdots e^{i(b\phi)} \vdots_D = e^{\frac{1}{2}(b[D-B]b)} \vdots e^{i(b\phi)} \vdots_B$$

where

$$I(g)=\int\frac{D\phi}{C_A}e^{-\frac{1}{2}(\phi A^{-1}\phi)+gW[\phi]}=\int d\sigma_{\phi,A}e^{gW[\phi]} \tag{41}$$

with normalization:

$$I(0)=\int\frac{D\phi}{C_A}e^{-\frac{1}{2}(\phi A^{-1}\phi)}=\int d\sigma_{\phi,A}=1.$$

Any path integral over Gaussian measure for analytical ϕ can be written in normal form with some Green function D:

$$W[\phi]=\int d\mu_\eta e^{i(b\phi)}=\int d\mu_\eta e^{-\frac{1}{2}(\eta D\eta)}\vdots e^{i(\eta\phi)}\vdots_D. \tag{42}$$

This path integral convenient to represent in the form:

$$W[\phi]=W_0+i(W_1\phi)-\frac{1}{2}\vdots\phi W_2\phi\vdots_D+\vdots W_I[\phi]\vdots_D$$

where

$$W_0=\int d\sigma_\eta e^{-\frac{1}{2}(\eta D\eta)},$$

$$i(W_1\phi)=\int d\sigma_\eta e^{-\frac{1}{2}(\eta D\eta)}i(\eta\phi),$$

$$\frac{1}{2}\vdots\phi W_2\phi\vdots_D=\frac{1}{2}\int d\sigma_\eta e^{-\frac{1}{2}(\eta D\eta)}\vdots(\eta\phi)(\eta\phi)\vdots,$$

$$\vdots W_I[\phi]\vdots_D=\int d\sigma_\eta e^{-\frac{1}{2}(\eta D\eta)}\vdots e_2^{i(\eta\phi)}\vdots_D=O(\vdots\phi^3\vdots_D),$$

$$e_2^z\equiv e^z-1-z-\frac{z^2}{2}.$$

Appendix B: Equations

Let us consider path integral (41) and make use of the following equivalent transformations. First, we shift the variable of integration $\phi(x)\longrightarrow\phi(x)+\xi(x)$. Second, we write the functional of interactions in the normal form with respect to Gauss measure for new kernel $B^{-1}(x_1,x_2)$, we obtain

$$\begin{aligned}I(g)&=\int\frac{D\phi}{C_A}e^{-\frac{1}{2}(\phi A^{-1}\phi)-(\phi A^{-1}\xi)-\frac{1}{2}(\xi A^{-1}\xi)+gW[\phi+\xi]}\\&=\frac{C_B}{C_A}\int\frac{D\phi}{C_B}e^{-\frac{1}{2}(\phi B^{-1}\phi)}e^{-\frac{1}{2}(\phi[A^{-1}-B^{-1}]\phi)-(\phi A^{-1}\xi)-\frac{1}{2}(\xi A^{-1}\xi)+gW[\phi+\xi]}\\&=\frac{C_B}{C_A}\int d\sigma_{\phi,B}e^{-\frac{1}{2}\vdots\phi[A^{-1}-B^{-1}]\phi\vdots_B-\frac{1}{2}([A^{-1}-B^{-1}]B)-(\phi A^{-1}\xi)-\frac{1}{2}(\xi A^{-1}\xi)}\\&=e^{gW_0+ig(W_I\phi)-\frac{g}{2}\vdots\phi W_2\phi\vdots_B+g\vdots W_I[\phi]\vdots_B}.\end{aligned} \tag{43}$$

The major contribution to the functional integral gives Gauss measure $d\sigma_{\phi,B}$, therefore the linear and quadratic terms over the integration variable $\phi(x)$ should be absent. Thus we obtain two equations

$$\text{Equation I:} \quad -(\phi A^{-1}\xi) + ig(W_{I\phi}) = 0, \tag{44}$$

$$\text{Equation II:} \quad -\frac{1}{2}\vdots(\phi[A^{-1} - B^{-1}]\phi)\vdots_B - \frac{g}{2}\vdots(\phi W_2\phi)\vdots_B = 0. \tag{45}$$

For more details see [5, 6].

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