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# Effective-potential expansion method for the many-body problem at finite temperatures.
## I. Basic formalism

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The effective-potential expansion method, namely, a variational approach to the many-body problem at zero temperature, is extended to nonzero temperatures by the introduction of a new trial density matrix in the Gibbs variational principle for the grand potential $\Omega$. The trial density matrix contains an effective potential as a variational parameter. We have given an expansion form for $\Omega$ in terms of the effective potential. Special care is taken to evaluate the entropy term correctly.

## I. INTRODUCTION

In condensed matter and plasma physics, one of the major problems is evaluation of the equilibrium thermodynamic properties of an interacting many-particle system. In the perturbation-theoretic approach, a formal analysis to calculate the grand potential $\Omega$ has already been given by the introduction of the thermal Green's function.[1] In general, however, the actual implementation is not easy and quantitatively good results can be obtained only in rare cases. Thus many alternative methods have been proposed so far. In particular, the imaginary-time path-integral formulation is a powerful and versatile approach.[2] The formulation provides a useful starting point to calculate the partition function directly in some simple systems with the use of the Monte Carlo methods.[3] It also gives the so-called Feynman inequality based on which a finite-temperature variational approach is formulated.[4] On the other hand, the finite-temperature density-functional theory is not couched on the inequality but on the Gibbs variational principle.[5,6]

The Gibbs variational principle is stated as follows. For any density matrix $\hat{\hat{\rho}}$, i.e., for any positive-definite $\hat{\hat{\rho}}$ with unit trace $\mathrm{Tr}\hat{\hat{\rho}}=1$, the functional

$$\Omega[\hat{\hat{\rho}}]=\mathrm{Tr}\hat{\hat{\rho}}(\hat{H}-\mu\hat{N}+\beta^{-1}\ln\hat{\hat{\rho}}) \tag{1.1}$$

satisfies

$$\Omega[\hat{\hat{\rho}}]\geq\Omega[\hat{\rho}]=-\beta^{-1}\ln\mathrm{Tr}e^{-\beta(\hat{H}-\mu\hat{N})}\;, \tag{1.2}$$

in which the equality holds only for $\hat{\hat{\rho}}=\hat{\rho}$. Here, $\hat{H}$ is the Hamiltonian of the system, $\mu$ is the chemical potential, $\hat{N}$ is the total number operator, $\beta=T^{-1}$,[7] and $\hat{\rho}$ is the grand canonical density matrix, given by

$$\hat{\rho}=e^{-\beta(\hat{H}-\mu\hat{N})}/\mathrm{Tr}e^{-\beta(\hat{H}-\mu\hat{N})}\;. \tag{1.3}$$

This is the principle which takes the place of the Rayleigh-Ritz variational principle at $T=0$, i.e., for the ground-state wave function.

The variational approach has been found quite successful in the calculation of the ground-state properties of the interacting many-body problem. In particular, the Jastrow trial function[8] is known to provide a rather accurate description of the ground-state wave function for many systems. There have been a lot of attempts to calculate the energy expectation value for the ground state with the Jastrow function either in the hypernetted-chain methods[9] or in the Monte Carlo methods.[10] Thus it would be very productive if we could extend the Jastrow's approach to the finite-temperature problem by giving some suitable trial $\hat{\hat{\rho}}$ including the correlation effect as in the Jastrow function. However, we soon realize that the entropy term $\beta^{-1}\mathrm{Tr}\hat{\hat{\rho}}\ln\hat{\hat{\rho}}$ is quite difficult to calculate in this approach. Further, the Jastrow-type trial function has a fundamental flaw in the finite-temperature problem due to the absence of the energy denominators in the definition of the correlation factor. According to the perturbation-theoretic approach, the correlation effect enters in the calculation of $\Omega$ in a power series of the matrix element $\langle n|\hat{V}|m\rangle$ of the interaction potential $\hat{V}$, but the actual expansion parameter is not $\langle n|\hat{V}|m\rangle$ alone but $\langle n|\hat{V}|m\rangle$ divided by the energy denominator $E_n^{(0)}-E_m^{(0)}$ at $T=0$ and $\langle n|\hat{V}|m\rangle/T$ at high temperatures, where $E_n^{(0)}$ is the eigenvalue of the noninteracting Hamiltonian $\hat{H}_0$. Since the Jastrow correlation factor is, in a sense, defined in terms of some average value of

$$\langle n|\hat{V}|m\rangle/(E_n^{(0)}-E_m^{(0)})$$

and has no energy denominators explicitly, the crossover between the energy denominator and $T$ with the increase of $T$ cannot be treated.

One of the authors has already proposed a variational method at $T=0$ with the energy denominators included explicitly in the definition of the correlation factor.[11] It is named the effective-potential expansion (EPX) method, because an effective potential $\hat{\hat{V}}$ is introduced as a variational parameter to construct a trial wave function and serves as an expansion parameter instead of the bare potential $\hat{V}$ in the perturbation-theoretic approach. Because of this change of the expansion parameter, the expansion series converges rapidly even in the strong-coupling region in many interesting systems. In fact, the EPX method is found to provide a much better description of the electron gas in the whole metallic-density region than the Jastrow-type approach.[12] Thus in this paper, we extend the EPX method to nonzero temperatures by giving an appropriate $\hat{\hat{\rho}}$. The actual manipulation of the terms in $\Omega[\hat{\hat{\rho}}]$ is illustrated in the companion paper [paper II (Ref. 13)] by the application of our method to a one-dimensional electron system with a repulsive δ-function interaction.

This paper is organized as follows. In Sec. II we make a quick review of the EPX at zero temperature and in Sec. III we give a form of $\hat{\hat{\rho}}$ which reduces to the EPX as $T$ approaches zero. In Sec. IV we show how to calculate the entropy term in the formal expression for $\Omega[\hat{\hat{\rho}}]$. In Sec. V we discuss two special cases to relate our formalism to other approaches. In Sec. VI we give an expansion form for $\Omega[\hat{\hat{\rho}}]$ explicitly up to second order of the effective potential. Calculations up to fourth order are done in Sec. VII. In Sec. VIII we summarize our results and suggest some systems to which our method can be applied successfully. Finally, in Sec. IX we discuss advantages as well as disadvantages of the present approach and indicate the direction along which our method may be improved upon. Some useful mathematical formulas are given in Appendixes A, B, and C.

## II. THE EFFECTIVE-POTENTIAL EXPANSION METHOD

We consider a system of $N$ particles interacting with one another through a two-body potential. The Hamiltonian of the system is written as

$$\hat{H}=\hat{H}_0+\hat{V}\ , \tag{2.1}$$

where $\hat{H}_0$ and $\hat{V}$ represent, respectively, the noninteracting and the interacting energies of the particles. In this paper, we need not specify $\hat{H}$ further. Our formalism can be applied equally well to both fermions and bosons. We can treat the electrons in the lattice, i.e., the Bloch electrons as well as those in the homogeneous systems like the electron gas.

In the EPX method, we take a trial function $|\tilde{\Phi}_0\rangle$ for the ground state as

$$\begin{aligned}|\tilde{\Phi}_0\rangle&=\hat{\hat{U}}(0,-\infty)|0\rangle\\&\equiv\sum_{n=0}^{\infty}\frac{1}{n!}\left[\sum_{m=1}^{\infty}\mu_m\hat{\hat{U}}_m(0,-\infty)\right]^n|0\rangle\ ,\end{aligned} \tag{2.2}$$

with $\hat{\hat{U}}_m(0,-\infty)$ defined by

$$\hat{\hat{U}}_m(0,-\infty)=\frac{(-i)^m}{m!}\int_{-\infty}^{0}e^{0^+t_1}dt_1\cdots\int_{-\infty}^{0}e^{0^+t_m}dt_m\,T_t[\hat{\hat{V}}(t_1)\cdots\hat{\hat{V}}(t_m)]_{L_m}\ , \tag{2.3}$$

where $\mu_m$'s are arbitrary parameters and $\hat{\hat{V}}(t)$ is defined as

$$\hat{\hat{V}}(t)=e^{i\hat{\hat{H}}_0t}\hat{\hat{V}}e^{-i\hat{\hat{H}}_0t}\ , \tag{2.4}$$

with some suitably chosen trial noninteracting Hamiltonian $\hat{\hat{H}}_0$ and effective interaction $\hat{\hat{V}}$. The state $|0\rangle$ is the normalized ground state of $\hat{\hat{H}}_0$; $T_t$ is the symbol for the time-ordered product in the usual sense; the subscript $L_m$ to the square bracket on the one hand denotes the instruction to consider only terms in which $m$ $\hat{\hat{V}}$'s in the bracket are connected with one another and, on the other hand declares to exclude any term in which $\hat{\hat{V}}$'s in the different square brackets are linked. The point here is that we can control the link-unlink properties in the correlation operator $\hat{\hat{U}}(0,-\infty)$ by the introduction of the $L_m$ operator. We also note that the Hartree and the Fock terms should be excluded in the definition of $\hat{\hat{V}}$, because these terms do not add any new intermediate state to $|\tilde{\Phi}_0\rangle$. The effect of these terms can be included in $\hat{\hat{H}}_0$ as we shall see an example in the following paper.[13] Elimination of the Fock term is quite helpful in avoiding the anomalous diagrams[14] which appear in the usual perturbation-theoretic approach.

The energy expectation value for the trial function (2.2) can be calculated in a similar way to the usual linked-cluster theorem[15] and the result is given by

$$\begin{aligned}\tilde{E}=\frac{\langle\tilde{\Phi}|\hat{H}|\tilde{\Phi}\rangle}{\langle\tilde{\Phi}|\tilde{\Phi}\rangle}&\equiv\langle 0|\hat{\hat{U}}^{\dagger}(0,\infty)\hat{H}\hat{\hat{U}}(0,-\infty)|0\rangle/\langle 0|\hat{\hat{U}}^{\dagger}(0,\infty)\hat{\hat{U}}(0,-\infty)|0\rangle\\&=\langle 0|\left[\sum_{m=1}^{\infty}\mu_m\hat{\hat{U}}_m^{\dagger}(0,\infty)\right]\hat{H}\left[\sum_{m'=1}^{\infty}\mu_{m'}\hat{\hat{U}}_{m'}(0,-\infty)\right]|0\rangle_C\ ,\end{aligned} \tag{2.5}$$

where $\hat{\hat{U}}_m(0,\infty)$ is defined by

$$\hat{\hat{U}}_m(0,\infty)=\frac{i^m}{m!}\int_0^{\infty}e^{-0^+t_1}dt_1\cdots\int_0^{\infty}e^{-0^+t_m}dt_m\,T_t[\hat{\hat{V}}(t_1)\cdots\hat{\hat{V}}(t_m)]_{L_m}\ , \tag{2.6}$$

and the subscript $C$ means that only connected diagrams linked to $\hat{H}$ should be considered in the evaluation of the expectation value. The expression (2.5) is a power series in $\hat{\hat{V}}$. Assuming that $\hat{\hat{V}}$ is a good expansion parameter, we evaluate $\tilde{E}$ up to a certain order in $\hat{\hat{V}}$ and then determine all the variational parameters included in the definition of $\hat{\hat{V}}$ and $\hat{\hat{H}}_0$ by minimizing $\tilde{E}$. (Usually we give some definite values for $\mu_m$'s by hand, though they can also be determined variationally in principle.)

## III. TRIAL DENSITY MATRIX

The functional (1.1) for the grand potential $\Omega[\hat{\hat{\rho}}]$ is reduced to the expectation value of $\hat{H}-\mu\hat{N}$ at zero temperature. A natural extension of the EPX method is obtained if we can give $\hat{\hat{\rho}}$ so as to reproduce the form of (2.5) for $\Omega[\hat{\hat{\rho}}]$ with the replacement of $\hat{H}$ by $\hat{H}-\mu\hat{N}$. Since the third equation in (2.5) shows that the operator $\hat{H}$ is sandwiched by the two correlation factors, one evolving from $t=-\infty$ to 0 and the other from 0 to $\infty$, we are tempted to express $\hat{\hat{\rho}}$ as a product of two factors, one defined in the interval $[0,\beta/2]$ and the other in $[\beta/2,\beta]$. (The latter can be converted into the interval $[-\beta/2,0]$.) From this consideration, we give $\hat{\hat{\rho}}$ as

$$\hat{\hat{\rho}}=\hat{\hat{F}}(\beta,0)/\mathrm{Tr}\hat{\hat{F}}(\beta,0)\ , \tag{3.1}$$

with

$$\begin{aligned}\hat{\hat{F}}(\beta,0)&=e^{-\beta(\hat{\hat{H}}_0-\mu\hat{N})}\hat{\hat{U}}(\beta,\beta/2)\hat{\hat{U}}(\beta/2,0)\\&=[e^{-(\beta/2)(\hat{\hat{H}}_0-\mu\hat{N})}\hat{\hat{U}}(\beta/2,0)]^2\equiv(e^{\hat{\hat{X}}}e^{\hat{\hat{Y}}})^2\ .\end{aligned} \tag{3.2}$$

Here the operators $\hat{\hat{U}}$, $\hat{\hat{X}}$, and $\hat{\hat{Y}}$ are, respectively, defined as

$$\hat{\hat{U}}(\tau,\tau')=\sum_{n=0}^{\infty}\frac{1}{n!}\left[\sum_{m=1}^{\infty}\mu_m\hat{\hat{U}}_m(\tau,\tau')\right]^n\ , \tag{3.3}$$

with

$$\begin{aligned}\hat{\hat{U}}_m(\tau,\tau')&=\frac{(-1)^m}{m!}\\&\quad\times\int_{\tau'}^{\tau}d\tau_1\cdots\int_{\tau'}^{\tau}d\tau_m T_\tau[\hat{\hat{V}}(\tau_1)\cdots\hat{\hat{V}}(\tau_m)]_{L_m}\ ,\end{aligned} \tag{3.4}$$

$$\hat{\hat{X}}=-\frac{\beta}{2}(\hat{\hat{H}}_0-\mu\hat{N})\ , \tag{3.5}$$

and

$$\hat{\hat{Y}}=\ln\hat{\hat{U}}(\beta/2,0)\ . \tag{3.6}$$

We have defined the operator $\hat{\hat{V}}(\tau)$ by

$$\hat{\hat{V}}(\tau)=e^{\tau(\hat{\hat{H}}_0-\mu\hat{N})}\hat{\hat{V}}e^{-\tau(\hat{\hat{H}}_0-\mu\hat{N})}\ , \tag{3.7}$$

and we can prove the following identity easily:

$$\hat{\hat{U}}(\tau-\sigma,\tau'-\sigma)=e^{-\sigma(\hat{\hat{H}}_0-\mu\hat{N})}\hat{\hat{U}}(\tau,\tau')e^{\sigma(\hat{\hat{H}}_0-\mu\hat{N})}\ . \tag{3.8}$$

Substituting (3.1) for $\hat{\hat{\rho}}$ into the functional (1.1), we obtain

$$\begin{aligned}\Omega[\hat{\hat{\rho}}]&=-\beta^{-1}\ln[\mathrm{Tr}\hat{\hat{F}}(\beta,0)]\\&\quad+\frac{\mathrm{Tr}\{\hat{\hat{F}}(\beta,0)[\hat{H}-\mu\hat{N}+\beta^{-1}\ln\hat{\hat{F}}(\beta,0)]\}}{\mathrm{Tr}[\hat{\hat{F}}(\beta,0)]}\ .\end{aligned} \tag{3.9}$$

With the use of (3.2), the first term in (3.9) is rewritten as

$$\begin{aligned}&-\beta^{-1}\ln[\mathrm{Tr}\hat{\hat{F}}(\beta,0)]\\&\qquad=\tilde{\Omega}_0-\beta^{-1}\ln\langle\hat{\hat{U}}(\beta/2,0)\hat{\hat{U}}(0,-\beta/2)\rangle_0\ ,\end{aligned} \tag{3.10}$$

where $\tilde{\Omega}_0$ is given by

$$\tilde{\Omega}_0=-\beta^{-1}\ln\mathrm{Tr}e^{-\beta(\hat{\hat{H}}_0-\mu\hat{N})} \tag{3.11}$$

and the average with the subscript 0 is defined as

$$\langle\hat{A}\rangle_0=\mathrm{Tr}(e^{\beta(\tilde{\Omega}_0-\hat{\hat{H}}_0+\mu\hat{N})}\hat{A})\ . \tag{3.12}$$

Employing the linked-cluster theorem, we can reduce the logarithmic term in (3.10) into

$$\begin{aligned}&\ln\langle\hat{\hat{U}}(\beta/2,0)\hat{\hat{U}}(0,-\beta/2)\rangle_0\\&\qquad=\langle\hat{\hat{U}}(\beta/2,0)\hat{\hat{U}}(0,-\beta/2)\rangle_{0C}-1\ ,\end{aligned} \tag{3.13}$$

where the subscript $C$ denotes to leave only connected terms. We can apply the same theorem to the second term in (3.9) and obtain

$$\begin{aligned}&\frac{\mathrm{Tr}\{\hat{\hat{F}}(\beta,0)[\hat{H}-\mu\hat{N}+\beta^{-1}\ln\hat{\hat{F}}(\beta,0)]\}}{\mathrm{Tr}[\hat{\hat{F}}(\beta,0)]}\\&\quad=\langle\hat{\hat{U}}(\beta/2,0)[\hat{H}-\mu\hat{N}+2\beta^{-1}\ln(e^{\hat{\hat{X}}}e^{\hat{\hat{Y}}})]\\&\qquad\times\hat{\hat{U}}(0,-\beta/2)\rangle_{0C}\ .\end{aligned} \tag{3.14}$$

Here the meaning of the subscript $C$ is a little different; we consider diagrams which link the terms in $\hat{\hat{U}}$ to those inside the square brackets.

## IV. BAKER-CAMPBELL-HAUSDORFF FORMULA

So far, the discussion has been quite formal and exact. In the actual calculation of $\Omega$, the term $\ln(e^{\hat{\hat{X}}}e^{\hat{\hat{Y}}})$ is most difficult to evaluate. Since the operator $\hat{\hat{Y}}$ can be expanded order by order in terms of $\hat{\hat{V}}$ through (3.3), (3.4), and (3.6), let us expand $\ln(e^{\hat{\hat{X}}}e^{\hat{\hat{Y}}})$ in terms of $\hat{\hat{Y}}$. For this purpose, we employ the following Baker-Campbell-Hausdorff formula valid for any operators (matrices) $\hat{\hat{X}}$ and $\hat{\hat{Y}}$:[16]

$$\begin{aligned}\ln(e^{\hat{\hat{X}}}e^{\hat{\hat{Y}}})&=\hat{\hat{X}}+\int_0^1 dt\,\Psi[e^{\mathrm{ad}(\hat{\hat{X}})}e^{t\,\mathrm{ad}(\hat{\hat{Y}})}]\hat{\hat{Y}}\\&=\hat{\hat{X}}+\sum_{n=0}^{\infty}\frac{\Psi_n[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}(\hat{\hat{Y}}),\cdots,\mathrm{ad}(\hat{\hat{Y}})]}{(n+1)!}\hat{\hat{Y}}\\&=\hat{\hat{X}}+\hat{\hat{Y}}+\tfrac{1}{2}[\hat{\hat{X}},\hat{\hat{Y}}]+\tfrac{1}{12}[\hat{\hat{X}},[\hat{\hat{X}},\hat{\hat{Y}}]]\\&\quad+\tfrac{1}{12}[\hat{\hat{Y}},[\hat{\hat{Y}},\hat{\hat{X}}]]+\cdots\ .\end{aligned} \tag{4.1}$$

Here $[\hat{\hat{X}},\hat{\hat{Y}}]=\hat{\hat{X}}\hat{\hat{Y}}-\hat{\hat{Y}}\hat{\hat{X}}$, the operator $\mathrm{ad}(\hat{\hat{X}})$ is defined by

$$[\mathrm{ad}(\hat{\hat{X}})]^n\hat{\hat{Y}}=\begin{cases}\hat{\hat{Y}}, & n=0,\\ [\mathrm{ad}(\hat{\hat{X}})]^{n-1}[\hat{\hat{X}},\hat{\hat{Y}}], & n\geq 1\end{cases} \tag{4.2}$$

and the functions $\Psi$ and $\Psi_n$ are, respectively, given by

$$\Psi(\alpha)=\frac{\alpha\ln\alpha}{\alpha-1} \tag{4.3}$$

and

$$\Psi_n[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}(\hat{\hat{Y}}),\cdots,\mathrm{ad}(\hat{\hat{Y}})] =\frac{d^n}{dt^n}\Psi[e^{\mathrm{ad}(\hat{\hat{X}})}e^{t\,\mathrm{ad}(\hat{\hat{Y}})}]\bigg|_{t=0} . \tag{4.4}$$

The first line of (4.1) is very useful and enables us to expand $\ln(e^{\hat{\hat{X}}}e^{\hat{\hat{Y}}})$ in terms of $\hat{\hat{Y}}$ as in the second line. A brief derivation of the formula (4.1) is recapitulated in Appendix A, an explicit expression for $\Psi_n$ is given in Appendix B, and useful identities are given in Appendix C.

With the use of (4.1), we can reduce (3.14) further as

$$\frac{\mathrm{Tr}\{\hat{\hat{F}}(\beta,0)[\hat{H}-\mu\hat{N}+\beta^{-1}\ln\hat{\hat{F}}(\beta,0)]\}}{\mathrm{Tr}[\hat{\hat{F}}(\beta,0)]}=\left\langle\hat{\hat{U}}(\beta/2,0)\left[\hat{H}-\hat{\hat{H}}_0+2\beta^{-1}\int_0^1 dt\,\Psi[e^{\mathrm{ad}(\hat{\hat{X}})}e^{t\,\mathrm{ad}(\hat{\hat{Y}})}]\hat{\hat{Y}}\right]\hat{\hat{U}}(0,-\beta/2)\right\rangle_{0C} . \tag{4.5}$$

One note is necessary here when we expand $\hat{\hat{Y}}$ in terms of $\hat{\hat{V}}$. Although we can control the link-unlink properties of $\hat{\hat{V}}$'s inside the operator $\hat{\hat{U}}(\beta/2,0)$ by the $L_m$ operator, we cannot do the same thing for the operator $\hat{\hat{Y}}$. We shall see an example in (6.6).

## V. SPECIAL CASES

If we take all the $\mu_m$'s to be zero in (3.3), $\hat{\hat{U}}(\beta/2,0)$ is the unit operator. Thus $\hat{\hat{Y}}$ is zero. Then the functional $\Omega$ is given by

$$\Omega[\hat{\hat{\rho}}]=\tilde{\Omega}_0+\langle\hat{H}-\hat{\hat{H}}_0\rangle_0 , \tag{5.1}$$

and this is, of course, larger than the exact value $\Omega[\hat{\rho}]$, namely,

$$-\beta^{-1}\ln\mathrm{Tr}e^{-\beta(\hat{\hat{H}}_0-\mu\hat{N})}+\langle\hat{H}-\hat{\hat{H}}_0\rangle_0 > -\beta^{-1}\ln\mathrm{Tr}e^{-\beta(\hat{H}-\mu\hat{N})} . \tag{5.2}$$

The inequality (5.2) is just the same as the one obtained by Feynman[2] and our problem is to choose the optimum noninteracting Hamiltonian $\hat{\hat{H}}_0$.

If we take all the $\mu_m$'s to be unity in (3.3), both $\hat{\hat{F}}(\beta,0)$ and $\hat{\hat{U}}(\beta,0)$ can be calculated formally by the same method as in the perturbation-theoretic method.[1] The only difference is in the fact that the Hamiltonian $\hat{H}$ is replaced by $\hat{\hat{H}}_0+\hat{\hat{V}}$ in the present case. Thus the result for $\hat{\hat{F}}(\beta,0)$ is

$$\hat{\hat{F}}(\beta,0)=e^{-\beta(\hat{\hat{H}}_0+\hat{\hat{V}}-\mu\hat{N})} , \tag{5.3}$$

and $\hat{\hat{U}}(\beta,0)$ is given by

$$\hat{\hat{U}}(\beta,0)=\hat{\hat{S}}(\beta,0)\equiv T_\tau\exp\left[-\int_0^\beta d\tau\,\hat{\hat{V}}(\tau)\right] . \tag{5.4}$$

The functional $\Omega$ is now calculated as

$$\Omega[\hat{\hat{\rho}}]=\tilde{\Omega}_0-\beta^{-1}[\langle\hat{\hat{S}}(\beta,0)\rangle_{0C}-1] +\langle\hat{\hat{S}}(\beta,0)(\hat{H}-\hat{\hat{H}}_0-\hat{\hat{V}})\rangle_{0C} . \tag{5.5}$$

In general the calculation of (5.5) is as difficult as that of the exact value $\Omega[\hat{\rho}]$. Besides, we know from the first that $\Omega[\hat{\hat{\rho}}]$ becomes minimum for $\hat{\hat{H}}_0+\hat{\hat{V}}$ equal to $\hat{H}$. Thus one may think that (5.5) is totally useless. However, there might be a situation in which $\hat{\hat{V}}$ serves as a good expansion parameter in the medium- or strong-coupling region of the bare potential $\hat{V}$. In that case the calculation up to a certain order in $\hat{\hat{V}}$ in (5.5) will be very useful. Unfortunately, we have not met such a situation until now. As long as we confine ourselves to the calculations up to second order in $\hat{\hat{V}}$, we come to know that the choice of $\mu_1=1$ and $\mu_m=0$ for $m\geq 2$ gives much better results.

## VI. EXPANSION UP TO SECOND ORDER

Hereafter we will consider the case of $\mu_1=1$ and $\mu_m=0$ for $m\geq 2$. Up to second order in $\hat{\hat{V}}$, (3.13) is expanded as

$$\begin{aligned}\langle\hat{\hat{U}}(\beta/2,0)\hat{\hat{U}}(0,-\beta/2)\rangle_{0C}-1 &=\langle\hat{\hat{U}}_1(\beta/2,0)\rangle_0+\langle\hat{\hat{U}}_1(0,-\beta/2)\rangle_0\\ &\quad+\langle\hat{\hat{U}}_1(\beta/2,0)\hat{\hat{U}}_1(0,-\beta/2)\rangle_{0C} ,\end{aligned} \tag{6.1}$$

where $\hat{\hat{U}}_1$ is defined in (3.4) with $m=1$. The terms like $\langle\hat{\hat{U}}_1(\beta/2,0)^2\rangle_{0C}$ are zero, because these two $\hat{\hat{U}}_1$'s are unlinked. By using the expansion form (B2) for $\Psi_0$, we can prove the following equation for any operator $\hat{A}$ easily:

$$\langle\Psi_0[\mathrm{ad}(\hat{\hat{X}})]\hat{A}\rangle_0=\langle\hat{A}\rangle_0 . \tag{6.2}$$

Thus we can reduce the first term in (6.1) as

$$\langle\hat{\hat{U}}_1(\beta/2,0)\rangle_0=\langle\Psi_0[\mathrm{ad}(\hat{\hat{X}})]\hat{\hat{U}}_1(\beta/2,0)\rangle_0=-\frac{\beta}{2}\langle\hat{\hat{V}}\rangle_0 . \tag{6.3}$$

To reach the final equation, we have used the identity (C3). The same result is given for $\langle\hat{\hat{U}}_1(0,-\beta/2)\rangle_0$.

In order to get an expansion form of (4.5), we have to expand $\hat{\hat{Y}}$ through (3.6). If we write

$$\hat{\hat{Y}}=\hat{\hat{Y}}^{(1)}+\frac{1}{2!}\hat{\hat{Y}}^{(2)}+\frac{1}{3!}\hat{\hat{Y}}^{(3)}+\cdots \,, \tag{6.4}$$

we obtain

$$\hat{\hat{Y}}^{(1)}=\hat{\hat{U}}_1(\beta/2,0)=-\int_0^{\beta/2}d\tau\,\hat{\hat{V}}(\tau) \tag{6.5}$$

and

$$\hat{\hat{Y}}^{(2)}=\hat{\hat{U}}_1(\beta/2,0)^2-\hat{\hat{Y}}^{(1)2} \,. \tag{6.6}$$

One might think that $\hat{\hat{Y}}^{(2)}$ is zero, but actually it is not zero. In the first term of (6.6), we consider only unlinked diagrams by the construction of the trial density matrix (3.1)–(3.4), but we have to include linked diagrams as well in the second one. Thus we have to be very careful about the link-unlink properties in the present formalism. With the use of (6.5) and (6.6), we have

$$\int_0^1 dt\,\Psi[e^{\mathrm{ad}(\hat{\hat{X}})}e^{t\,\mathrm{ad}(\hat{\hat{Y}})}]\hat{\hat{Y}}=-\frac{\beta}{2}\hat{\hat{V}}+\tfrac{1}{2}\Psi_0[\mathrm{ad}(\hat{\hat{X}})]\hat{\hat{U}}_1(\beta/2,0)^2-\tfrac{1}{2}\Psi_0[\mathrm{ad}(\hat{\hat{X}})]\left[T_\tau\int_0^{\beta/2}d\tau_1\int_0^{\beta/2}d\tau_2\hat{\hat{V}}(\tau_1)\hat{\hat{V}}(\tau_2)\right] , \tag{6.7}$$

where we have employed the identities (C3) and (C4). If the two $\hat{\hat{V}}$'s are unlinked in the third term, the contribution is just canceled by the counterdiagram in the second term. Thus we have to include only the connected diagrams in the third term of (6.7) and need not consider the second term. Substituting (6.7) into (4.5), we have an expansion as

$$\begin{aligned}&\frac{\mathrm{Tr}\{\hat{\hat{F}}(\beta,0)[\hat{H}-\mu\hat{N}+\beta^{-1}\ln\hat{\hat{F}}(\beta,0)]\}}{\mathrm{Tr}[\hat{\hat{F}}(\beta,0)]}\\&\quad=\langle\hat{H}-\hat{\hat{H}}_0-\hat{\hat{V}}\rangle_0-\beta^{-1}\langle\Psi_0[\mathrm{ad}(\hat{\hat{X}})]\left[T_\tau\int_0^{\beta/2}d\tau_1\int_0^{\beta/2}d\tau_2\hat{\hat{V}}(\tau_1)\hat{\hat{V}}(\tau_2)\right]\rangle_{0C}\\&\qquad+\langle\hat{\hat{U}}_1(\beta/2,0)(\hat{H}-\hat{\hat{H}}_0-\hat{\hat{V}})\rangle_{0C}+\langle(\hat{H}-\hat{\hat{H}}_0-\hat{\hat{V}})\hat{\hat{U}}_1(0,-\beta/2)\rangle_{0C}+\langle\hat{\hat{U}}_1(\beta/2,0)(\hat{H}-\hat{\hat{H}}_0)\hat{\hat{U}}_1(0,-\beta/2)\rangle_{0C} \,.\end{aligned} \tag{6.8}$$

Since the Hartree and the Fock terms are not included in the definition of $\hat{\hat{V}}$, the terms like $\langle\hat{\hat{U}}_1(\beta/2,0)^2(\hat{H}-\hat{\hat{H}}_0)\rangle_{0C}$ vanish.

Collecting terms in (6.1) and (6.8) and using (6.2) again, we obtain the following form for $\Omega$:

$$\begin{aligned}\Omega[\hat{\rho}]=\tilde{\Omega}_0&+\langle\hat{H}-\hat{\hat{H}}_0\rangle_0+\langle\hat{\hat{U}}_1(\beta/2,0)(\hat{H}-\hat{\hat{H}}_0-\hat{\hat{V}})\rangle_{0C}+\langle(\hat{H}-\hat{\hat{H}}_0-\hat{\hat{V}})\hat{\hat{U}}_1(0,-\beta/2)\rangle_{0C}\\&+\langle\hat{\hat{U}}_1(\beta/2,0)(\hat{H}-\hat{\hat{H}}_0)\hat{\hat{U}}_1(0,-\beta/2)\rangle_{0C}-\beta^{-1}\langle\hat{\hat{U}}_1(\beta/2,0)\hat{\hat{U}}_1(0,-\beta/2)\rangle_{0C}\\&-\beta^{-1}\langle T_\tau\int_0^{\beta/2}d\tau_1\int_0^{\beta/2}d\tau_2\hat{\hat{V}}(\tau_1)\hat{\hat{V}}(\tau_2)\rangle_{0C} \,.\end{aligned} \tag{6.9}$$

It is not difficult to see that as $T$ goes to zero, (6.9) approaches the expression (2.5) expanded up to second order in $\hat{\hat{V}}$ with $\hat{H}$ replaced by $\hat{H}-\mu\hat{N}$, $\mu_1=1$, and $\mu_m=0$ for $m\geq 2$. At high temperatures, i.e., when $\beta$ is small, the actual expansion parameter in (6.9) is easily seen to be $\beta\hat{\hat{V}}/2$. Since this parameter is small for small $\beta$, (6.9) provides an accurate description for $\Omega$.

If we write $\hat{\hat{U}}_1$ in terms of $\hat{\hat{V}}$, (6.9) can be reduced further as

$$\begin{aligned}\Omega[\hat{\rho}]=\tilde{\Omega}_0&+\langle\hat{H}-\hat{\hat{H}}_0\rangle_0-\int_0^{\beta}d\tau\langle\hat{\hat{V}}(\tau)(\hat{H}-\hat{\hat{H}}_0-\hat{\hat{V}})\rangle_{0C}\\&+\int_0^{\beta/2}d\tau_1\int_{-\beta/2}^{0}d\tau_2\langle\hat{\hat{V}}(\tau_1)(\hat{H}-\hat{\hat{H}}_0)\hat{\hat{V}}(\tau_2)\rangle_{0C}\\&-\frac{1}{2!\beta}\langle T_\tau\int_0^{\beta}d\tau_1\int_0^{\beta}d\tau_2\hat{\hat{V}}(\tau_1)\hat{\hat{V}}(\tau_2)\rangle_{0C} \,.\end{aligned} \tag{6.10}$$

This expression is more convenient than (6.9) for practical purposes.

## VII. EXPANSION UP TO FOURTH ORDER

Let us consider the third-order terms. It is clear that (3.13) does not give any contribution. We divide the contribution from (4.5) into three components:

$$\Omega^{(3)}=\sum_{i=1}^{3}\Omega_i^{(3)} \tag{7.1}$$

with

$$\begin{aligned}\Omega_1^{(3)}=&\frac{1}{2!}\langle\hat{\hat{U}}_1(\beta/2,0)^2(\hat{H}-\hat{\hat{H}}_0)\hat{\hat{U}}_1(0,-\beta/2)\rangle_{0C}\\&+\frac{1}{2!}\langle\hat{\hat{U}}_1(\beta/2,0)(\hat{H}-\hat{\hat{H}}_0)\hat{\hat{U}}_1(0,-\beta/2)^2\rangle_{0C} \,,\end{aligned} \tag{7.2}$$

$$\Omega_2^{(3)}=\frac{2}{\beta}\langle\hat{\hat{U}}_1(\beta/2,0)\Psi_0[\mathrm{ad}(\hat{\hat{X}})]\hat{\hat{Y}}^{(1)}\hat{\hat{U}}_1(0,-\beta/2)\rangle_{0C} \,, \tag{7.3}$$

and

$$\Omega_3^{(3)}=\frac{2}{\beta}\frac{1}{3!}\langle \Psi_0[\mathrm{ad}(\hat{\hat{X}})]\hat{\hat{Y}}^{(3)}\rangle_{0C}+\frac{2}{\beta}\frac{1}{2!2!}\langle \Psi_1[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}(\hat{\hat{Y}}^{(2)})]\hat{\hat{Y}}^{(1)}\rangle_{0C}+\frac{2}{\beta}\frac{1}{2!2!}\langle \Psi_1[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}(\hat{\hat{Y}}^{(1)})]\hat{\hat{Y}}^{(2)}\rangle_{0C}$$
$$+\frac{2}{\beta}\frac{1}{3!}\langle \Psi_2[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}(\hat{\hat{Y}}^{(1)}),\mathrm{ad}(\hat{\hat{Y}}^{(1)})]\hat{\hat{Y}}^{(1)}\rangle_{0C}$$
$$+\frac{2}{\beta}\frac{1}{2!}\langle \hat{\hat{U}}_1(\beta/2,0)\{\Psi_0[\mathrm{ad}(\hat{\hat{X}})]\hat{\hat{Y}}^{(2)}+\Psi_1[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}(\hat{\hat{Y}}^{(1)})]\hat{\hat{Y}}^{(1)}\}\rangle_{0C}$$
$$+\frac{2}{\beta}\frac{1}{2!}\langle \{\Psi_0[\mathrm{ad}(\hat{\hat{X}})]\hat{\hat{Y}}^{(2)}+\Psi_1[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}(\hat{\hat{Y}}^{(1)})]\hat{\hat{Y}}^{(1)}\}\hat{\hat{U}}_1(0,-\beta/2)\rangle_{0C} . \tag{7.4}$$

We cannot simplify (7.2) any further, but (7.3) is reduced to

$$\Omega_2^{(3)}=-\langle \hat{\hat{U}}_1(\beta/2,0)\hat{\hat{V}}\hat{\hat{U}}_1(0,-\beta/2)\rangle_{0C} \tag{7.5}$$

with the use of the identity (C3). Similarly, using an identity for $\Psi_2$ as obtained for $\Psi_1$ in (C4), we can rewrite $\Omega_3^{(3)}$ into

$$\Omega_3^{(3)}=\frac{2}{\beta}\frac{1}{3!}\langle \Psi_0[\mathrm{ad}(\hat{\hat{X}})](\hat{\hat{Y}}^{(3)}-\hat{\hat{Z}}^{(3)})\rangle_{0C}+\frac{2}{\beta}\frac{1}{2!2!}\langle \{\Psi_1[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}(\hat{\hat{Y}}^{(2)})]-\Psi_1[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}(\hat{\hat{Z}}^{(2)})]\}\hat{\hat{Y}}^{(1)}\rangle_{0C}$$
$$+\frac{2}{\beta}\frac{1}{2!2!}\langle \Psi_1[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}(\hat{\hat{Y}}^{(1)})](\hat{\hat{Y}}^{(2)}-\hat{\hat{Z}}^{(2)})\rangle_{0C}+\frac{2}{\beta}\frac{1}{2!}\langle \hat{\hat{U}}_1(\beta,0)\Psi_0[\mathrm{ad}(\hat{\hat{X}})](\hat{\hat{Y}}^{(2)}-\hat{\hat{Z}}^{(2)})\rangle_{0C} , \tag{7.6}$$

where $\hat{\hat{Z}}$ is defined by

$$\hat{\hat{Z}}=\ln\left[T_\tau\exp\left[-\int_0^{\beta/2}d\tau\,\hat{\hat{V}}(\tau)\right]\right]=\hat{\hat{Z}}^{(1)}+\frac{1}{2!}\hat{\hat{Z}}^{(2)}+\frac{1}{3!}\hat{\hat{Z}}^{(3)}+\cdots . \tag{7.7}$$

The first term of (7.6) is transformed further as

$$\frac{1}{3!}\langle \Psi_0[\mathrm{ad}(\hat{\hat{X}})](\hat{\hat{Y}}^{(3)}-\hat{\hat{Z}}^{(3)})\rangle_{0C}=-\frac{1}{3!}\langle \hat{\hat{S}}^{(3)}\rangle_{0C}-\frac{1}{2!2!}\int_0^{\beta/2}d\tau\langle \hat{\hat{V}}(\tau)\hat{\hat{S}}^{(2)}+\hat{\hat{S}}^{(2)}\hat{\hat{V}}(\tau)\rangle_{0C}$$
$$=-\frac{1}{3!}\langle \hat{\hat{S}}^{(3)}\rangle_{0C}-\frac{\beta}{8}\left\langle \hat{\hat{S}}^{(2)}(e^{2\,\mathrm{ad}(\hat{\hat{X}})}+1)\frac{1-e^{-\mathrm{ad}(\hat{\hat{X}})}}{\mathrm{ad}(\hat{\hat{X}})}\hat{\hat{V}}\right\rangle_{0C} , \tag{7.8}$$

where $\hat{\hat{S}}^{(j)}$ is defined through

$$T_\tau\exp\left[-\int_0^{\beta/2}d\tau\,\hat{\hat{V}}(\tau)\right]=1+\sum_{j=1}^{\infty}\frac{1}{j!}\hat{\hat{S}}^{(j)} . \tag{7.9}$$

In deriving (7.8), we have used the following identities valid for any operators $\hat{A}$ and $\hat{B}$:

$$\langle f[\mathrm{ad}(\hat{\hat{X}})]\hat{A}\rangle_0=\langle \hat{A}\rangle_0 , \tag{7.10}$$

and

$$\langle \hat{A}g[\mathrm{ad}(\hat{\hat{X}})]\hat{B}\rangle_{0C}=\langle \{g[-\mathrm{ad}(\hat{\hat{X}})]\hat{A}\}\hat{B}\rangle_{0C} , \tag{7.11}$$

provided that $f(x)$ is analytic at $x=0$ with $f(0)=1$. [Equation (6.2) is a special case of (7.10).] Other terms in (7.8) can be calculated in a similar way and the final form for $\Omega_3^{(3)}$ is obtained as

$$\Omega_3^{(3)}=\left[\frac{\beta}{2}\right]^2\left\langle \hat{\hat{V}}\frac{1}{\mathrm{ad}(\hat{\hat{X}})}\hat{\hat{V}}\frac{1}{\mathrm{ad}(\hat{\hat{X}})}\hat{\hat{V}}\right\rangle_{0C}$$
$$=\frac{1}{3!\beta}\left\langle T_\tau\int_0^{\beta}d\tau_1\int_0^{\beta}d\tau_2\int_0^{\beta}d\tau_3\hat{\hat{V}}(\tau_1)\hat{\hat{V}}(\tau_2)\hat{\hat{V}}(\tau_3)\right\rangle_{0C} . \tag{7.12}$$

We can perform a similar reduction for the fourth-order terms and find that at least up to forth order in $\hat{\hat{V}}$, $\Omega[\hat{\hat{\rho}}]$ is provided faithfully by the following expression:

$$\Omega[\hat{\hat{\rho}}]=\tilde{\Omega}_0+\langle \hat{\hat{U}}(\beta/2,0)(\hat{H}-\tilde{\hat{H}}_0)\hat{\hat{U}}(0,-\beta/2)\rangle_{0C}-\frac{1}{\beta}[\langle \hat{\hat{S}}(\beta,0)\rangle_{0C}-1]$$
$$+\frac{2}{\beta}\langle [\hat{\hat{S}}(\beta/2,0)-\hat{\hat{U}}(\beta/2,0)]\Psi_0[\mathrm{ad}(\hat{\hat{X}})][\hat{\hat{S}}(0,-\beta/2)-\hat{\hat{U}}(0,-\beta/2)]\rangle_{0C} , \tag{7.13}$$

where $\hat{\hat{U}}$ is defined in (3.3) and (3.4) with $\mu_1=1$ and $\mu_m=0$ for $m\geq 2$ and $\hat{\hat{S}}$ is given by

$$\hat{\hat{S}}(\tau,\tau')=T_\tau\exp\left[-\int_\tau^{\tau'}d\tau\,\hat{\hat{V}}(\tau)\right] . \tag{7.14}$$

We have not confirmed yet whether (7.13) still applies beyond fourth order, but we anticipate that (7.13) may be a good approximate expression for $\Omega$ up to infinite order.

## VIII. SUMMARY

The central result of this paper is (6.10) for the grand potential $\Omega$. This is a direct extension of the EPX method in the two-body approximation[17] to finite temperatures. Since at high temperatures the expansion parameter in (6.10) is $\beta\hat{\hat{V}}/2$ and is much smaller than that at $T=0$ which is $\hat{\hat{V}}$ divided by a suitable energy denominator, the two-body approximation, i.e., the cutoff of the series for $\Omega$ at second order in $\hat{\hat{V}}$, becomes much more reliable at these temperatures compared to the case of $T=0$. Thus it is almost certain that our present method will provide a very precise temperature-dependent exchange-correlation energy $E_{\mathrm{xc}}(n,T)$ as a function of the electron density $n$ in the whole temperature region for the electron gas, i.e., the system in which electrons are confined in a uniform neutralizing background and interact with one another through a Coulomb potential. In fact, $E_{\mathrm{xc}}(n,T)$ is a very important quantity in the finite-temperature density-functional calculations.[6] We plan to supply our results for $E_{\mathrm{xc}}$ in the future.

Besides the electron gas, our method can be applied successfully to any system at high temperatures. Of course, at high enough temperatures, one needs not resort to our method but to the usual perturbation-theoretic approach and obtains the same results. However, the point here is that with just the same labor to calculate the terms in the usual perturbation series, one can obtain the results valid in much wider applicable ranges of both $T$ and the strength of the bare potential, if one employs our formalism. An example is given in the companion paper.[13]

If we start with $\hat{\hat{H}}_0$ not describing the normal state but some condensed state like superconductivity, we can naturally obtain some type of a gap equation at a finite temperature. By solving the gap equation, we can discuss the many-body effects on the transition temperature. This is another area to which we plan to apply our method.

## IX. DISCUSSION

The many-body effects in many-electron systems are usually separated into two, i.e., the exchange and the correlation effects. The former is the consequence of the Pauli exclusion principle. This principle is satisfied completely only when each direct term is accompanied by its exchange partner. In the perturbation-theoretic approach, it is usually quite difficult to include all the direct and the exchange terms on the equal footing, because some partial sum is almost always necessary and in such a partial sum the exchange terms are neglected or treated quite roughly. In our method, the partial sum is done implicitly by the choice of the effective potential. The direct and the exchange diagrams are defined on the basis of this effective potential. Thus, as far as the direct and exchange terms are included in pairs, the Pauli principle is satisfied completely in our method, even if we cut the series for $\Omega$ at some finite order in the effective potential. As a byproduct of this procedure, the convergence of the series is sometimes found to be very rapid, even though each higher-order direct term itself is large. Such a case occurs when the contribution of each direct term is almost cancelled by that of its exchange partner. Although this situation imposes the so-called negative-spin problem for the Monte Carlo methods[3] and is avoided, we welcome such a case. In this sense, our method is complementary to the Monte Carlo ones.

The correlation effect in the metallic state is characterized by the change of the many-body wave function in the Hilbert space in which there is a continuous spectrum of the energy eigenvalues located without any energy gap from the ground-state energy. In the correlation problem of the continuous spectrum, the energy denominator plays a very important role in the construction of the wave function. Thus the theories[9,10] based on the Jastrow wave function[8] cannot be so accurate, because they do not include the energy denominators in their formulations from the beginning. In fact, quantities like the total energy in which all the electrons participate may be calculated rather well even by such theories, but quasiparticle properties near the Fermi surface will not be evaluated properly by them. The same criticism might also be applied to the Monte Carlo methods,[3] because they can treat only finite-number systems in which the spectrum of the energy eigenvalues is discrete. On the other hand, our method as well as the perturbation-theoretic approach can study the correlation effect in the continuous spectrum of excited states. In particular, our method will provide well-balanced values for both the exchange and the correlation effects with their full complexities from the weak- to at least the medium-coupling regions.

An apparent disadvantage of our method to the perturbation-theoretic approach is that we cannot take an accurate account of low-lying collective modes, because such collective modes can be included either by an explicit sum of some particular terms up to infinite order or by the use of the frequency- as well as momentum-dependent effective potential. At present, we have not succeeded in either way. An example is given in the companion paper[13] in which we show that we cannot reproduce the contribution from the spin waves very accurately in the strong-coupling region, though we succeeded in obtaining the correct behavior qualitatively. We need to improve on our method in this direction.

Another direction to develop our method can be found by the comparison of (6.10) with (5.5). As we have mentioned, the expansion parameter is $\beta\hat{\hat{V}}/2$ for (6.10) at high temperatures, while for (5.5), it is $\beta\hat{\hat{V}}$ which is worse. Thus (6.10) gives a better result than (5.5) when we compare the calculations up to second order in $\hat{\hat{V}}$. The reason why the factor 2 appears in the former case is that in (3.2) we have divided the interval $(0,\beta)$ into 2. If we divide the interval into $M$ instead of 2, we may expand with the expansion parameter $\beta\hat{\hat{V}}/M$. A systematic increase of $M$ will give progressively better results. Nevertheless, (5.5) also seems to be very important and may provide a very good starting point to include some particular terms up to an infinite order for the description of collective modes.

### APPENDIX A: DERIVATION OF FORMULA (4.1)

Consider the function, defined by

$$\hat{g}(s,t)\equiv\exp[s\hat{\Gamma}(t)]\ , \qquad \text{(A1)}$$

with

$$\hat{\Gamma}(t)\equiv\ln(e^{\hat{\hat{X}}}e^{t\hat{\hat{Y}}}) \ . \tag{A2}$$

By taking the derivative with respect to $s$, we obtain

$$\hat{\Gamma}(t)=\hat{g}(s,t)^{-1}\frac{\partial\hat{g}(s,t)}{\partial s} \ . \tag{A3}$$

We also take the derivative with respect to $t$ and define the function as

$$\hat{h}(s,t)\equiv\hat{g}(s,t)^{-1}\frac{\partial\hat{g}(s,t)}{\partial t} \ , \tag{A4}$$

By taking the difference between the derivative of (A3) with respect to $t$ and that of (A4) with respect to $s$, we obtain

$$\frac{\partial\hat{h}}{\partial s}=\frac{d\hat{\Gamma}}{dt}-\mathrm{ad}(\hat{\Gamma})\hat{h} \ . \tag{A5}$$

With the initial condition $\hat{h}(0,t)=0$, this equation is solved iteratively to give

$$\hat{\hat{Y}}=\hat{h}(1,t)=\Phi[-\mathrm{ad}(\hat{\Gamma})]\frac{d\hat{\Gamma}}{dt} \ , \tag{A6}$$

with

$$\Phi(\alpha)=\sum_{n=1}^{\infty}\frac{\alpha^{n-1}}{n!}=\frac{e^{\alpha}-1}{\alpha} \ . \tag{A7}$$

Therefore we have

$$\frac{d\hat{\Gamma}}{dt}=\Phi[-\mathrm{ad}(\hat{\Gamma})]^{-1}\hat{\hat{Y}}=\Psi[e^{\mathrm{ad}(\hat{\Gamma})}]\hat{\hat{Y}} \ , \tag{A8}$$

in which $\Psi$ is defined in (4.3).

Now we show

$$e^{\mathrm{ad}(\hat{\Gamma})}=e^{\mathrm{ad}(\hat{\hat{X}})}e^{t\,\mathrm{ad}(\hat{\hat{Y}})} \ . \tag{A9}$$

For the purpose, we note the following identities valid for any operators $\hat{V}$ and $\hat{W}$:

$$e^{\hat{V}}\hat{W}e^{-\hat{V}}=e^{\mathrm{ad}(\hat{V})}\hat{W} \tag{A10}$$

and

$$e^{\hat{V}}e^{\hat{W}}e^{-\hat{V}}=\exp[e^{\mathrm{ad}(\hat{V})}\hat{W}] \ . \tag{A11}$$

With the use of (A10), (A11), and the definition for $\hat{\Gamma}$ in (A2), we have

$$\begin{aligned}\exp[e^{\mathrm{ad}(\hat{\Gamma})}\hat{W}]&=e^{\hat{\Gamma}}e^{\hat{W}}e^{-\hat{\Gamma}}\\&=e^{\hat{\hat{X}}}\exp[e^{t\,\mathrm{ad}(\hat{\hat{Y}})}\hat{W}]e^{-\hat{\hat{X}}}\\&=\exp[e^{\mathrm{ad}(\hat{\hat{X}})}e^{t\,\mathrm{ad}(\hat{\hat{Y}})}\hat{W}] \ .\end{aligned} \tag{A12}$$

Since (A12) holds for any $\hat{W}$, (A9) should be valid. By substituting (A9) into (A8) and integrating both sides of (A8) with the initial condition $\hat{\Gamma}(0)=\hat{\hat{X}}$, we obtain (4.1).

## APPENDIX B: EXPRESSION FOR $\Psi_n$

With the definitions of (4.3) and (4.4), we readily obtain the expression for $\Psi_0$ as

$$\Psi_0[\mathrm{ad}(\hat{\hat{X}})]=\Psi[e^{\mathrm{ad}(\hat{\hat{X}})}]=\frac{\mathrm{ad}(\hat{\hat{X}})}{1-e^{-\mathrm{ad}(\hat{\hat{X}})}} \ . \tag{B1}$$

The expansion form

$$\Psi_0[\mathrm{ad}(\hat{\hat{X}})]=1+\tfrac{1}{2}\mathrm{ad}(\hat{\hat{X}})+\sum_{p=1}^{\infty}K_{2p}[\mathrm{ad}(\hat{\hat{X}})]^{2p} \tag{B2}$$

is useful in the actual calculation, where $K_{2p}$ is the coefficient of the $2p$th-order term in the series

$$\frac{x}{1-e^{-x}}=1+\tfrac{1}{2}x+\sum_{p=1}^{\infty}K_{2p}x^{2p} \ . \tag{B3}$$

Introducing

$$\hat{A}(t)=e^{\mathrm{ad}(\hat{\hat{X}})}e^{t\,\mathrm{ad}(\hat{\hat{Y}})} \ , \tag{B4}$$

we can derive the expression for $\Psi_1[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}(\hat{\hat{Y}})]$ as

$$\begin{aligned}\Psi_1[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}(\hat{\hat{Y}})]&=\frac{d}{dt}\left[\ln\hat{A}(t)\left[1+\frac{1}{\hat{A}(t)-1}\right]\right]\bigg|_{t=0}\\&=-\ln\hat{A}(0)\frac{1}{\hat{A}(0)-1}\hat{A}'(0)\frac{1}{\hat{A}(0)-1}\\&\quad+\frac{d}{dt}\ln\hat{A}(t)\bigg|_{t=0}\frac{\hat{A}(0)}{\hat{A}(0)-1} \ .\end{aligned} \tag{B5}$$

With the use of (4.1), the term $(d/dt)\ln\hat{A}(t)|_{t=0}$ is calculated as

$$\begin{aligned}\frac{d}{dt}\ln\hat{A}(t)|_{t=0}&=\Psi_0[\mathrm{ad}(\mathrm{ad}(\hat{\hat{X}}))]\mathrm{ad}(\hat{\hat{Y}})\\&=\mathrm{ad}(\Psi_0[\mathrm{ad}(\hat{\hat{X}})]\hat{\hat{Y}}) \ ,\end{aligned} \tag{B6}$$

where the second equality can be derived through Jacobi's identity for any operator $\hat{W}$:

$$[\mathrm{ad}(\hat{\hat{X}}),\mathrm{ad}(\hat{\hat{Y}})]\hat{W}=\mathrm{ad}([\hat{\hat{X}},\hat{\hat{Y}}])\hat{W} \ . \tag{B7}$$

Then we can rewrite (B5) as

$$\begin{aligned}\Psi_1[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}(\hat{\hat{Y}})]&=-\Psi_0[\mathrm{ad}(\hat{\hat{X}})]\mathrm{ad}(\hat{\hat{Y}})\frac{1}{e^{\mathrm{ad}(\hat{\hat{X}})}-1}\\&\quad+\mathrm{ad}(\Psi_0[\mathrm{ad}(\hat{\hat{X}})]\hat{\hat{Y}})\frac{1}{1-e^{-\mathrm{ad}(\hat{\hat{X}})}} \ .\end{aligned} \tag{B8}$$

We can perform a similar calculation for $\Psi_n$ and the result is

$$\Psi_n[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}(\hat{\hat{Y}}),\cdots,\mathrm{ad}(\hat{\hat{Y}})]=\frac{1}{1-e^{-\mathrm{ad}(\hat{\hat{X}})}}\mathrm{ad}(\Psi_{n-1}[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}(\hat{\hat{Y}}),\cdots,\mathrm{ad}(\hat{\hat{Y}})]\hat{\hat{Y}})$$
$$+\sum_{k=1}^{n-1}\sum_{l=1}^{n-k}\sum_{m}\frac{(-1)^l n!}{k!m_1!\cdots m_l!}\hat{\ell}_{m_1}\cdots\hat{\ell}_{m_l}$$
$$\times\frac{1}{e^{\mathrm{ad}(\hat{\hat{X}})}-1}\mathrm{ad}(\Psi_{k-1}[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}(\hat{\hat{Y}}),\cdots,\mathrm{ad}(\hat{\hat{Y}})]\hat{\hat{Y}})\ . \tag{B9}$$

Here $\hat{\ell}_m$ is defined by

$$\hat{\ell}_m=\frac{1}{1-e^{-\mathrm{ad}(\hat{\hat{X}})}}[\mathrm{ad}(\hat{\hat{Y}})]^m\ , \tag{B10}$$

and the last summation is taken under the condition

$$\sum_{j=1}^{l} m_j=n-k,\quad m_j\geq 1\ . \tag{B11}$$

## APPENDIX C: USEFUL IDENTITIES FOR $\Psi_n$

By the same method as is known well in the usual perturbation-theoretic approach,[1] we can prove

$$e^{-(\beta/2)(\hat{\hat{H}}_0-\mu\hat{N}+\hat{\hat{V}})}=e^{\hat{\hat{X}}}T_\tau\exp\left[-\int_0^{\beta/2}d\tau\,\hat{\hat{V}}(\tau)\right]\equiv e^{\hat{\hat{X}}}e^{\hat{\hat{Z}}}\ , \tag{C1}$$

where $\hat{\hat{X}}$ are $\hat{\hat{Z}}$ are, respectively, defined in (3.5) and (7.7). By taking the logarithm of (C1) and applying the Baker-Campbell-Hausdorff formula (4.1), we obtain the identity

$$-\frac{\beta}{2}\hat{\hat{V}}=\sum_{n=0}^{\infty}\frac{\Psi_n[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}(\hat{\hat{Z}}),\cdots,\mathrm{ad}(\hat{\hat{Z}})]}{(n+1)!}\hat{\hat{Z}} \tag{C2}$$

Expanding $\hat{\hat{Z}}$ in the power of $\hat{\hat{V}}$ and comparing terms order by order in (C2), we have a series of identities:

$$\Psi_0[\mathrm{ad}(\hat{\hat{X}})]\left[-\int_0^{\beta/2}d\tau\,\hat{\hat{V}}(\tau)\right]=-\frac{\beta}{2}\hat{\hat{V}}\ , \tag{C3}$$

$$\Psi_0[\mathrm{ad}(\hat{\hat{X}})]\left[T_\tau\int_0^{\beta/2}d\tau_1\int_0^{\beta/2}d\tau_2\hat{\hat{V}}(\tau_1)\hat{\hat{V}}(\tau_2)-\left[-\int_0^{\beta/2}d\tau\,\hat{\hat{V}}(\tau)\right]^2\right]$$
$$+\Psi_1\left[\mathrm{ad}(\hat{\hat{X}});\mathrm{ad}\left[-\int_0^{\beta/2}d\tau\,\hat{\hat{V}}(\tau)\right]\right]\left[-\int_0^{\beta/2}d\tau\,\hat{\hat{V}}(\tau)\right]=0\ , \tag{C4}$$

and so on. Note that these identities can also be proven directly by the integral of $\tau$ with the use of the relation

$$\hat{\hat{V}}(\tau)=e^{-(2\tau/\beta)\mathrm{ad}(\hat{\hat{X}})}\hat{\hat{V}}\ . \tag{C5}$$

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