A variational expansion for the free energy of a bosonic system

2002 J. Phys. A: Math. Gen. 35 21

(http://iopscience.iop.org/0305-4470/35/1/302)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **35** (2002) 21–32 PII: S0305-4470(02)21985-X

A variational expansion for the free energy of a bosonic system

Wen-Fa Lu[1,2,3], **Sang Koo You**[4], **Jino Bak**[1,3], **Chul Koo Kim**[1,3] **and Kyun Nahm**[5]

[1] Institute of Physics and Applied Physics, Yonsei University, Seoul 120-749, Korea
[2] Department of Physics and Institute for Theorectical Physics, Shanghai Jiao Tong University, Shanghai 200030, People's Republic of China
[3] Center for Strongly Correlated Materials Research, Seoul National University, Seoul 151-742, Korea
[4] Max-Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany
[5] Department of Physics, Yonsei University, Wonju 220-710, Korea

E-mail: wenfalu@online.sh.cn

Received 5 February 2001, in final form 14 August 2001
Published 21 December 2001
Online at stacks.iop.org/JPhysA/35/21

Abstract

In this paper, a variational perturbation scheme for nonrelativistic many-fermion systems is generalized to a bosonic system. By calculating the free energy of an anharmonic oscillator model, we investigated this variational expansion scheme for its efficiency. Using the modified Feynman rules for the diagrams, we obtained the analytical expression of the free energy up to the fourth order. Our numerical results at various orders are compared with the exact and other relevant results.

PACS numbers: 11.15.Bt, 11.10.−z

1. Introduction

For calculating the free energy of a system, there exist usually two basic methods, the conventional perturbative and the variational methods [1]. In fact, these two methods are standard in calculations of many physics problems. However, it is well known that the former is useful only for small perturbing potentials, whereas the latter lacks systematic schemes to control its accuracy, albeit it is valid for any potential. In order to overcome these difficulties and improve the variational method, a variational perturbation idea of properly combining the two methods was pioneered by Koehler in lattice dynamics [2] and Seznec and Zinn-Justin [3] on an anharmonic oscillator decades ago. Later, the idea was extended to path integrals by Feynman and Kleinert [4] as well as Okopińska [4] and further developed by other authors [5–7][6]. Very recently, three of the present authors and their collaborator (You *et al*) presented

[6] Here we are far from exhausting the relevant literature.

a variational perturbation scheme for a nonrelativistic many-fermion system in the functional integral formalism [8]. In order to test the efficiency of the method, You *et al* [8] provided a model numerical calculation at zero temperature up to the second order. Obviously, this test is limited and wider investigation is necessary for the variational perturbation scheme.

Actually, the scheme in [8] is a Taylor series expansion based on the variational result obtained in the spirit of the Feynman variational principle [1]. This scheme can improve the variational method if used judicially. We note that there exists no work performing the same scheme for bosonic systems. Although Okopińska [9] and Krzyweck [6] established two kinds of expansion schemes, the optimized expansions and the cumulant expansions respectively, whose lowest order results are the variational results, they are really not based on the variational results because the variational procedure was performed at the truncated order. Further, improvement to the variational method is notoriously difficult and different schemes will have their own advantages over others. So it is worthwhile generalizing the scheme in [8] to bosonic systems.

For the above two purposes, an anharmonic oscillator will be an effective laboratory. For a one-dimensional anharmonic oscillator, the Hamiltonian is

$$H(t) = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2(t) + \lambda x^4(t). \tag{1}$$

Here, x is the space position, p the momentum, t the time and m, ω and λ are the mass, frequency and coupling strength, respectively. Such an anharmonic oscillator is probably the simplest model which does not have an exact analytic solution. Its exact free energy was obtained numerically [6, 10]. Moreover, there exist many approximation methods to calculate its free energy [4, 6, 9, 11]. All of these make equation (1) an ideal candidate for our purpose. Therefore, in this paper, we will generalize the scheme in [8], taking the simple anharmonic oscillator (equation (1)) as a laboratory and investigate the Taylor expansion scheme on the free energy based on the variational result obtained from the Feynman variational principle [1].

Simultaneously, the anharmonic oscillator itself is useful in chemical physics [12] and many physics problems, such as thermal expansion, phonon softening and structural phase transitions [13]. Although its free energy was calculated using many methods, their numerical (approximate and exact) results[7] were focused mainly on the case of the reduced temperature T less than 1, except for [10] which provided accurate results for a moderate T. Therefore, we also test whether our scheme can produce reliable results for a moderate temperature range.

We will work within the functional integral formalism [14]. The next section generalizes the scheme in [8] to calculate the free energy of a system with potential $V(x)$. In section 3, we carry out the scheme on the anharmonic oscillator (equation (1)). Section 4 presents calculations of the free energy for equation (1) up to the fourth order and makes comparisons with the exact and various approximate results, such as variational, cumulant-expansion and optimized-expansion results. Conclusions are given in section 5.

2. A variational expansion of free energies for bosonic systems

For a system with the Hamiltonian $H(t) = \frac{1}{2m}p^2 + V[x(t)]$ with $V[x(t)] = \frac{1}{2}m\omega^2 x^2(t) + V_I[x(t)]$, the generating functional is [14]

$$Z[J] = \int_{x(0)=x(\beta)} \mathcal{D}[x(\tau)] \exp\left\{-\int_0^\beta \left[\tfrac{1}{2}mx(\tau)\left(-\partial_\tau^2\right)x(\tau) + V[x(\tau)] - J(\tau)x(\tau)\right]\mathrm{d}\tau\right\} \tag{2}$$

[7] In this paper, an anharmonic oscillator does not include the double-well potential case.

where $\tau = \mathrm{i}t$ is the imaginary time, $\partial_\tau \equiv \frac{\partial}{\partial\tau}$, $\beta = \frac{1}{\kappa T}$ with κ the Boltzmann constant (we will consider it as unity for convenience) and T the temperature. J is an arbitrary external source and the symbol $\mathcal{D}[x(\tau)]$ represents the functional measure. In equation (2), $x(0) = x(\beta)$ means that the functional integral should be executed over all the closed paths [14]. To introduce a variational parameter Ω, one can rewrite the classical action functional $S[x]$ in the Euclidean spacetime in equation (2) as [3, 6, 9]

$$\begin{aligned} S[x, J] &= \int_0^\beta \left[\tfrac{1}{2}mx(\tau)\left(-\partial_\tau^2 + \Omega^2\right)x(\tau) - J(\tau)x(\tau) - \tfrac{1}{2}m\Omega^2x^2(\tau) + V[x(\tau)]\right]\mathrm{d}\tau \\ &\equiv S_0[x, J] + S_D[x] \end{aligned} \tag{3}$$

with $S_0[x, J] = \int_0^\beta \left[\frac{1}{2}mx(\tau)\left(-\partial_\tau^2 + \Omega^2\right)x(\tau) - J(\tau)x(\tau)\right]\mathrm{d}\tau$ and $S_D[x] = \int_0^\beta \left[-\frac{1}{2}m\Omega^2x^2(\tau) + V[x(\tau)]\right]\mathrm{d}\tau$. Thus, $Z[J]$ can be rewritten as

$$\begin{aligned} Z[J] &= \int_{x(0)=x(\beta)} \mathcal{D}[x(\tau)]\exp\{-S_0[x, J] - S_D[x]\} \\ &= \exp\left\{-\int_0^\beta \left[-\tfrac{1}{2}m\Omega^2\delta_{J_\tau}^2 + V\left[\delta_{J_\tau}\right]\right]\mathrm{d}\tau\right\}\int_{x(0)=x(\beta)} \mathcal{D}[x(\tau)]\exp\{-S_0[x, J]\} \\ &= (\mathrm{Det}(G^{-1}))^{-\frac{1}{2}}\exp\left\{-\int_0^\beta \left[-\tfrac{1}{2}m(\Omega^2 - \omega^2)\delta_{J_\tau}^2\right.\right. \\ &\quad \left.\left. + V_I\left[\delta_{J_\tau}\right]\right]\mathrm{d}\tau\right\}\exp\left\{\tfrac{1}{2}J_\tau G_{\tau\tau'}J_{\tau'}\,\mathrm{d}\tau\,\mathrm{d}\tau'\right\} \end{aligned} \tag{4}$$

where $J_\tau = J(\tau)$, $\delta_{J_\tau} \equiv \frac{\delta}{\delta J_\tau}$, G^{-1} represents the operator $-\partial_\tau^2 + \Omega^2$ with the propagator $G_{\tau\tau'} = G(\tau, \tau')$ and Det means the determinant. In the third step of equation (4), we have carried out the Gaussian functional integration [14]. Note that $G_{\tau\tau'}$ can be expanded into a series owing to the closed-path requirement in the functional integral, equation (2) [14, 15]. To calculate the free energy, we express the partition function $Z \equiv Z[J = 0]$ in the following form:

$$\begin{aligned} Z &= \int_{x(0)=x(\beta)} \mathcal{D}[x(\tau)]\exp\{-S_0[x, J = 0]\}\frac{\int_{x(0)=x(\beta)}\mathcal{D}[x(\tau)]\,\exp\{-S_0[x, J = 0] - S_D[x]\}}{\int_{x(0)=x(\beta)}\mathcal{D}[x(\tau)]\,\exp\{-S_0[x, J = 0]\}} \\ &= (\mathrm{Det}(G^{-1}))^{-\frac{1}{2}}\left\langle\exp\left\{-\int_0^\beta\left[-\tfrac{1}{2}m(\Omega^2 - \omega^2)\delta_{J_\tau}^2 + V_I[\delta_{J_\tau}]\right]\mathrm{d}\tau\right\}\right\rangle_G \qquad (5) \\ &= (\mathrm{Det}(G^{-1}))^{-\frac{1}{2}}\exp\left\{-\int_0^\beta\left\langle-\tfrac{1}{2}m(\Omega^2 - \omega^2)\delta_{J_\tau}^2 + V_I[\delta_{J_\tau}]\right\rangle_G\mathrm{d}\tau\right\} \\ &\quad \times\left\langle\exp\left\{-\int_0^\beta\left[-\tfrac{1}{2}m(\Omega^2 - \omega^2)\delta_{J_\tau}^2 + V_I\left[\delta_{J_\tau}\right]\right.\right.\right. \\ &\quad \left.\left.\left. - \left\langle-\tfrac{1}{2}m(\Omega^2 - \omega^2)\delta_{J_\tau}^2 + V_I[\delta_{J_\tau}]\right\rangle_G\right]\mathrm{d}\tau\right\}\right\rangle_G. \qquad (6) \end{aligned}$$

Here, we have used the following notation and relation

$$\begin{aligned} \langle O[x]\rangle_G &\equiv \frac{\int_{x(0)=x(\beta)}\mathcal{D}[x(\tau)]O[x]\exp\left\{-\int_0^\beta\frac{1}{2}mx(\tau)\left(-\partial_\tau^2 + \Omega^2\right)x(\tau)\,\mathrm{d}\tau\right\}}{\int_{x(0)=x(\beta)}\mathcal{D}[x(\tau)]\exp\left\{-\int_0^\beta\frac{1}{2}mx(\tau)\left(-\partial_\tau^2 + \Omega^2\right)x(\tau)\,\mathrm{d}\tau\right\}} \\ &= O[\delta_J]\exp\left\{\tfrac{1}{2}J_\tau G_{\tau\tau'}J_{\tau'}\,\mathrm{d}\tau\,\mathrm{d}\tau'\right\}_{J=0} \equiv \langle O[\delta_J]\rangle_G. \end{aligned} \tag{7}$$

Obviously, when $V_I[x(t)]$ is not zero, it will be impossible to obtain an analytically exact partition function and, hence, one has to design some scheme to produce an approximate

solution. For the case of small V_I, one can take $\Omega = \omega$, make a Taylor series expansion to the exponential in equation (5) and then truncate the series at some order to approximate Z. This is just the conventional perturbation theory and the propagator $G_{\tau\tau'}$ is the bare propagator. When V_I is not so small, the above perturbation method is no longer valid. In such a case, an effective alternative is the variational method which is based on the Feynman variational principle. In the following, we briefly introduce the variational method.

Exploiting Jensen's inequality [1, 8], one can have

$$\left\langle \exp\left\{-\int_0^\beta \left[-\tfrac{1}{2}m(\Omega^2-\omega^2)\delta_{J_\tau}^2 + V_I[\delta_{J_\tau}]\right] \mathrm{d}\tau\right\}\right\rangle_G \geqslant \exp\left\{-\int_0^\beta \left\langle -\tfrac{1}{2}m(\Omega^2-\omega^2)\delta_{J_\tau}^2 + V_I[\delta_{J_\tau}]\right\rangle_G \mathrm{d}\tau\right\}. \tag{8}$$

By substituting the above equation into equation (6) leads to a relation for the lower limit of the partition function, i.e.,

$$Z \geqslant (\mathrm{Det}(G^{-1}))^{-\frac{1}{2}} \exp\left\{-\int_0^\beta \left\langle -\tfrac{1}{2}m(\Omega^2-\omega^2)\delta_{J_\tau}^2 + V_I[\delta_{J_\tau}]\right\rangle_G \mathrm{d}\tau\right\}. \tag{9}$$

Hence, the free energy is

$$F = -\frac{1}{\beta}\ln(Z) \leqslant \frac{1}{2\beta}\ln(\mathrm{Det}(G^{-1})) + \frac{1}{\beta}\int_0^\beta \left\langle -\tfrac{1}{2}m(\Omega^2-\omega^2)\delta_{J_\tau}^2 + V_I[\delta_{J_\tau}]\right\rangle_G \mathrm{d}\tau \equiv \bar{F}. \tag{10}$$

Obviously, making $\bar{F}$ of the last equation the absolute minimum will lead to a minimum upper limit of the free energy F_0 with the variationally extremized condition,

$$\frac{\delta\bar{F}}{\delta\Omega^2} = 0 \tag{11}$$

and the stabilized condition

$$\frac{\delta^2\bar{F}}{(\delta\Omega^2)^2} \geqslant 0. \tag{12}$$

The parameter Ω which renders $\bar{F}$ absolutely minimized will be chosen from three possibilities: the non-zero solution of equation (11), zero and ∞. $\bar{F}$ with such an Ω is just F_0, the variational result of F. This procedure is essentially the same as in [16] for equation (1).

Entering the above variational result into equation (6) and taking the logarithm, we obtain the following expression for F:

$$F = F_0 - \frac{1}{\beta}\ln[\langle\exp\{-[S_D[\delta_J] - \langle S_D[\delta_J]\rangle_G]\}\rangle_G]. \tag{13}$$

Now, we make a Taylor series expansion of the exponential in the last equation and the average $\langle\cdots\rangle_G$ can be calculated order by order by borrowing the Feynman diagram technique [14][8]. The logarithmic operation in equation (13) is equivalent to discarding disconnected diagrams [14]. Consequently, we have

$$F = F_0 + \sum_2^\infty F^{(n)} \tag{14}$$

with the nth order correction to the variational result

$$F^{(n)} = (-1)^{n+1}\frac{1}{\beta}\frac{1}{n!}\langle[S_D[\delta_J]|_{\tau=\tau_1} - \langle S_D[\delta_J]|_{\tau=\tau_1}\rangle_G]\cdots[S_D[\delta_J]|_{\tau=\tau_i} - \langle S_D[\delta_J]|_{\tau=\tau_i}\rangle_G] \cdots[S_D[\delta_J]|_{\tau=\tau_n} - \langle S_D[\delta_J]|_{\tau=\tau_n}\rangle_G]\rangle_{G,C}. \tag{15}$$

[8] Now the diagrams are no longer bare Feynman diagrams in the sense of perturbation theory owing to $\Omega \neq \omega$ which has been variationally determined.

Here, the subscript C means that only the connected diagrams have their contributions to the free energy [14]. Equation (14) corresponds to a systematic Feynman-diagram-like expansion and from it, one can estimate the approximate values of the free energy F order by order. Thus, we have finished the generalization of the scheme in [8] to a bosonic case. In this scheme, the parameter Ω is variationally determined before the series expansion is performed and it is identical for all orders. Obviously, this is a Taylor series expansion around the variational result and so we call it the variational expansion. Because the ith factor in equation (15) ($i = 1, 2, \ldots, n$) has the term $-\langle S_D[\delta_J]|_{\tau=\tau_i}\rangle_G = -\int_0^\beta \left\langle -\frac{1}{2}m\Omega^2\delta^2_{J_{\tau_i}} + V\left[\delta_{J_{\tau_i}}\right]\right\rangle_G \mathrm{d}\tau_i$, which has a negative sign against the major part of F_0, one can expect to get a simplified diagram rule, as will be shown for the system (equation (1)) in the next section. Next, we apply the above procedure to the anharmonic oscillator and make a comparison with existing results in the literature.

3. Application to the anharmonic oscillator

For the system, $V[x(t)] = \frac{1}{2}m\omega^2x^2(t) + \lambda x^4(t)$ (equation (1)), the procedure from equations (8) to (12) yields easily the variational free energy F_0,

$$F_0 = \frac{1}{\beta}\ln\left(2\sinh\left(\frac{\beta\Omega}{2}\right)\right) - \frac{3\lambda}{4m^2\Omega^2}\coth^2\left(\frac{\beta\Omega}{2}\right) \tag{16}$$

with the variationally extremized condition $\left(\frac{\delta\bar{F}}{\delta\Omega^2} = 0\right)$

$$\Omega^2 = \omega^2 + \frac{6\lambda}{m^2\Omega}\coth\left(\frac{\beta\Omega}{2}\right). \tag{17}$$

Here, owing to the periodicity of the path in equation (2), we have used the following propagator

$$G_{\tau\tau'} = \frac{1}{\beta}\sum_{-\infty}^{\infty}\frac{1}{m\left(\omega_n^2 + \Omega^2\right)}\mathrm{e}^{-\mathrm{i}\omega_n(\tau-\tau')} = \frac{1}{2m\Omega}\frac{\cosh\left(\frac{\beta\Omega}{2} - \Omega|\tau-\tau'|\right)}{\sinh\left(\frac{\beta\Omega}{2}\right)} \tag{18}$$

with ω_n the Matsubara frequency [14, 15]. Equation (16) coupled with equation (17) are just the variational result of F in [16].

Using the relation $\frac{1}{2}m^2(\omega^2 - \Omega^2) = -6\lambda G_{\tau\tau}$ from equation (17), we have

$$\begin{aligned}\langle S_D[\delta_J]\rangle_G &= \int_0^\beta \left\langle \tfrac{1}{2}m(\omega^2-\Omega^2)\delta^2_{J_\tau} + \lambda\delta^4_{J_\tau}\right\rangle_G \mathrm{d}\tau \\ &= \int_0^\beta \left[\tfrac{1}{2}m(\omega^2-\Omega^2)G_{\tau\tau} + 3\lambda G_{\tau\tau}G_{\tau\tau}\right]\mathrm{d}\tau = -\int_0^\beta 3\lambda G_{\tau\tau}G_{\tau\tau}\,\mathrm{d}\tau.\end{aligned} \tag{19}$$

So, for any i, one has

$$\begin{aligned}
&\left\langle \cdots S_D[\delta_J]|_{\tau=\tau_i} - \left\langle S_D[\delta_J]|_{\tau=\tau_i}\right\rangle_G] \cdots \right\rangle_{G,C} \\
&\quad = \left\langle \cdots \int_0^\beta \left[\tfrac{1}{2}m(\omega^2-\Omega^2)\delta^2_{J_{\tau_i}} + \lambda\delta^4_{J_{\tau_i}} - \left\langle -\tfrac{1}{2}m(\omega^2-\Omega^2)\delta^2_{J_{\tau_i}} + \lambda\delta^4_{J_{\tau_i}}\right\rangle_G \mathrm{d}\tau_i \cdots \right\rangle_{G,C} \\
&\quad = \left\langle \cdots \int_0^\beta \left[\tfrac{1}{2}m(\omega^2-\Omega^2)\left(\left(\overset{\circ}{\delta}_{J_{\tau_i}}\right)^2 + G_{\tau_i\tau_i}\right) + \lambda\left(\left(\overset{\circ}{\delta}_{J_{\tau_i}}\right)^4 + 6G_{\tau_i\tau_i}\left(\overset{\circ}{\delta}_{J_{\tau_i}}\right)^2 \right.\right.\right. \\
&\qquad \left.\left.\left. + 3G_{\tau_i\tau_i}G_{\tau_i\tau_i}\right) + 3\lambda G_{\tau_i\tau_i}G_{\tau_i\tau_i}\right]\mathrm{d}\tau_i \cdots \right\rangle_{G,C} \\
&\quad = \left\langle \cdots \int_0^\beta [\lambda\left(\left(\overset{\circ}{\delta}_{J_{\tau_i}}\right)^4 \cdots \right\rangle_{G,C} \qquad (20)
\end{aligned}$$

where, the symbol $\circ$ in $\overset{\circ}{\delta}$ means that the functional derivative with the index i takes effect on $\exp\left\{\frac{1}{2}J_\tau G_{\tau\tau'}J_{\tau'}\,\mathrm{d}\tau\,\mathrm{d}\tau'\right\}$ only if it makes up a pair with any other functional derivative with the index $j \neq i$ to yield $G_{\tau_i\tau_j}$. In going to the second step of the last equation, a concrete analysis has led to the following equivalent properties ($\Leftrightarrow$ means equivalence):

$$\delta^2_{J_{\tau_i}} \Leftrightarrow \left(\overset{\circ}{\delta}_{J_{\tau_i}}\right)^2 + G_{\tau_i\tau_i} \qquad \delta^4_{J_{\tau_i}} \Leftrightarrow \left(\overset{\circ}{\delta}_{J_{\tau_i}}\right)^4 + 6G_{\tau_i\tau_i}\left(\overset{\circ}{\delta}_{J_{\tau_i}}\right)^2 + 3G_{\tau_i\tau_i}G_{\tau_i\tau_i}. \qquad (21)$$

In terms of the Feynman diagram language, it implies that only the legs which come from different vertices can connect each other.

Substituting equation (20) into equation (14), we can estimate the higher order corrections to F_0 in equation (16) with the help of the diagram technique [14]. The free energy for equation (1) is now

$$F = F_0 - \frac{1}{\beta}\left\langle \exp\left\{-\int_0^\beta \lambda\left(\overset{\circ}{\delta}_{J_\tau}\right)^4 \mathrm{d}\tau\right\}\right\rangle_{G,C} = F_0 + \sum_2^\infty F^{(n)} \qquad (22)$$

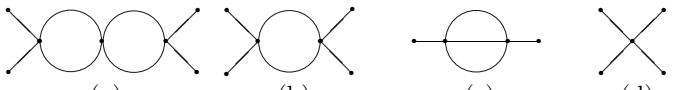
with the nth order correction,

$$F^{(n)} = (-1)^{n+1}\frac{1}{\beta}\frac{\lambda^n}{n!}\left\langle \int_0^\beta \mathrm{d}\tau_1\left(\overset{\circ}{\delta}_{J_{\tau_1}}\right)^4 \cdots \int_0^\beta \mathrm{d}\tau_n\left(\overset{\circ}{\delta}_{J_{\tau_n}}\right)^4 \right\rangle_{G,C}. \qquad (23)$$

Here, the modified Feynman rules for drawing diagrams are quite simple and they are as follows:

(1) Propagator, $G_{\tau_1\tau_2}$; (2)  Vertex, $-\lambda\int_0^\beta d\tau$.

For the nth order, there is an additional total factor $-\frac{1}{\beta n!}$. From equation (23), it is evident that there will be no cactus diagrams appearing at any higher order, which is demonstrated by the diagrams in the next section. This simplifying feature of diagrams is similar to what occurs in the fermionic case [8]. A further analysis indicates that there exist the following four types of building bricks for any nth order connected diagrams ($n > 2$):



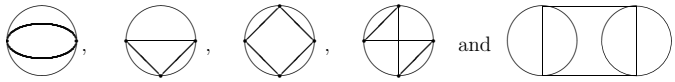
which correspond to the four kinds of partitionings of the integer '4': (a) 2 + 2, (b) 2 + 1 + 1, (c) 3 + 1 and (d) 1 + 1 + 1 + 1, respectively. In this figure, the intermediate vertex of the brick (a) has two legs connected with one vertex and the other two legs with a different vertex, the left (or right) vertex of the brick (b) has two legs connected with one vertex and the other two

legs of it connected with two other different vertices respectively, the left (or right) vertex of the brick (c) has three legs connected with one vertex and the other leg of it connected with a different vertex and the vertex of the brick (d) will have its legs connected with four different vertices, respectively. These four bricks are helpful for drawing various distinct diagrams at any order as one can see from the five diagrams drawn in the next section. For example, none of them contains the brick (d), the second-order diagram consists of only the brick (a), as does the first diagram of the fourth-order diagrams (4a).

In the next section, we calculate the free energy up to the fourth order from equation (22).

4. Analytical expressions and numerical results up to the fourth order

According to the last section, the topologically non-equivalent diagrams at the second, third and fourth orders can be drawn as follows:



2nd 3rd 4th (4a) 4th (4b) 4th (4c)

For these five diagrams from left to right, their symmetry factors (the number of topologically equivalent diagrams appearing in the expansion) are $N_2 = 4!$, $N_3 = \frac{3!}{3\cdot 2}\cdot\left(2\cdot C_4^2\right)^3$, $N_{4a} = \frac{4!}{4\cdot 2}\cdot\left(2\cdot C_4^2\right)^4$, $N_{4b} = \frac{4!}{4\cdot 2}\cdot\left(C_4^2\cdot 2\cdot C_4^2\right)^2\cdot 2^4$ and $N_{4c} = \frac{4!}{4\cdot 2}\cdot\left(C_4^3\cdot 3!\cdot C_4^3\right)^2\cdot 2$, respectively. Thus, one can easily write down the corrections $F^{(2)}$, $F^{(3)}$ and $F^{(4)}$ according to the above diagrams and then calculate them as

$$F^{(2)} = -\frac{1}{\beta}\frac{\lambda^2}{2!}N_2\int_0^\beta \mathrm{d}\tau_1\,\mathrm{d}\tau_2 G^4_{\tau_1\tau_2}$$
$$= -\frac{3\lambda^2}{64m^4\Omega^5}\sinh^{-4}\left(\frac{\beta\Omega}{2}\right)[6\beta\Omega + 8\sinh(\beta\Omega) + \sinh(2\beta\Omega)] \tag{24}$$

$$F^{(3)} = \frac{1}{\beta}\frac{\lambda^3}{3!}N_3\int_0^\beta \mathrm{d}\tau_1\,\mathrm{d}\tau_2\,\mathrm{d}\tau_3 G^2_{\tau_1\tau_2}G^2_{\tau_2\tau_3}G^2_{\tau_3\tau_1}$$
$$= \frac{9\lambda^3}{512m^6\Omega^8}\sinh^{-6}\left(\frac{\beta\Omega}{2}\right)\{-48 + 32\beta^2\Omega^2 + [-3 + 8\beta^2\Omega^2]\cosh(\beta\Omega)$$
$$+ 48\cosh(2\beta\Omega) + 3\cosh(3\beta\Omega) + 108\beta\Omega\sinh(\beta\Omega)\} \tag{25}$$

and

$$F^{(4)} = -\frac{1}{\beta}\frac{\lambda^4}{4!}\int_0^\beta \mathrm{d}\tau_1\,\mathrm{d}\tau_2\,\mathrm{d}\tau_3\tau_4\left\{N_{4a}G^2_{\tau_1\tau_2}G^2_{\tau_2\tau_3}G^2_{\tau_3\tau_4}G^2_{\tau_4\tau_1}\right.$$
$$\left. + N_{4b}G^2_{\tau_1\tau_2}G^2_{\tau_3\tau_4}G_{\tau_2\tau_3}G^2_{\tau_2\tau_4}G_{\tau_1\tau_3}G^2_{\tau_1\tau_4} + N_{4c}G^3_{\tau_1\tau_2}G^3_{\tau_3\tau_4}G_{\tau_2\tau_3}G_{\tau_4\tau_1}\right\}$$
$$= -\frac{3\lambda^4}{32\,768\beta m^8\Omega^{12}}\sinh^{-8}\left(\frac{\beta\Omega}{2}\right)\{6291 - 181\,320\beta^2\Omega^2 + 25\,920\beta^4\Omega^4$$
$$+ 6[71 + 13\,156\beta^2\Omega^2 + 2688\beta^4\Omega^4]\cosh(\beta\Omega) + 48[-134 + 2115\beta^2\Omega^2$$
$$+ 6\beta^4\Omega^4]\cosh(2\beta\Omega) - 432\cosh(3\beta\Omega) + 864\beta^2\Omega^2\cosh(3\beta\Omega)$$
$$+ 141\cosh(4\beta\Omega) + 6\cosh(5\beta\Omega) - 191\,394\beta\Omega\sinh(\beta\Omega)$$
$$+ 129\,456\beta^3\Omega^3\sinh(\beta\Omega) + 42\,568\beta\Omega\sinh(2\beta\Omega) + 12\,672\beta^3\Omega^3\sinh(2\beta\Omega)$$
$$+ 37\,750\beta\Omega\sinh(3\beta\Omega) + 1600\beta\Omega\sinh(4\beta\Omega)\}. \tag{26}$$

These analytical expressions of equations (24)–(26) are the main results in this section. In order to obtain them, we have had to handle the absolute value symbol in the expression of

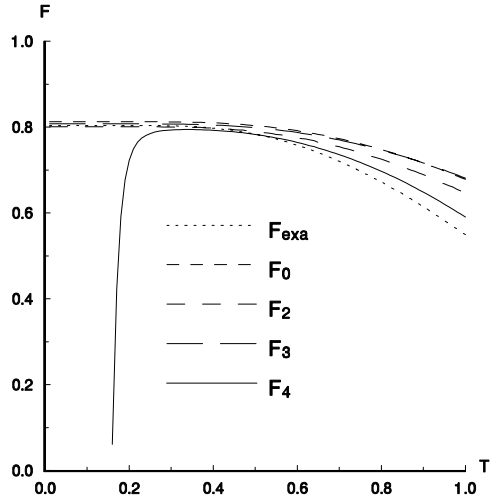


Figure 1. For the case of $T < 1$ and $\lambda = 1$, F_2, F_3 and F_4, the free energies up to the second, the third and the fourth orders, are compared with the variational result F_0 and the exact free energy. The exact results were calculated according to $F = -T \ln\left[\sum_n \mathrm{e}^{-E_n/T}\right]$ and table V in [6]. Here, E_n represents the nth eigenenergy for the system (1). We took $m = \omega = 1$. In this figure, when $T > 0.6$, the curve for F_3 almost coincides with the curve for F_0.

$G_{\tau\tau'}$ (see equation (18)). It is straightforward to calculate the integrals in $F^{(2)}$ and $F^{(3)}$ by dividing the integration domains into 2! and 3! parts, respectively. As for $F^{(n)}$ ($n \geqslant 4$), a multi-dimensional integration domain which exceeds our direct intuition, is involved. However, for any n-dimensional integration domain, one can divide it into $n!$ sub-domains so that, for each sub-domain, the relation $\tau_{i_1} \leqslant \tau_{i_2} \leqslant \tau_{i_3} \leqslant \cdots \leqslant \tau_{i_j} \cdots \leqslant \tau_{i_{n-3}} \leqslant \tau_{i_{n-2}} \leqslant \tau_{i_{n-1}} \leqslant \tau_{i_n}$ holds. Then, mimicking the calculation of $F^{(3)}$, one can find the following equivalent relation

$$\int_0^\beta \mathrm{d}\tau_1 \cdots \mathrm{d}\tau_n \Leftrightarrow \sum_P \int_0^\beta \mathrm{d}\tau_{i_n} \int_0^{\tau_{i_n}} \mathrm{d}\tau_{i_1} \int_{\tau_{i_1}}^{\tau_{i_n}} \mathrm{d}\tau_{i_2} \int_{\tau_{i_2}}^{\tau_{i_n}} \mathrm{d}\tau_{i_3} \cdots \int_{\tau_{i_{n-3}}}^{\tau_{i_n}} \mathrm{d}\tau_{i_{n-2}} \int_{\tau_{i_{n-2}}}^{\tau_{i_n}} \mathrm{d}\tau_{i_{n-1}} \qquad (27)$$

where the letter 'P' below the summation symbol means that the summation is carried out over all the $n!$ sub-domains. Equation (27) allows one to obtain equation (26) with the aid of the computer software Mathematica.

Using the above results, we can now readily calculate the free energy up to the fourth order: $F_2 = F_0 + F^{(2)}$, $F_3 = F_0 + F^{(2)} + F^{(3)}$ and $F_4 = F_0 + F^{(2)} + F^{(3)} + F^{(4)}$. In the following, we will numerically compare them with existing results to examine the reliability of our scheme.

First, we compare our results with the exact results obtained from [6]. Using $F = -T \ln\left[\sum_n \mathrm{e}^{-E_n/T}\right]$ (E_n is the nth eigenenergy of equation (1)), letting $m = \omega = 1$ and for $T < 1$, one can calculate the exact free energies from table V in [6]. For this case, we plot figure 1 with $\lambda = 1$. In figure 1, the dotted, short-dashed, medium-dashed, long-dashed and solid curves are the exact free energy F_{exa}, F_0, F_2, F_3 and F_4, respectively. Figure 1 indicates that: (i) when the temperature is near zero, F_2 and F_3 are very to close to F_{exa}, whereas F_4 is unbounded from below; (ii) when the temperature is greater than 0.5 or so, F_2 and F_4 provide substantial corrections to F_0 and F_4 gives better results than F_2 does, while F_3 is close to F_0. Here, we note that the invalidity of F_4 at very low temperature is not unexpected. Since the present scheme is basically the Taylor expansion of the free energy, the smallness of

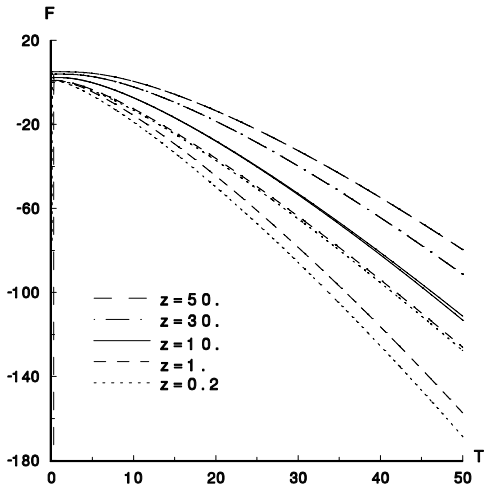


Figure 2. For the case of $T > 1$ and for several values of z, F_4 are compared with F_0. We use the same types of curves to represent F_4 and F_0 and the latter is always above the former. But for the cases $z = 30$ and 50, F_4 almost coincides with F_0, and for the cases $z = 1.0$ and 0.2, F_4 is much lower than F_0.

Table 1. Our results F_2, F_3 and F_4 are compared with the variational result F_0 and the accurate free energies F_{accu} provided by Okopińska ($z = 10$).

T	F_4	F_{accu}	F_0	F_2	F_3
1	2.262 259	2.262 259 515 64	2.262 452	2.262 2504	2.262 261
2	2.063 913	2.063 915 755 14	2.064 409	2.063 8734	2.063 925
3	1.555 676	1.555 697 188 63	1.556 991	1.555 5342	1.555 747
4	0.780 8495	0.780 936 961 496	0.783 6171	0.780 5129	0.781 1028
5	−0.209 9735	−0.209 722 583 045	−0.205 0294	−0.210 593	−0.209 3154
10	−7.377 75	−7.372 498 233 58	−7.348 171	−7.379 3287	−7.367 283
20	−28.039 25	−27.967 003 646 9	−27.861 47	−28.007 4342	−27.921 05
30	−53.507 69	−53.226 914 316 5	−52.997 67	−53.327 8138	−53.087 86

the temperature prevents and competes with the convergence process of the perturbation and finally wins over at the fourth order.

Then, we can compare our results with the accurate free energies, F_{accu}, from Okopińska's optimized variational method [10]. In order to compare with Okopińska's data, we used the definitions of the dimensionless quantities in [10], that is, $m = 1$, $z = \frac{1}{2}\omega^2\lambda^{-\frac{2}{3}}$, $\Omega\lambda^{-\frac{1}{3}} \to \Omega$, $T\lambda^{-\frac{1}{3}} \to T$ and $F_i\lambda^{-\frac{1}{3}} \to F_i$[9]. For the case of $z = 10$, which corresponds to $\lambda = 0.011\,18$ in the dimensionlized system of [6], we give the comparison in table 1[10]. From this table, one can see that F_4 has a better agreement with F_{accu} than F_2, F_3 and F_0 except for $T = 30$.

Thirdly, to show the improvement of F_0 by higher order corrections, for the range of $1 < T < 50$, we plotted the results in figure 2 to compare F_4 with F_0 in the cases $z = 0.2$, 1, 10, 30 and 50. In figure 2, we use the same types of curve to represent F_4 and F_0 and between the curves of the same type, F_4 is always the lower. Also, figure 2 shows that F_4 almost coincides with F_0 for $z = 30$ and 50 and the differences between F_0 and F_4 are quite large for both $z = 1$

[9] In [10], there is a typo on the rescaling expression of T, and here it is corrected.
[10] The data of the accurate free energies were provided by Okopińska, the author of [10].

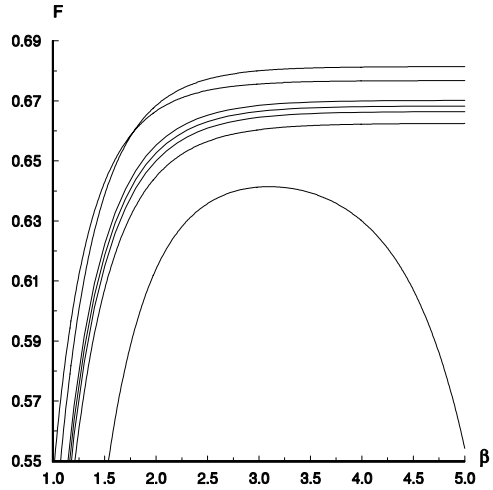


Figure 3. Our results F_2, F_3 and F_4 are compared with the the second- and third-order results by the optimized expansion which were provided by Okopińska ($z = 0$). In this figure, from top to bottom (for large values of β), the first, the second, the sixth and the seventh curves are the variational, the third-, the second- and the fourth-order results of our scheme, respectively. The third and the fourth curves are the second- and the third-order results of the optimized expansion respectively, and the fifth curve is the exact result.

Table 2. Our results F_2 and F_3 are compared with the variational result F_0, the first- and third-order results F_1^{Kr} and F_3^{Kr} obtained by the cumulant expansions (F_2 and F_3 in table 2 of [6]) and the exact free energies $F_{\rm exa}$. In this table, $m = \omega = 1$.

λ	β	F_0	F_1^{Kr}	F_3	F_3^{Kr}	$F_{\rm exa}$	F_2
1.0	5.0	0.812 491	0.811 88	0.807 364	0.803 882	0.803 758	0.800 767
5.0	5.0	1.244 312	1.243 53	1.235 5	1.224 94	1.224 59	1.216 996
50.0	5.0	2.547 58	2.546 75	2.529 673	2.500 67	2.499 71	2.480 384
500.0	10.0	5.425 756	5.425 36	5.387 961	5.322 11	5.319 9	5.276 719
20000.0	3.0	18.501 66	18.500 3	18.373 14	18.144 9	18.137	17.988 22

and $z = 0.2$. From figure 2, we learn that : (i) for a given temperature, with the increase of z, i.e., with weakening coupling, the corrections of F_4 to F_0 get smaller; (ii) for a given z, with increasing T, the corrections of F_4 to F_0 become larger; (iii) the quite large differences between F_0 and F_4 imply that our scheme becomes invalid with decreasing z or increasing coupling strength (for a fixed ω^2). The third point is similar to the optimized expansion [9].

Finally, taking $m = \omega = 1$, we compare our results with those obtained from the cumulant expansions [6] in table 2. In table 2, the free energies F_2 and F_3 are ours, the free energies F_1^{Kr} and F_3^{Kr} are the first- and third-order results from the cumulant expansion in [6] (i.e., F_1 and F_2 of table 2 in [6]). The temperature in this table is lower than 1 and the corresponding z is small. So we did not include F_4 in the table due to its invalidity. This table indicates that our F_2 and F_3 are nearer to the exact value than F_1^{Kr}, but not as good as F_3^{Kr}. This reflects that the convergence of our expansion is not as fast as in the cumulant expansions in [6]. As for the optimized expansions, Okopińska [9] compared the free energy with the exact results in the case of both $\omega = 0$ (i.e., the smallest z) and reduced temperature less than 1 and demonstrated a fast convergence. Here, in figure 3, our results

are compared at various orders with figure 2 in [9][11]. In figure 3, from top to bottom (for large values of β), the first, second, sixth and seventh curves are the variational, the third-, the second- and the fourth-order results of our scheme, respectively. The third and the fourth curves are the second- and the third-order results of the optimized expansion, and the fifth curve is the exact result. The variational result is just the first-order result in the optimized expansion. From this figure, our third-order result is not so good as the results in the optimized expansion, and our second-order result is almost as good as the second-order results in the optimized expansion. This figure simultaniously indicates the invalidity of our fourth-order result. Thus, the optimized expansion also has a better convergence than our results. Additionally, the optimized expansion approaches the exact result monotonically in orders, whereas our results oscillate with orders. However, we want to emphasize that our scheme is not as complicated as the optimized and cumulant expansions. The crucial difference between our expansion and the optimized or the cumulant expansions is that our scheme performs the variational procedure at the lowest order and, accordingly, the parameter Ω is identical for all orders, whereas in both the optimized and the cumulant expansions [6, 9], the variational procedures are performed at their truncated order, and, consequently, Ω at one order is different from the next. It is this difference that gives rise to the simplicity and slow convergence of our scheme and the fast convergence and complication of the optimized or cumulant expansions.

5. Conclusion and discussion

In this paper, we have generalized the scheme in [8] to a bosonic case and taking the anharmonic oscillator (equation (1)) as a laboratory, provided a wide test of its efficiency. Our investigations demonstrate that the present scheme can substantially improve the variational result even in the second order and when the reduced temperature is greater than 0.5 or so and the reduced coupling parameter λ is not strong (or z is small), the free energy for equation (1) up to the fourth order in our expansion gives good agreement with the accurate result. We also demonstrate that for the free energy of equation (1), when the reduced temperature approachs zero, or the reduced coupling λ is strong (or z is small), the fourth-order result is invalid. Thus, from our investigations here, one can see the efficiency and limitations of our scheme. Here, we also note that the present scheme is much simpler than the optimized and cumulant expansions, albeit it does not converge as fast as they do. We believe that a simple scheme is often necessary and useful because the non-perturbative method beyond the Gaussian approximation is extremely complicated in general. Additionally, we gave the approximate free energy of the system (equation (1)) for a moderate temperature range. Although the exact results for the moderate temperature exist in the literature [10], our results can be readily used, as a basis of quantitative comparison, when some other approximate methods produce the free energy for the same temperature range.

In general, it should be noted that the variational perturbation theory yields an asymptotic rather than a convergent series [14], and hence a particular range of validity in a specific problem has no universality. As for any specific problem, the present scheme should always be used with a judicial examination of the true physical property. We believe that the present paper can provide a qualitative reference for an application of our scheme. In particular, when a specific problem is too complicated to treat beyond the Gaussian approximation with other expansions, we believe that our scheme can provide a simple and viable tool to treat it.

Finally, we want to point out that, although we only treated the quantum-mechanical anharmonic oscillator in this paper, it is straightforward to apply our method to

[11] The data from the optimized expansions were also provided by Okopińska.

finite-temperature scalar field theory [15]. Especially, when it is generalized to the ϕ^6 models [17], we expect the simplicity of the method to still hold there.

Acknowledgments

W-FL acknowledges A Okopińska for providing her accurate data and would like to thank H S Park for his help. This project was supported by the Korea Research Foundation (99-005-D00011). The work of W-FL was also supported in part by the National Natural Science Foundation of China under grant no 19875034.

References

[1] Feynman R P and Hibbs A R 1965 *Quantum Mechanics and Path Integrals* (New York: McGraw-Hill)
Feynman R P 1972 *Statistical Mechanics—a Set of Lectures* (New York: Addison-Wesley)
[2] Koehler T R 1968 *Phys. Rev.* **165** 942
[3] Seznec R and Zinn-Justin J 1979 *J. Math. Phys.* **20** 1398
[4] Feynman R P and Kleinert H 1986 *Phys. Rev.* A **34** 5080
Kleinert H 1993 *Phys. Lett.* A **173** 332 and the references therein
Okopińska A 1987 *Phys. Rev.* D **35** 1835
[5] Ibañez-Meiar R, Mattingly A, Ritschel U and Stevenson P M 1992 *Phys. Rev.* D **45** 2893
Sissakian A N, Solovtsov I L and Shevchenko O Y 1993 *Phys. Lett.* B **313** 367
Lee G H and Yee J H 1997 *Phys. Rev.* D **56** 6573
[6] Krzyweck J 1997 *Phys. Rev.* A **56** 4410
[7] You S K, Jeon K J, Kim C K and Nahm K 1998 *Eur. J. Phys.* **19** 179
[8] You S K, Kim C K, Nahm K and Noh H S 2000 *Phys. Rev.* C **62** 045503
[9] Okopińska A 1987 *Phys. Rev.* D **36** 2415
Duncan A and Jones H F 1993 *Phys. Rev.* D **47** 2560
Vlachos K and Okopińska A 1994 *Phys. Lett.* A **186** 375
(Vlachos K and Okopińska A 1993 *Preprint* hep-th/9311145)
Vlachos K and Okopińska A 1998 *Phys. Lett.* A **249** 259
[10] Okopińska A 1987 *Phys. Rev.* D **36** 1273
[11] Giachetti R and Tognetti V 1985 *Phys. Rev. Lett.* **55** 912
Giachetti R and Tognetti V 1986 *Phys. Rev.* B **33** 7674
Wang Y R 1990 *Phys. Rev.* A **41** 4493
[12] Kilpatrick J E and Kilpatrick M F 1948 *J. Chem. Phys.* **16** 781
[13] Bunde A and Diederich S 1979 *Phys. Rev.* B **19** 4069
Kerr W C and Bishop A R 1986 *Phys. Rev.* B **34** 6295
Monga M R and Pathak K N 1978 *Phys. Rev.* B **18** 5859
[14] Ramond P 1990 *Field Theory: A Modern Primer* (New York: Addison-Wesley) (revised printing)
Negele J W and Orland H 1988 *Quantum Many-Particle System* (New York: Addison-Wesley)
[15] Das A 1997 *Finite Temperature Field Theory* (Singapore: World Scientific)
[16] Haugerud H and Ravndal F 1991 *Phys. Rev.* D **43** 2736
[17] Stevenson P M and Roditi I 1986 *Phys. Rev.* D **33** 2305
Funke M and Kümmel H G 1994 *Phys. Rev.* D **50** 991
Lu W F, Ni G J and Wang Z G 1998 *J. Phys. G: Nucl. Part. Phys.* **24** 673