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On optimal mean-field descriptions in finite-temperature many-body theories: Use of thermal Brillouin and Bruckner conditions

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Abstract. Although the structural similarity between the properties of a thermal trace and the zero-temperature expectation values for quantum systems has been known for quite some time, not all the practical computational methods in the thermal field theories exploit this correspondence explicitly. Using a thermal field theory derived by us, which introduces the thermal analogues of normal ordering and Wick's expansion, a very close resemblance between zero-temperature and finite-temperature field theories can be established. We use this apparatus in this paper to derive optimal conditions of mean-field and correlated descriptions of thermally averaged quantities. It is shown that the optimal mean-field conditions for the free energy is equivalent to the minimum value for the average energy. The optimality conditions turn out to be exact thermal analogues of the Brillouin conditions. The optimal mean-field condition to generate the minimum value of the ratio Z/Z_0, where Z and Z_0 are the exact and the mean-field partition functions, yields the exact thermal analogue of the Brückner condition. In a similar vein, we generalize the thermal Brillouin condition to include correlated functions used in the evaluation of the thermal trace. The optimal choice of the correlated ground states leads to many-particle generalizations of the thermal Brillouin conditions. In the context of the path-integral methods for determining Z, we envisage use of a local optimal mean field that depends on each point on the path – leading to local thermal analogues of Brillouin and Brückner conditions. To derive these conditions, we have used another apparatus of field theory derived recently by us that uses concepts of normal ordering and Wick expansion with respect to a path-integral measure (rather than the measure implied by thermal trace). We hope to demonstrate in our discussions that this way of formulating thermal many-body problems enables us to exploit deep similarities between thermal and zero-temperature situations which are difficult to discern in the traditional methods. Illustrative examples by way of deriving thermal Brillouin and Bruckner conditions for typical Fermionic and Bosonic problems are presented.

Keywords. Optimal mean-field description; finite-temperature many-body theory; thermal Brillouin condition; Brückner conditions.

1. Introduction

Quantum many-body systems in equilibrium at a finite temperature display complex and fascinating behaviour that seems inexhaustible in its richness and variety. It is no wonder therefore that there exist in the literature several general methodologies for computing equilibrium thermal properties of quantum systems. We may mention here just a few among them as being of direct relevance to us: the finite-temperature perturbation theories (Bloch and de Dominicis 1958; Balian and de Dominicis 1960;

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Balian *et al* 1960), the temperature Green's function method (Matsubara 1955), the complex time-path formalisms (Martin and Schwinger 1957; Niemi and Semenoff 1984), the path-integral methods (Feynman and Kleinert 1986; Giachetti and Tognetti 1986; Lee *et al* 1991), and the recently emerging developments of thermofield dynamics (Arimitsu and Umezawa 1985, 1987; Umezawa and Yamanaka 1988). Although a close correspondence between the properties of thermal traces of the finite-temperature statistical mechanics with those of the zero-temperature expectation values in quantum mechanics has been known for quite some time (Araki and Woods 1963), not all the finite-temperature formalisms mentioned above exhibit this feature in a manifest and transparent manner. To keep this correspondence explicit is, however, highly desirable since this would encourage very fruitful reciprocal fertilization of both finite-temperature statistical–mechanical methodologies and zero-temperature quantum mechanical formulations.

The path-integral methods (Feynman and Kleinert 1986; Giachetti and Tognetti 1986; Lee *et al* 1991) and the formalisms of thermofield dynamics (Arimitsu and Umezawa 1985, 1987; Umezawa and Yamanaka 1988) are rather special in the sense of bringing out the correspondence mentioned above. The path-integral methods employ integration over the paths with a suitable measure to perform the thermal traces which has a correspondence with the ordinary integration over co-ordinates (or other suitable degrees of freedom) for computing the expectation values. The manipulations in the path-integral methods can thus, with appropriate notational innovations, be mapped onto a zero-temperature formalism. Likewise, in the thermofield dynamic formulations, one replaces the thermal trace as an expectation value over a properly defined "thermal vacuum". To establish a complete correspondence, it then becomes necessary to "double" all the degrees of freedom. In the occupation number representation, as befitting a finite-temperature field theory, one replaces the system Hamiltonian $H(\mathbf{a},\mathbf{a}^\dagger)$ by a modified Hamiltonian $\tilde{H} = H(\mathbf{a},\mathbf{a}^\dagger) - H(\tilde{\mathbf{a}},\tilde{\mathbf{a}}^\dagger)$, where the set of tilde variables $\tilde{\mathbf{a}}/\tilde{\mathbf{a}}^\dagger$ are exact replicas of the system variables $\mathbf{a}/\mathbf{a}^\dagger$.

Despite the possibility of discerning the kinship of both path-integral and thermofield dynamical methods to zero-temperature formalisms, their operational details are sufficiently different compared with the zero-temperature field theoretic treatments, so that it seems worth formulating finite-temperature many-body theories *involving the physical variables only* – using manipulations that are structurally closer in spirit to those invoked in zero-temperature many-body theories.

We have proposed very recently a finite-temperature many-body theory, called the thermal cluster cumulant theory by us (Sanyal *et al* 1992, 1993) which may be looked upon as a finite-temperature generalization of the zero-temperature time-dependent coupled cluster theory. It should be mentioned that there are both closed shell (Monkhorst 1977; Hoodbhoy and Negele 1978; Arponen 1983; Sebastian 1985; Arponen *et al* 1987; Prasad 1988) and open shell (Mukherjee 1986; Guha *et al* 1989; Guha and Mukherjee 1991) formalisms. Our normal-ordered thermal generalizations are akin to the open shell formalisms mentioned above. The formalism combines the advantages of both finite-temperature perturbation theories (Bloch and de Dominicis 1958; Balian and de Dominicis 1960; Balian *et al* 1960) and formalisms of thermofield dynamics (Feynman and Kleinert 1986; Giachetti and Tognetti 1986; Lee *et al* 1991) but has the simplicity of using only the physical variables in the manipulations. It can also be applied in situations where the use of a path-integral method seems

the more convenient (Mandal *et al*, to be published). This development offers the possibility of exploiting a much more direct algebraic homomorphy between the finite-temperature and zero-temperature formalisms. In fact, by invoking the finite-temperature analogues of normal ordering, contractions and Wick's expansion, the correspondence can be made very close – as has been recently illustrated by applying the formalism for computing partition functions of interacting quantum systems (Sanyal *et al* 1992, 1993). The apparatus of this new thermal field theory is, however, of quite general utility which allows us to treat thermal traces at par with expectation values for a much wider range of situations. The purpose of the present paper is to indicate and explore several such possibilities. Just as one invokes optimal mean-field functions in the zero-temperature formalisms – either in the sense of best energy (Hartree or Hartree–Fock descriptions), or in the sense of best overlap with the exact functions (maximal overlap or Brückner function) – one may analogously envisage finding the conditions for optimal mean-field descriptions for generating best thermally averaged energies (thermal Hartree or Hartree–Fock conditions) and the best mean-field description of the free energies (which may be deemed as thermal Brückner conditions) from our thermal field theory. It is even possible to go beyond the mean-field descriptions and formulate general thermal Brillouin conditions for correlated models, which are the natural finite-temperature analogues of the so-called k-particle Brillouin conditions formulated more than a decade ago (Kutzelnigg 1979, 1980). In the path-integral methods for partition functions, one often invokes a "smearing procedure" (Feynman and Kleinert 1986; Giachetti and Tognetti 1986; Lee *et al* 1991), amounting to the choice of a "local" mean-field potential on each point on the path, which finds its natural use in our thermal field theory as generating "local" thermal Brillouin and Brückner conditions. These relations, in our opinion, offer useful insight as regards the various optimal choices in a variety of situations that would have been pretty hard to discern with the other formalisms currently in use.

The paper is organized as follows. In § 2, we delineate the appropriate thermal analogues of the normal ordering and Wick's theorem and summarize the contents of our formulation of the thermal field theory. This section will also serve to introduce the terminology and notations to be used later in the paper. In § 3, we derive the thermal Brillouin and Brückner conditions as alternative optimal defining relations for the mean-field descriptions. In § 4, we discuss the appropriate generalizations of the thermal Brillouin conditions for models beyond the mean fields. In § 5, we introduce the concept of "local" mean fields in the context of path-integral formalisms and derive the "local" thermal Brillouin and Brückner conditions in the framework of path integrals. Section 6 contains our concluding remarks.

2. Thermal normal ordering and thermal wick expansion in a finite-temperature many-body theory

2.1 *Matsubara formula for thermal traces as the analogue of Wick's reduction for expectation values*

To provide the basis for the development to follow, we start out with the well-known formula for computing the thermal trace of a time-ordered product of Bose/Fermi

operators:

$$\ll T[A_1(\tau_1)A_2(\tau_2)\ldots A_n(\tau_n)] \gg$$
$$\equiv Tr\exp[-\beta(H_0-\mu N)]\; T[A_1(\tau_1)A_2(\tau_2)\ldots A_n(\tau_n)]/Z_0$$
$$= \sum_{\substack{\text{all pairs}\\(ij)}} \prod (-1)^{\eta_{ij}} \ll T[A_i(\tau_i)A_j(\tau_j)] \gg, \tag{1}$$

where each pair involves one creation and one annihilation operator of each type and η_{ij} is the parity of permutation needed to bring two Fermi-type operators A_i and A_j side by side in evaluating the pair average $\ll T[A_i(\tau_i)A_j(\tau_j)] \gg$. Z_0 is the partition function of the "unperturbed" system, characterized by a one-electron Hamiltonian H_0,

$$H_0 = \sum_k \varepsilon_k [a_k^\dagger a_k], \tag{2}$$

N is the number operator,

$$N = \sum_k [a_k^\dagger a_k], \tag{3}$$

and μ is the chemical potential of the interacting system. The operators $A_i(\tau_i)$ are either defined in the ordinary interaction picture,

$$A_i(\tau_i) = \exp(iH_0\tau_i)A_i\exp(-iH_0\tau_i), \tag{4}$$

or in the "interaction picture" involving "imaginary time",

$$A_i(\tau_i) = \exp(H_0\tau_i)A_i\exp(-H_0\tau_i) \tag{5}$$

Expression (1) was derived by many authors in the context of finite-temperature perturbation theory (Matsubara 1955; Bloch and de Dominicis 1958; Balian and de Dominicis 1960; Balian *et al* 1960) and is generally known as the Matsubara formula. It bears a striking resemblance to the familiar zero-temperature Wick reduction formula of the vacuum expectation value of a T-ordered product of operators as a sum of product of T-ordered pairs. In analogy with the notion of contractions, we may define $\ll T[A_i(\tau_i)A_j(\tau_j] \gg$ as a thermal contraction

$$\text{Def:} \ll T[A_i(\tau_i)A_j(\tau_j)] \gg \equiv \{\overbrace{A_i(\tau_i)A_j(\tau_j)}\}_\beta \tag{6}$$

2.2 *Notion of thermal normal ordering and thermal Wick expansion*

Unlike in the path-integral method where a suitable measure takes care of the thermal trace, or in the method of thermofield dynamics where a doubling of the degrees of freedom achieves the correspondence with the zero-temperature situations, we shall envisage a procedure where a T-product of operators admits of an expansion involving suitably defined thermal normal products and multiple thermal contractions – a perfect finite-temperature analogue of Wick's theorem. The thermal normal products should have the property of (i) commuting (anticommuting) under the thermal normal

ordering symbol for Bose (Fermi) operators, and (ii) having vanishing thermal averages. Such an expansion, if it exists, would automatically generate the Matsubara formula, (1), since only the completely contracted terms in the expansion will survive on taking the thermal trace. We have shown recently, while formulating our thermal cluster cumulant theory (Sanyal *et al* 1992, 1993), that such a thermal Wick's expansion is indeed possible. It should be obvious that the thermal normal ordering is not a normal ordering in the usual sense, since the thermal trace of $A_i^\dagger(\tau_i)A_j(\tau_j)$ with $\tau_i > \tau_j$ and A_j a destruction is non-zero.

We shall illustrate the theorem by taking up concrete examples. For the general proof we refer to our more elaborate papers (Sanyal *et al* 1992, 1993). Let us consider first the bosonic systems. We define the thermal normal product $\{A_1(\tau_1)A_2(\tau_2)\}_\beta$ as follows:

$$\begin{aligned}\text{Def:}\{A_1(\tau_1)A_2(\tau_2)\}_\beta &= T[A_1(\tau_1)A_2(\tau_2)] - \ll T[A_1(\tau_1)A_2(\tau_2)] \gg \\ &\equiv T[A_1(\tau_1)A_2(\tau_2)] - \{\overbrace{A_1(\tau_1)A_2(\tau_2)}\}_\beta \end{aligned} \tag{7}$$

We note that our development follows a path complementary to what is done in the zero-temperature many-body theory: we define the thermal normal order as the difference of the T-ordered product and the thermal contraction – to ensure the vanishing of $\langle\{A_1(\tau_1)A_2(\tau_2)\}_\beta\gg$; the zero-temperature theories define normal ordering first and introduce the contraction as the difference between the T-ordered product and the normal order. For three operators, we can construct the thermal normal product in terms of T-product of these operators and $\{\cdots\}_\beta$ products of two operators, keeping a manifest symmetry in the expression with respect to all the three variables. We thus write:

$$\begin{aligned}\{A_1(\tau_1)A_2(\tau_2)A_3(\tau_3)\}_\beta &= C_1\, T[A_1(\tau_1)A_2(\tau_2)A_3(\tau_3)] \\ &+ C_2\{\overbrace{A_1(\tau_1)A_2(\tau_2)}\}_\beta A_3(\tau_3) + C_3\{\overbrace{A_1(\tau_1)A_3(\tau_3)}\}_\beta A_2(\tau_2) \\ &+ C_4 A_1(\tau_1)\{\overbrace{A_2(\tau_2)A_3(\tau_3)}\}_\beta. \end{aligned} \tag{8}$$

Since we want the functional definition of $\{\cdots\}_\beta$ to be independent of the number of variables, (8) should reduce to the definition, (7), if one of the variables is deleted. Thus, for example, if we delete $A_1(\tau_1)$, we get

$$\begin{aligned}\{A_1(\tau_1)A_2(\tau_2)A_3(\tau_3)\}_\beta &= C_1\, T[A_1(\tau_1)A_2(\tau_2)A_3(\tau_3)] \\ &+ C_4 A_1(\tau_1)\{\overbrace{A_2(\tau_2)A_3(\tau_3)}\}_\beta, \end{aligned} \tag{9}$$

which shows that $C_1 = -C_4 = 1$. From symmetry, it follows therefore that

$$\begin{aligned}\{A_1(\tau_1)A_2(\tau_2)A_3(\tau_3)\}_\beta &= T[A_1(\tau_1)A_2(\tau_2)A_3(\tau_3)] \\ &- \{\overbrace{A_1(\tau_1)A_2(\tau_2)}A_3(\tau_3)\}_\beta - \{\overbrace{A_1(\tau_1)A_2(\tau_2)A_3(\tau_3)}\}_\beta \\ &- \{A_1(\tau_1)\overbrace{A_2(\tau_2)A_3(\tau_3)}\}_\beta, \end{aligned} \tag{10}$$

where $\{\overbrace{A_1(\tau_1)A_2(\tau_2)A_3(\tau_3)}\}_\beta$ etc. are compact symbols for $\{\overbrace{A_1(\tau_1)A_3(\tau_2)A_2(\tau_3)}\}_\beta$. It is easily verified that the thermal trace of $\{A_1(\tau_1)A_2(\tau_2)A_3(\tau_3)\}_\beta$ is zero.

This procedure can be followed for any number of operators, and we may write (Sanyal *et al* 1992, 1993)

$$\{A_1(\tau_1)A_2(\tau_2)\dots A_n(\tau_n)\}_\beta = T[A_1(\tau_1)A_2(\tau_2)\dots A_n(\tau_n)] - \Big[\{\overbrace{A_1(\tau_1)A_2(\tau_2)}A_3(\tau_3)\dots A_n(\tau_n)\}_\beta + \text{all other single contractions}\Big] - \Big[\{A_1(\tau_1)A_2(\tau_2)A_3(\tau_3)A_n(\tau_n)\dots\}_\beta + \text{all other double contractions}\Big] - \text{all possible other multiple contractions.} \tag{11}$$

Equation (11) is the thermal Wick expansion for n boson operators.

For proving the analogous theorem for fermion operators (denoted by C_i), we first show that the anticommuting property of fermion variables under the T-symbol may be simulated faithfully by the following mapping:

$$C_i(\tau_i) \leftrightarrow \gamma_i A_i(\tau_i) \tag{12a}$$

$$C_i^\dagger(\tau_i) \leftrightarrow \gamma_i^* A_i^\dagger(\tau_i), \tag{12b}$$

where $A_i/A_i^\dagger$ are boson operators and γ_i and γ_i^* are the Grassmann numbers which are taken from a set of even number of Grassmann numbers. All Grassmann numbers anticommute (Berezin 1966) among themselves and we take them to commute with the bosonic operators in (12):

$$\gamma_i\gamma_j = -\gamma_j\gamma_i \forall_{i,j} \tag{13}$$

We have arbitrarily assigned one particular $\gamma_j (j \neq i)$ for each i as the conjugate γ_i^*; this is possible since by choice the total number of Grassmann numbers is even.

$$\ll T[C_i(\tau_i)C_j(\tau_j)] \gg \leftrightarrow \vartheta(\tau_i - \tau_j)\gamma_i\gamma_j A_i(\tau_i)A_j(\tau_j) - \vartheta(\tau_j - \tau_i)\gamma_j\gamma_i A_j(\tau_j)A_i(\tau_i) = \gamma_i\gamma_j\, T[A_i(\tau_i)A_j(\tau_j)]. \tag{14}$$

From the anticommuting properties of C_is under a T-symbol and γ_is, we then find

$$T[C_j(\tau_j)C_i(\tau_i)] \leftrightarrow \gamma_j\gamma_i\, T[A_j(\tau_j)A_i(\tau_i)] = -\gamma_i\gamma_j\, T[A_i(\tau_i)A_j(\tau_j)] = -\,T[C_i(\tau_i)C_j(\tau_j)]. \tag{15}$$

Hence, we may write for $T[C_1(\tau_1)\dots C_n(\tau_n)]$, the mapped expression

$$T[C_1(\tau_1)\dots C_n(\tau_n)] = \gamma_1\dots\gamma_n\, T[A_1(\tau_1)\dots A_n(\tau_n)]. \tag{16}$$

If we now write the T-product of the bosons in terms of thermal normal products and introduce the symbols

$$\{\overbrace{C_1(\tau_1)C_2(\tau_2)C_3(\tau_3)}\}_\beta = \gamma_1\gamma_2\gamma_3\{\overbrace{A_1(\tau_1)A_2(\tau_2)A_3(\tau_3)}\}_\beta \tag{17}$$

and the analogous ones for multiple contractions, then it follows that

$$\begin{aligned}\{C_1(\tau_1)C_2(\tau_2)\dots C_n(\tau_n)\}_\beta = {} & T[C_1(\tau_1)C_2(\tau_2)\dots C_n(\tau_n)] \\ & - \Big[\{\overbrace{C_1(\tau_1)C_2(\tau_2)C_3(\tau_3)}\}_\beta + \text{all other single contractions}\Big] \\ & - \Big[\{\overbrace{C_1(\tau_1)\overbrace{C_2(\tau_2)\overbrace{C_3(\tau_3)\overbrace{C_n(\tau_n)\dots}}}}\}_\beta + \text{all other} \\ & \qquad \text{double contractions}\Big] - \text{all the rest of other multiple} \\ & \qquad\qquad \text{contractions.}\end{aligned} \tag{18}$$

Clearly, the Matsubara formula for fermions *with the correct phases* follows from (18), since the only nonvanishing terms in the thermal trace of a T-product would be the set of completely contracted terms. The phases are taken care of by signs generated by the Grassmann numbers used in the definitions (17), above and the like. A zero-temperature analogue of the thermal Wick expansion may be obtained by setting the variables $\tau_1,\dots,\tau_n$ as $\tau_n = 0$, $\tau_n = \varepsilon$, $\tau_{n-2} = 2\varepsilon$, etc, and let $\varepsilon \to 0_+$.

$$\{D_1 D_2 \cdots D_n\}_\beta = D_1 D_2 \cdots D_n - \text{all posible contractions,} \tag{19}$$

where the D_is are either Bose or Fermi operators. The contractions $\{\overline{D_i D_j}\}_\beta$ are defined as

$$\{\overbrace{D_i D_j}\}_\beta = \ll D_i D_j \gg. \tag{20}$$

Equations (11), (18) and (19) are the central building blocks of our thermal field theory, and they would replace the zero-temperature Wick's expansion in all of our subsequent developments.

3. Optimal thermal mean-field formulations: Thermal Brillouin and Brückner conditions

3.1 *Preliminaries*

The grand partition function Z for any interacting many-particle system is central to any statistical mechanical description at a finite temperature $1/\beta$:

$$Z = \mathrm{Tr}\exp[-\beta(H-\mu N)] \equiv \mathrm{Tr}\exp(-\beta K), \tag{21}$$

where μ is the chemical potential for the system.

Z is a multiplicatively separable quantity since the operator $\exp(-\beta K)$ is a multiplicatively separable operator. Two important extensive (i.e. additively separable)

properties of the system are thermally averaged energy $E = \ll H \gg$ and the free energy F, defined by

$$\mu \ll N \gg - \frac{\partial \ln Z}{\partial \beta} = E \tag{22}$$

$$-\frac{\ln Z}{\beta} = F. \tag{23}$$

In actual applications, it is seldom possible to exactly compute the trace of $\exp(-\beta K)$. What is feasible (and what is usually done) is to partition H into H_0 (of the type shown in (2)) and a "perturbation" V, and compute Z in terms of thermal traces with respect to the unperturbed Hamiltonian H_0. Thus, for example, we may write $\exp(-\beta K)$ as (Matsubara 1955)

$$\exp(-\beta K) = \exp(-\beta K_0)\, T\left[\exp\left(\int_0^\beta - V_I(\tau)\mathrm{d}\tau\right)\right], \tag{24}$$

where

$$K_0 = H_0 - \mu N \tag{25}$$

$$V_I(\tau) = \exp(\tau K_0)\, V \exp(-\tau K_0) \tag{25b}$$

and get

$$Z/Z_0 = \mathrm{Tr}\left[\exp[-\beta K_0]\, T\left[\exp\left(\int_0^\beta - V_I(\tau)\mathrm{d}\tau\right)\right] \Big/ \mathrm{Tr}\exp[-\beta K_0]\right]$$

$$\equiv \ll T\left[\exp\left(\int_0^\beta - V_I(\tau)\mathrm{d}\tau\right)\right] \gg. \tag{26}$$

Using our thermal Wick's expansion, It is possible in principle to compute the right-hand side of (26) to any desired order in perturbation theory. However, just as in the Dyson expansion of a unitary operator where the unitarity is lost under a truncation of the series, the multiplicative separability of Z/Z_0 is lost under a truncation of the series in (26). To obviate this difficulty, one introduces the extensive quantity called the cumulant (Kubo 1957, 1962) in the thermodynamic perturbation theories (Bloch and de Dominicis 1958; Balian and de Dominicis 1960; Balian *et al* 1960)

$$Z/Z_0 = \exp(C), \tag{27}$$

where the cumulant C is written as a perturbation series

$$C = C_1 + C_2 + C_3 + \ldots \tag{28}$$

By expanding Z/Z_0 orderwise in both (26) and (28), and comparing like-powers in V_I, C_ns can be recursively generated. A nonperturbative access to C is achieved in our thermal cluster cumulant theory (Sanyal *et al* 1992, 1993). In either case, the strategy is to truncate the T-ordered exponential in (26) in an appropriate manner – but perform the thermal trace exactly, involving the Boltzmann factor $\exp(-\beta K_0)$. The latter is most easily achieved in terms of the eigenfunctions of H_0. The lowest energy eigenfunction $|\phi\rangle$ of H_0 defines the mean-field function. The optimal choice

of H_0 is not unique: we may, e.g., demand H_0 to be so chosen that $E = \ll H \gg$ has the lowest value. Or, alternatively, one may impose some optimal conditions on Z/Z_0 in the sense of providing the ratio of minimum magnitude.

We should mention here that there was an earlier coupled cluster inspired formulation for the calculation of partition function (Altenbokum *et al* 1987), which required an explicit knowledge of the spectra of H. Our method is more natural and more compact, and is direct in the sense of not requiring an explicit knowledge of the spectrum of H.

3.2 *The thermal Brillouin condition: Optimal choice for average energy*

We shall derive now the conditions for generating the optimal $|\phi\rangle$ for providing the lowest value of $\ll H \gg$. This will lead to the thermal Hartree (Hartree–Fock) function $|\phi\rangle$ for bosons (fermions). The interesting aspect of our derivation is the demonstration that if we minimize the mean-field value F_0 for the free energy, it follows automatically that $\ll H \gg$ is minimized with respect to the parameters of variation, for fixed average orbital occupancies.

Let us take $\mathbf{a}/\mathbf{a}^\dagger$ to be the set of destruction/creation operators for the system. To find out the optimal $|\phi\rangle$, we start out with a trial $|\phi_t\rangle$ – defined with respect to $\mathbf{a}/\mathbf{a}^\dagger$ and some trial parameters – and induce a unitary transformation on the set $\mathbf{a}/\mathbf{a}^\dagger$:

$$\mathbf{a} \to \mathbf{b} = u^\dagger \mathbf{a} u, \tag{29a}$$

$$\mathbf{a}^\dagger \to \mathbf{b}^\dagger = u^\dagger \mathbf{a}^\dagger u, \tag{29b}$$

$$|\phi_t\rangle \to u^\dagger |\phi_t\rangle. \tag{30}$$

$u^\dagger$ induces a transformation on $|\phi_t\rangle$ which keeps its form unchanged but changes its parameters and transforms $\mathbf{a}/\mathbf{a}^\dagger$ to $\mathbf{b}/\mathbf{b}^\dagger$. $H(\mathbf{a}, \mathbf{a}^\dagger)$ can be explicitly written in terms of $\mathbf{b}/\mathbf{b}^\dagger$; using (29),

$$H(\mathbf{a}, \mathbf{a}^\dagger) \equiv H(\mathbf{b}, \mathbf{b}^\dagger). \tag{31}$$

Let us now assume that we take as our new unperturbed ground state the function $u^\dagger|\phi_t\rangle$, with an unperturbed K_0^t, and rewrite $H(b, b^\dagger)$ in thermal normal order with respect to this unperturbed description. The general form of this transcription is given by

$$H(\mathbf{b}, \mathbf{b}^\dagger) = \ll H \gg + \sum_k \epsilon_k \{b_k^\dagger b_k\}_\beta + V_\beta, \tag{32}$$

where $\ll H \gg$ is computed as

$$\ll H \gg \equiv \frac{\mathrm{Tr}\exp(-\beta K_0^t) H}{\mathrm{Tr}\exp(-\beta K_0^t)} \tag{33}$$

with

$$K_0^t = \{H_0\}_\beta + \ll H \gg - \mu N. \tag{34}$$

The values of the contractions $n_k = \{\overbrace{b_k^\dagger b_k}\}_\beta$ are given by

$$n_k = [\exp(\beta(\epsilon_k - \mu)) \pm 1]^{-1} \tag{35}$$

for fermions (bosons). μ should be determined from the condition that $\ll N \gg$ has a fixed assigned value $\bar{N}$.

We now define the mean-field free energy F_0 by

$$F_0 = -\frac{1}{\beta}\ln(Z_0), \tag{36}$$

where Z_0 is given by

$$Z_0 = \mathrm{Tr}\exp(-\beta K_0'). \tag{37}$$

It can be shown by straightforward computation that F_0 is explicitly given by

$$F_0 = \ll H \gg + \frac{1}{\beta}\left[\sum_k n_k \ln n_k \pm (1 \mp n_k)\ln(1 \mp n_k)\right] - \mu\sum_k n_k \tag{38}$$

with upper (lower) signs for fermions (bosons).

The variation in F_0 is induced by the variations induced by $u^\dagger$ in $u^\dagger|\phi_t\rangle$, and affects (38) in two ways: (i) the parameters describing $|\phi_t\rangle$ change, thus affecting the expression of H; (ii) the values of ε_ks change as a result of the variations and this changes the contributions from n_k. We shall take account of both these types of changes below while varying F_0.

The precise form for $u^\dagger$ depends on the form of the function $|\phi_t\rangle$. For fermions, $|\phi_t\rangle$ is a single Slater determinant, so that $u^\dagger \sim \exp[\Sigma_{\alpha p} t_{\alpha p}(a_p^\dagger a_\alpha - a_\alpha^\dagger a_p)]$, where $\{\alpha\}$ and $\{p\}$ are the holes and particles defined with respect to $|\phi_t\rangle$. This is Thouless's way of parametrizing a Slater determinant (Thouless 1960). For bosons, $|\phi_t\rangle$ is generally a product of displaced Gaussians, so that $u^\dagger$ is of the form

$$u^\dagger \sim \exp\left[\sum_k s_k(a_k^\dagger - a_k) + \frac{t_k}{2}(a_k^{\dagger 2} - a_k^2)\right].$$

Generically, we may write $u^\dagger \sim \exp[\Sigma t_i(e_i^\dagger - e_i)]$, where t_is are real and e_is are those products of creation/annihilation operators which are needed to parametrize $|\phi_t\rangle$.

The variation of F_0 can now be written as

$$\delta F_0 = \sum_i \left.\frac{\partial F_0}{\partial t_i}\right|_{\mathbf{n}} \delta t_i + \sum_k \frac{\partial F_0}{\partial n_k}\delta n_k. \tag{39}$$

The first term of the right of (39) indicates the variation of F_0 keeping the sets $\{n_k\}$ fixed.

Using (35) and (38), we find

$$\delta F_0 = \sum_i \left.\frac{\partial \ll H \gg}{\partial t_i}\right|_{\mathbf{n}} \delta t_i + \sum_i \left[\frac{\partial \ll H \gg}{\partial n_k} - \mu\right]\delta n_k - \sum_k (\varepsilon_k - \mu)\delta n_k. \tag{40}$$

When rewriting $H(\mathbf{b}, \mathbf{b}^\dagger)$ in thermal normal order, we generate thermal contractions involving n_ks. $\ll H \gg$ is the fully contracted term; $\{H_0\}_\beta$ has one contraction less than in $\ll H \gg$, since $\{H_0\}_\beta$ is a one-body operator, containing $\Sigma_k \varepsilon_k \{b_k^\dagger b_k\}_\beta$.

From (32), it then follows that

$$\frac{\partial \ll H \gg}{\partial n_k} = \varepsilon_k. \tag{41}$$

We thus obtain from (41) the important relation

$$\delta F_0 = \sum_i \left.\frac{\partial \ll H \gg}{\partial t_i}\right|_{\mathbf{n}} \delta t_i. \tag{42}$$

The minimizing condition for F_0 with respect to the parameters t_i then take the form

$$\partial F_0 = 0 \equiv \left.\frac{\partial \ll H \gg}{\partial t_i}\right|_{n}. \tag{43}$$

We have thus shown that the best mean-field description of F_0 leads to the best mean-field description of $\ll H \gg$, keeping $\mathbf{n}$ fixed at values defined for these t_is.

Let us now find out the explicit minimizing condition for $\ll H \gg$. For this, let us assume that the nth unperturbed state $|n_t\rangle$ is generated from $|\phi_t\rangle$ by the action of suitable excitation operator $Y_n^\dagger$:

$$|n_t\rangle = Y_n^\dagger |\phi_t\rangle. \tag{44}$$

$\ll H \gg$ is given by

$$\ll H \gg = \frac{\mathrm{Tr}\exp(-\beta K_0)H}{\mathrm{Tr}\exp(-\beta K_0)} = \frac{\sum_n \exp(-\beta \bar{E}_n^0)\langle \phi_t | Y_n u H u^\dagger Y_n^\dagger | \phi_n \rangle}{\sum_n \exp(-\beta \bar{E}_n^0)\langle \phi_t | Y_n Y_n^\dagger | \phi_t \rangle}, \tag{45}$$

where $\bar{E}_n^0 = E_n^0 - \mu \langle n_t | N | n_t \rangle$, with E_n^0 as the unperturbed energy for $|n_t\rangle$. For optimal choice of the parameters, $\mathbf{a} \equiv \mathbf{b}$, $|\phi_t\rangle$ is the desired $|\phi\rangle$, and the first-order variation of (45) should be zero with respect to the parameters. We find

$$\begin{aligned}
\sum_i \left.\frac{\partial \ll H \gg}{\partial t_i}\right|_{\mathbf{n}} \delta t_i = {} & \frac{\sum_n \exp(-\beta \bar{E}_n^0)\langle \phi_t | Y_n \sum_i \delta t_i (e_i - e_i^\dagger) H Y_n^\dagger | \phi_t \rangle}{\sum_n \exp(-\beta \bar{E}_n^0)\langle \phi_t | Y_n Y_n^\dagger | \phi_t \rangle} + \text{h.c.} \\
& - \frac{\ll H \gg \sum_n \exp(-\beta \bar{E}_n^0)\langle \phi_t | Y_n \sum_i \delta t_i (e_i - e_i^\dagger) Y_n^\dagger | \phi_t \rangle}{\sum_n \exp(-\beta \bar{E}_n^0)\langle \phi_t | Y_n Y_n^\dagger | \phi_t \rangle} + \text{h.c.} \\
\equiv {} & \sum_i [\ll (e_i - e_i^\dagger) H \gg \delta t_i + \text{h.c.}] \\
& - \left[\ll H \gg \sum_i \ll e_i - e_i^\dagger) \gg \delta t_i + \text{h.c.} \right].
\end{aligned} \tag{46}$$

The elements $e_i/e_i^\dagger$ are products of suitable creation/annihilation operators and have no common indices in the products. They may thus be taken to be in thermal normal order. Thus $\ll e_i \gg$ etc. are all zero. We thus find that the thermal mean-field conditions are equivalent to

$$\ll e_i H \gg = \ll H e_i^\dagger \gg = 0 \tag{47}$$

for all e_i needed to parameterize $|\phi_t\rangle$. For this to be satisfied, H obviously cannot have terms in it having $e_i/e_i^\dagger$.

If we write H in thermal normal order in long hand as

$$H = \ll H \gg + \sum_k \varepsilon_k \{b_k^\dagger b_k\}_\beta + \sum_j h_j e_j, \tag{48}$$

where e_js are the various generators contributing to V_β, then we infer from (47) that the best mean-field condition (in the sense of energy) is given by

$$h_i = h_i^\dagger = 0, \forall \text{ all } i \text{ needed to parameterize } |\phi_t\rangle. \tag{49}$$

This is the abstract form for the thermal Brillouin conditions.

As concrete illustrations, let us work out the thermal Brillouin conditions for the thermal Hartree–Fock function for fermions and for the thermal Gaussian Hartree function for bosons.

Let us assume that for fermions H is given by

$$H = \sum_{IJ} \langle I|k|J\rangle b_I^\dagger b_J + \frac{1}{2} \sum_{I,J,K,L} \langle IJ|v|KL\rangle b_I^\dagger b_J^\dagger b_L b_K), \tag{50}$$

where $b_I/b_I^\dagger$ are defined with respect to the optimal orbitals. I is a generic index. Writing H in thermal normal order, we have

$$H = \ll H \gg + \sum_{IJ} \langle I|k|J\rangle \{b_I^\dagger b_J\}_\beta + \sum_{I,K} [\langle IK|v|JK\rangle - \langle IK|v|KJ\rangle n_k \{b_I^\dagger J_J\}_\beta$$

$$+ \frac{1}{2} \sum_{I,J,K,L} \langle IJ|v|KL\rangle \{b_I^\dagger b_J^\dagger b_L b_K\}_\beta, \tag{51}$$

where $n_k = \ll b_k^\dagger b_k \gg$. Defining a one-body mean-field Hermitian operator f by the relation

$$\langle I|f|J\rangle = \langle I|k|J\rangle + \sum_k [\langle IK|v|JK\rangle - \langle IK|v|KJ\rangle] n_k, \tag{52}$$

we may write H in thermal normal order as

$$H = \ll H \gg + \sum_{I,J} \langle I|f|J\rangle \{b_I^\dagger b_J\}_\beta + \frac{1}{2} \sum_{I,J,K,L} \langle IJ|v|KL\rangle \{b_I^\dagger b_J^\dagger b_L b_K\}_\beta. \tag{53}$$

The products $\{b_I^\dagger b_J\}_\beta$ and $\{b_I^\dagger b_J^\dagger b_L b_K\}_\beta$ are the elements of the type $\{e_j\}_\beta$ introduced in (40). The parameters $\{e_i\}_\beta$ needed to parametrize $|\phi\rangle$ are of the form $\{b_p^\dagger b_\alpha\}_\beta$ with α holes and p particles. Hence the thermal Brillouin condition for Fermions is equivalent to

$$\langle p|f|\alpha\rangle = \langle \alpha|f|p\rangle = 0, \forall \alpha, p. \tag{54}$$

One may impose somewhat more general variational conditions on $|\phi\rangle$ in the finite-temperature case. For the zero-temperature case, operators of the form $b_p^\dagger b_q$ or $b_\beta^\dagger b_\alpha$

for $p=q$, $\alpha=\beta$ give zero contributions when appearing in $\delta u^\dagger|\phi\rangle$. In contrast, for the finite-temperature case, $\delta u^\dagger \Sigma Y_n^\dagger|\phi\rangle$ is generally non-zero for the above operators appearing in $\delta u^\dagger$. We have exclude the $p=q$ or $\alpha=\beta$ choice, since they are not variations in the proper sense. The associated thermal Brillouin conditions then demand

$$\langle p|f|q\rangle = \langle q|f|p\rangle = 0, \forall p \neq q, \tag{55}$$

$$\langle \alpha|f|\beta\rangle = \langle \beta|f|\alpha\rangle = 0, \hbar\alpha \neq \beta. \tag{56}$$

These conditions essentially imply that the thermal Hartree–Fock orbitals diagonalize the operator f. This feature is used in the temperature Green's function formalisms (Feter and Walecka 1971); our derivations provide an alternative rationale for its use from variational arguments.

For the bosonic systems with non-number-conserving interactions, we may induce a Bogolyubov transformation on the creation/annihilation operators to generate the optimal orbitals. As a concrete case, let us take the case of an anharmonic oscillator, with cubic and quartic perturbation:

$$H = a^\dagger a + (1/2) + 2^{-3/2}\gamma(a^\dagger + a)^3 + \lambda/4(a^\dagger + a)^4. \tag{57}$$

The unperturbed frequency is scaled to the value 1. With respect to the vacuum $|0\rangle$ as the ground state of $(a^\dagger a + \frac{1}{2})$, we introduce a transformation

$$|\phi\rangle \sim \exp(sa^\dagger + \tfrac{1}{2}ta^{\dagger 2})|0\rangle \tag{58}$$

to generate a new Gaussian, and introduce new boson operators $b/b^\dagger$ for which $|\phi\rangle$ is vacuum:

$$b = (1-t^2)^{-1/2}(a - t\,a^\dagger - s), \tag{59a}$$

$$b^\dagger = (1-t^2)^{-1/2}(a^\dagger - t\,a - s), \tag{59b}$$

where we restrict ourselves only to the real parametrizations of s, t. We note that s and t are, respectively, related to the shift and width parameter of the Gaussian.

To determine the optimal s and t parameters, we rewrite H in terms of boson variables $b/b^\dagger$ and bring H in thermal normal order. H in this new thermal normal order is given by:

$$\begin{aligned} H = {} & \ll H \gg + (2\omega)^{-1}[\omega^2 + (1 + 6\sqrt{2}\gamma\omega' + 24\lambda\omega'^2) + (6\lambda/\omega)(2n+1)]\{b^\dagger b\}_\beta \\ & + \omega^{-3/2}[(8\lambda\omega)\omega'^3 + (3\sqrt{2}\gamma\omega)\omega'^2 + (\omega + 6\lambda(2n+1))\omega' + (3\gamma/2\sqrt{2})(2n+1)]\{b^\dagger + b\}_\beta \\ & - (2\omega)^{-2}[\omega^3 - (1 + 6\sqrt{2}\gamma\omega' + 24\lambda\omega'^2)\omega - 6\lambda(2n+1)]\{b^{\dagger 2} + b^2\}_\beta \\ & + [(\gamma/(2\omega)^{3/2}) + (4\sqrt{22}\lambda\omega'/(2\omega)^{3/2})]\{b^{\dagger 3} + b^3 + 3b^{\dagger 2}b + 3b^\dagger b^2\}_\beta \\ & + (\lambda/(2\omega)^2)\{b^{\dagger 4} + b^4 + 4b^{\dagger 3}b + 4b^\dagger b^3 + 6b^{\dagger 2}b^2\}_\beta, \end{aligned} \tag{60}$$

where

$$\omega = (1-t)/(1+t) \text{ and } \omega' = s/(1-t)$$

$$n = \ll b^\dagger b \gg = 1/[\exp(\beta\omega) - 1].$$

$\ll H \gg$ is given by

$$\ll H \gg = \tfrac{1}{2} + ((1+\omega^2)/2\omega)n + [(3\gamma\omega'/\sqrt{2\omega}) + (6\lambda\omega'^2/\omega)(2n+1) + (3\lambda/\omega^2)n(n+1) + (3\lambda/4\omega^2) + (1-\omega)^2/4\omega + \omega^2 + 2\sqrt{2\gamma\omega^3} + 4\lambda\omega'. \tag{61}$$

From (61), the minimizing conditions for $\ll H \gg$ with respect to ω and ω' (equivalently s and t), for fixed n, are:

$$\omega^3 - (1 + 6\sqrt{2\gamma\omega'} + 24\lambda\omega'^2)\omega - 6\lambda(2n+1) = 0, \tag{62a}$$

$$(8\lambda\omega)\omega'^3 + (3\sqrt{2\gamma\omega})\omega'^2 + [\omega + 6\lambda(2n+1)]\omega' + (3\lambda/2\sqrt{2})(2n+1) = 0 \tag{62b}$$

Using these conditions, H gets simplified to

$$H = \ll H \gg + \omega\{b^\dagger b\}_\beta + \eta\{b^{\dagger 3}/3! + b^3/3! + b^{\dagger 2}b/2! + b^\dagger b^2/2!\}_\beta + \alpha\{b^{\dagger 4}/4! + b^4/4! + b^{\dagger 3}b/3! + b^\dagger b^3/3! + b^{\dagger 2}b^2/2!2!\}_\beta, \tag{63}$$

where $\eta = [\gamma + 4\sqrt{2\lambda\omega'}]\ ((6/2\omega)^{3/2})$ and $\alpha = 6\lambda/\omega^2$ (Sanyal *et al* 1993).

We note that we have no terms containing $b^\dagger, b, b^{\dagger 2}$ and b^2 in the thermally normal ordered expression with respect to the thermal Hartree function $|\phi\rangle$. This is the boson equivalent of (49). Also, the same Hamiltonian is obtained if we equate the coefficients of $b^\dagger, b, b^{\dagger 2}$ and b^2 of H in (60) to zero, since $b^\dagger$ and $b^{\dagger 2}$ are needed to parametrize the shifted Gaussians. The consistency of the thermal Brillouin condition is thus verified.

3.3 *The thermal Bruckner condition*

We recall from §2·1 that Z/Z_0 is given by

$$Z/Z_0 = \ll T\left[\exp - \int_0^\beta V_I(\tau)\mathrm{d}\tau\right] \gg.$$

Let us now try to find out an optimal $|\phi\rangle$ in such a way that Z_0 is closest to the value Z. From Gibbs' Bogolyubov inequality (Feynman 1972), we know that

$$Z \geqslant Tr \exp(-\beta \bar{H}_0)\exp(-\beta \ll V \gg). \tag{64}$$

Since in our formulation of thermal field theory, V is in thermal normal order, $\ll V \gg = 0$. Hence

$$Z/Z_0 \geqslant 1 \tag{65}$$

Thus if we minimize Z/Z_0 for describing an optimal $|\phi\rangle$, we would obtain a function which is optimal in the sense of providing the mean-field free energy that is closest to the exact free energy.

We may write a compact non-perturbative representation of Z/Z_0 using our cluster cumulant theory (Sanyal *et al* 1992, 1993). If we expand $T[\exp(-\int_0^\beta V_I(\tau)\mathrm{d}\tau)]$ in thermal normal order and collect all the connected operators together, then the entire

expression can be regrouped again as a thermally normal-ordered product of a connected entity (Sanyal *et al* 1992, 1993)

$$T\left[\exp-\int_0^\beta V_{\rm I}(\tau)\mathrm{d}\tau\right]=\{\exp(S_{\rm I}(\beta)+X_{\rm I}(\beta))\}_\beta, \tag{66}$$

where $S_{\rm I}(\beta)$ contains operators which excite or de-excite and $X_{\rm I}(\beta)$ contains diagonal operators. Differential equations for directly determining $S_{\rm I}(\beta)$ and $X_{\rm I}(\beta)$ can be written down; they are the working equations for the thermal cluster cumulant theory.

Z/Z_0 is given by the zero-body component X_1^0 of $X_{\rm I}$:

$$Z/Z_0=\exp(X_1^0) \tag{67}$$

since only the zero-body part of the T-ordered exponential survives in Z/Z_0.

For our purpose, it is sufficient to note that $S_{\rm I}(\beta)$ and $X_{\rm I}(\beta)$ can be expressed as

$$S_{\rm I}(\beta)=\sum_{j\in nd} s_j\{e_j\}_\beta \tag{68}$$

$$X_{\rm I}(\beta)=\sum_{j\in d} x_j\{e_j\}_\beta, \tag{68b}$$

where *nd* and *d* denote non-diagonal and diagonal components of a Lie algebra, generated by the elements of Lie algebra of H.

The first-order variation of Z/Z_0 is given by

$$\delta(Z/Z_0)=\sum_i \delta t_i[\ll(e_i-e_i^\dagger)_\beta\{\exp(S_{\rm I}(\beta)+X_{\rm I}(\beta))\}_\beta\gg - (Z/Z_0)\ll(e_i-e_i^\dagger)_\beta\gg]. \tag{69}$$

Using (68), and noting that $e_i/e_i^\dagger$ are non-diagonal by construction, we have

$$\delta(Z/Z_0)=\sum_i \delta t_i[\ll\{\overbrace{e_i e_j^\dagger}\}_\beta\gg s_i^\dagger-\ll\{e_i^\dagger e_i\}_\beta\gg s_i]. \tag{70}$$

The minimizing condition for Z/Z_0 is hence given by

$$\delta(Z/Z_0)=0\Rightarrow s_i^\dagger=s_i=0. \tag{71}$$

In analogy with the zero-temperature formalism, we may call this relation a thermal Brückner condition.

For fermions, the thermal Brückner conditions can be expressed as

$$\langle I|s_1|J\rangle=0,\forall I\neq J, \tag{72}$$

where $\langle I|s_1|J\rangle$ is the coefficient of $\{b_{\rm I}^\dagger b_{\rm I}\}_\beta$ appearing in $S_{\rm I}(\beta)$. For the bosonic Hamiltonian with cubic plus quartic perturbation, we can write $S_{\rm I}(\beta)$ as

$$S_{\rm I}(\beta)=\sum_{k\neq l} S_{k,l}\{b^{\dagger k}b^l\}_\beta \tag{73}$$

and the thermal Brückner conditions take the form

$$s_{1,0} = s_{0,1} = s_{2,0} = s_{0,2} = 0. \tag{74}$$

The maximal overlap condition (Kümmel *et al* 1978) of the zero temperature formalism is replaced here by the minimum ratio condition of Z/Z_0 for the thermal Brückner orbitals. We note that, analogous to the zero-temperature Brückner condition, we cannot determine the Brückner function $|\phi\rangle$ directly. We may, however, find an approximation to it for Z of a given form (i.e. a given choice of $S(\beta)$ and $X(\beta)$).

4. Generalization of thermal Brillouin conditions for models beyond mean-field description

4.1 *Preliminaries*

As we have emphasized in § 3, our approach to evaluate Z/Z_0 has been to truncate the T-ordered exponential $T[\exp(-\int_0^\beta V_I(\tau)d\tau)]$, followed by the exact evaluation of the thermal trace involving the eigenfunctions of H_0. In the next step of the hierarchy, we may envisage using correlated functions for evaluating the trace. This will presumably rectify the defects in the description of Z entailed in the truncation of the T-ordered exponential. Use of optimal parameters in the correlated description of the ground state would lead to higher-body thermal Brillouin conditions – in a way analogous to the zero-temperature conditions (Kutzelnigg 1979, 1980).

We shall generate correlated functions using the unitary cluster ansatz of the coupled-cluster theory (Kutzelnigg 1977, 1992; Bartlett and Noga 1988). Denoting the functions $|\phi_t\rangle$ and $Y_n^\dagger|\phi_t\rangle$ generically as $|n_t\rangle$ ($|0_t\rangle \equiv |\phi_t\rangle$), we may introduce correlated functions $e^{\sigma_t}|n_t\rangle$ for the evaluation of the thermal trace. e^{σ_t} is a unitary cluster operator. The ground-state function $|\psi_{gr}\rangle$ is parametrized by $e^{\sigma_t}|\phi_t\rangle$. For a general function $|\psi_{gr}\rangle$, the operators defining the σ_t (the various m-hole, m-particle excitations) do not form a closed Lie-algebra of finite dimension, unlike for the mean-field parametrization. As a result, a straightforward generalization for the correlated trace is not very illuminating. We instead use an alternative strategy where we use a transformed mean field (correlated mean field is more picturesque though slightly misnomeric) to establish the group closure property.

4.2 *Modified trace formula with correlated basis and the associated variational conditions*

The partition function Z using the correlated basis is given by

$$Z = \sum_n \langle n_t|\exp(-\sigma_t)\exp(-\beta K)\exp(\sigma_t)|n_t\rangle. \tag{75}$$

Introducing the dressed Hamiltonian L_t and the operator $\bar{L}_t$ via

$$L_t = \exp(-\sigma_t)H\exp(\sigma_t); \quad \bar{L}_t = \exp(-\sigma_t)H\exp(\sigma_t), \tag{76}$$

we may rewrite Z as

$$Z = \sum_n \langle n_t | \exp(-\beta L_t) | n_t \rangle. \tag{77}$$

If we now partition L_t into a zero-body plus a one-body part, denoted L_t^0, and the rest as $\tilde{V}_t$, then we can rewrite Z as

$$Z = \sum_n \langle n_t | \exp(-\beta L_t^0)\, T\left[\exp\left\{-\int_0^\beta \tilde{V}_I(\tau)\mathrm{d}\tau\right\}\right] | n_t \rangle. \tag{78}$$

If we introduce a correlated mean field-value $\tilde{Z}_0^t$ defined as

$$\tilde{Z}_0^t = \sum_n \langle n_t | \exp(-\beta L_t^0) | n_t \rangle, \tag{79}$$

then we have

$$\begin{aligned} Z/\tilde{Z}_0^t = & \left\{\sum_n \langle n_t | \exp(-\beta L_t^0)\, T\left[\exp - \int_0^\beta \tilde{V}_I(\tau)\mathrm{d}\tau\right] | n_t \rangle\right\} \Big/ \left\{\sum_n \langle n_t | \exp(-\beta L_t^0) | n_t \rangle\right\} \\ = & \left\langle\left\langle T\left[\exp - \int_0^\beta \tilde{V}_I(\tau)\mathrm{d}\tau\right]\right\rangle\right\rangle \sigma_t. \end{aligned} \tag{80}$$

Equation (80) indicates that it is fruitful to introduce thermal traces $\ll A \gg_{\sigma_t}$ with correlated basis as

$$\ll A \gg_{\sigma_t} = \sum_n \langle n_t | \exp(-\beta L_t^0) A | n_t \rangle / \sum_n \langle n_t | \exp(-\beta L_t^0) | n_t \rangle. \tag{81}$$

The unknown parameters in evaluating (81) are the orbitals and the parameters of σ_t. Since in (80) and (81) we still have uncorrelated basis $|n_t\rangle$, the group property of the generators defining $|\phi_t\rangle$ can still be properly utilized.

For choosing the optimal $|\phi_t\rangle$ as well as σ_t in the sense of generating the best average energy $\ll H \gg$ leads to the generalization of the mean-field thermal Brillouin conditions. We have

$$\begin{aligned} \ll H \gg &= \sum_n \langle n_t | \exp(-\sigma_t) \exp(-\beta H) H \exp(\sigma_t) | n_t \rangle \\ &\equiv \sum_n \langle n_t | \exp(-\beta L_t)\, L_t | n_t \rangle \\ &= \sum_n | n_t | \exp(-\beta L_t^0)\, T\left[\exp - \int_0^\beta \tilde{V}_I(\tau)\mathrm{d}\tau\right] L_t | n_t \rangle. \end{aligned} \tag{82}$$

In analogy with the mean-field thermal trace, we define $\ll L_t \gg_{\sigma_t}$ as

$$\ll L_t \gg_{\sigma_t} = \sum_n \langle n_t | \exp(-\beta L_t^0)\, L_t | n_t \rangle. \tag{83}$$

Since by choice L_t^0 is a constant plus a sum of one-body operators, the Matsubara formula for the trace would hold good even in (83). Thus it would be convenient to rewrite L_t^0 as well as L_t in thermal normal order. In exact analogy with the optimal mean-field description, the variation of $\ll L_t \gg$ with respect to the orbitals for fixed n_ks leads to (cf (36))

$$\delta \ll L_t \gg_{\sigma_t} = \sum_i \ll (e_i - e_i^\dagger)[L_t] \gg \delta t_i - \ll L_t \gg \sum_i (e_i - e_i^\dagger) \gg \delta t_i + \text{h.c.} \tag{84}$$

We now express L_t in thermal normal order as

$$L_t = \sum_j l_j \{e_j\}_\beta. \tag{85}$$

Then the optimality of $|\phi\rangle$ leads to the following condition (cf (62)),

$$\delta \ll L_t \gg_\sigma \equiv 0 = \sum_i [\ll \{e_i e_i^\dagger\}_\sigma \gg l_i^\dagger - \ll \{e_i^\dagger e_i\}_\beta \gg l_i], \tag{86}$$

leading to the thermal Brillouin condition for the matrix elements of the effective operator L_t:

$$l_i^\dagger = l_i = 0, \quad \forall i \text{ needed to parametrize } |\phi\rangle. \tag{87}$$

Obviously, we cannot use (87) above the obtain $l_i^\dagger$ or l_i, since they involve cluster amplitudes σ. If we write $\ll L_t \gg_{\sigma_t}$ as

$$\ll L_t \gg_{\sigma_t} = \left\{ \sum_n \langle n_t | \exp(-\beta \varepsilon_n^0)\, L_t | n_t \rangle \right\} \Big/ \left\{ \sum_n \langle n_t | \exp(-\beta \varepsilon_n^0) | n_t \rangle \right\} \tag{88}$$

with ε_t^0 as the eigenvalues of the operator L_t^0 for the functions $|n_t\rangle$, then the variation of $\ll L_t \gg_{\sigma_t}$ with respect to σ_t for fixed n_ks can be written as

$$\begin{aligned} \delta_{\sigma_t} \ll L_t \gg_{\sigma_t} &= \left\{ \sum_n \langle n_t | \exp(-\beta \varepsilon_n^0) \delta [\exp(-\sigma_t) H \exp(\sigma_t)] | n_t \rangle \right\} \Big/ \tilde{Z}_0^t \\ &\equiv \sum_n \langle n_t | \exp(-\beta \varepsilon_n^0) \delta \sigma_t\, L_t | n_t \rangle / \tilde{Z}_0^t. \end{aligned} \tag{89}$$

If we write the variation $\delta \sigma_t$ as

$\delta \sigma_t = \sum_j \delta r_j (e_j - e_j^\dagger)$, then the optimality of σ leads to

$$l_j^\dagger = l_j = 0, \quad \forall j \text{ used to define } \sigma. \tag{90}$$

These are the analogues of the thermal Brillouin conditions going beyond the mean-field description.

5. "Local" thermal Brillouin and Brückner conditions in the path-integral-based thermal many-body theories

5.1 *Basic preliminaries*

In the path-integral approach to the evaluation of the partition function, a very widely adopted strategy is to use an auxiliary potential *which depends on each point on the path* and choose it in some optimal sense to expedite the convergence of the perturbative expansion of the partition function (Feynman and Kleinert 1986; Giachetti and Tognetti 1986; Lee *et al* 1991). We have recently extended this method (Mandal *et al*, to be published) to formulate a non-perturbative theory via a generalized version of the thermal cluster cumulant methodology. This method requires for its performance the concept of new forms of normal ordering and Wick's expansion *that depend on the choice of the measure used in the path-integral description.* This concept is, however, of quite general validity and may be used to advantage for defining optimal local potentials defined by certain local analogues of thermal Brillouin and Brückner conditions.

In the next subsection, we give a succinct summary of the basic expressions of the path-integral approach to partition function – emphasizing only those aspects which are of direct relevance to us.

5.2 *Path-integral formulation of Z: A brief resume*

We shall specialize our discussion to bosons only, and for the sake of simplicity we present expressions for the one-dimensional case only. The many-dimensional generalization is straightforward, but computationally demanding.

Following the classic derivation of Feynman (Feynman and Hibbs 1965), the partition function Z for interacting Bosonic system is given by

$$Z = \oint D[x] \exp\left(- \int_0^\beta [(1/2)\dot{x}^2(\tau) + V(x)]\mathrm{d}\tau \right), \tag{91}$$

where we have taken μ be zero. $D(x)$ is the measure for the path-integral and the possible paths are taken to be periodic, with period $\Omega = 2\pi/\beta$. Moreover, the cyclical path-integral symbol denotes that all the cyclical periodic paths have to be considered.

Expanding $x(\tau)$ as a Fourier series with period Ω,

$$x(\tau) = x_0 + \sum_{n \neq 0} (x_n \exp(in\Omega\tau) + \text{h.c.}) \equiv x_0 + y, \tag{92}$$

we may rewrite Z as

$$Z = \int_{-\infty}^{+\infty} \mathrm{d}x_0 \exp(-\beta V(x_0))/(2\pi\beta)^{1/2} \oint D[y] \exp\left(- \int_0^\beta [(1/2)\dot{y}^2 + {}^{V}(x_0 + y) - V(x_0)]\mathrm{d}\tau \right). \tag{93}$$

Expanding $V(x_0 + y)$ as a Taylor series around x_0, we have

$$Z = \int_{-\infty}^{+\infty} dx_0 \exp(-\beta V(x_0))/(2\pi\beta)^{1/2} \oint D[y] \exp\left(-\int_0^\beta\right) \dot{y}^2 + [(1/2)\, W^2(x_0) y^2 + \sum_{m=3}^{\infty} \frac{1}{m!} V^{(m)} y^m] d\tau, \quad (94)$$

where $V^{(m)}$ denotes $\left.\frac{\partial^2 V}{\partial x^m}\right|_{x_0}$ and $W(x_0) = \left.\frac{\partial^2 V}{\partial x^2}\right|_{x_0}$. Since y is periodic in the integral over τ, the linear term in the Taylor expansion gives zero contribution and is hence omitted in (94) above. The Hamiltonian in the integral over τ is that of a harmonic oscillator *with an x_0-dependent frequency $W(x_0)$*, plus an anharmonicity correction. Taking the latter part as a perturbation, a series expansion of Z can be determined. Defining $\xi(x_0)$ and $\xi^0(x_0)$ as

$$\xi(x_0) = \oint D[y] \exp\left(-\int_0^\beta\right) [(1/2)\dot{y}^2 + (1/2)\, W^2(x_0) y^2 + \sum_{m=3}^{\infty} \frac{1}{m!} V^{(m)} y^m] d\tau$$

$$\equiv \oint D[y] \exp\left(-\int_0^\beta\right) H_{x_0}(y) d\tau, \quad (95)$$

$$\xi^0(x_0) = \oint D[y] \exp\left(-\int_0^\beta\right) [(1/2)\dot{y}^2 + (1/2)\, W^2(x_0) y^2] d\tau$$

$$\equiv \oint D[y] \exp\left(-\int_0^\beta\right) H^0_{x_0}(y) d\tau, \quad (96)$$

we can find out $\xi(x_0)$ as a perturbation series involving $\xi^0(x_0)$. We first note that $\xi(x_0)/\xi^0(x_0)$ involves a path-integral involving the following normalized Gaussian weight factor $\tilde{D}[y]$:

$$\tilde{D}[y] \equiv D[y] \exp\left(-\int_0^\beta\right) [1/2]\dot{y}^2 + (1/2)\, W^2(x_0) y^2] d\tau / \xi(x_0) \quad (97a)$$

with

$$\oint \tilde{D}[y] = 1. \quad (97b)$$

Hence, using the property of the Gaussian integrals, any integral of the form $\oint \tilde{D}[y]\, y(\tau_1) \ldots y(\tau_n)$ may be written as a sum over products of pair averages:

$$\ll y(\tau_1) \ldots y(\tau_n) \gg_{\tilde{D}} = \oint \tilde{D}[y]\, y(\tau_1) \ldots y(\tau_n) = \sum_{\substack{i,j \\ \text{pairs}}} \prod \ll y(\tau_i) y(\tau_j) \gg_{\tilde{D}}. \quad (98)$$

Using (98), one may expand the $\Sigma_{m=3}^{\infty}(1/m!)\, V^{(m)} y^m d\tau$ in the expression for $\xi(x_0)/\xi^0(x_0)$ and get the perturbation expansion in terms of the pair averages $\ll y(\tau_i) y(\tau_j) \gg_{\tilde{D}}$. To expedite the convergence of the expansion, one often adds and substracts another quadratic potential $(1/2)\omega' y^2$ and demands that ω' be determined from the condition that $\ll \Sigma_{m=3}^{\infty}(1/m!)\, V^{(m)} y^m d\tau \gg$ be zero. This in a way determines an optimal x_0-dependent potential.

In our path-integral-based cluster cumulant theory (Mandal *et al* 1994), we posit a cluster ansatz for the exponential in $\xi(x_0)$ and define suitable normal ordering and Wick's expansion. We shall show now that we can use these concepts to define intuitively optimal local potential by imposing local thermal Brillouin and Brückner conditions.

5.3 *Normal ordering and Wick's expansion relative to a measure D*

We start out by noting the striking resemblance of (98) with the Matsubara formula, (1). The measure $\tilde{D}[y]$ in (98) replaces the thermal trace in (1). Since no explicit property of thermal trace was ever required in our thermal cluster cumulant theory, except at the end where the values of thermal contractions are needed to evaluate the relevant quantity, we may define in a perfectly analogous manner the following quantities defined with respect to the measure $\tilde{D}$:

$$\{\overbrace{y(\tau_1)y(\tau_2)}\}_{\tilde{D}} \equiv \ll T[y(\tau_1)y(\tau_2)] \gg_{\tilde{D}}, \tag{99}$$

$$\{y(\tau_1)y(\tau_2)\}_{\tilde{D}} = T[y(\tau_1)y(\tau_2)] - \{\overbrace{y(\tau_1)y(\tau_2)}\}_{\tilde{D}}. \tag{100}$$

In (99) and (100) we have exploited the well-known fact that in the expression for path integrals the products $y(\tau_1)y(\tau_2)$ automatically remain time-ordered (Feynman and Hibbs 1965). Equation (99) defines a contraction with respect to the measure $\tilde{D}$, and (100) defines an analogous normal ordering to be called $\tilde{D}$ normal ordering by us (Mandal *et al* 1994). It can then be shown that the following Wick's expansion holds good:

$$\begin{aligned}\{y(\tau_1)\ldots y(\tau_n)\}_{\tilde{D}} = {} & T[y(\tau_1)\ldots y(\tau_n)\} \\ & - [\{\overbrace{y(\tau_1)y(\tau_2)\ldots y(\tau_n)}\}_{\tilde{D}} + \text{all other single contractions}] \\ & - [\{\overbrace{y(\tau_1)\overbrace{y(\tau_2)y(\tau_3)}y(\tau_4)}\ldots\}_{\tilde{D}} + \text{all other double contractions}] \\ & - \text{all other multiple contractions.}\end{aligned} \tag{101}$$

In (101), we have used the symbol $\{\overbrace{y(\tau_1)\overbrace{y(\tau_2)y(\tau_3)}y(\tau_4)}\ldots y(\tau_n)\}_{\tilde{D}}$ to denote $\{\overbrace{y(\tau_1)y(\tau_3)}\}_{\tilde{D}}\{y(\tau_2)\ldots y(\tau_n)\}_{\tilde{D}}$ and its obvious generalizations. Using (101), we can perform not only perturbative expansions of $\xi(x_0)/\xi^0(x_0)$ but also formulate non-perturbative generalizations. Moreover, we can use improved descriptions by defining optimal local potentials.

5.4 *Choice of optimal local potentials: Local thermal Brillouin and thermal Brückner conditions*

Let us define creation annihilation operators $a/a^\dagger$ in (95) and (96) defined via

$$y = \frac{1}{2W[(x_0)]^{1/2}}[a + a^\dagger], \tag{102}$$

$$\dot{y} = \frac{W(x_0)}{i2^{1/2}}[a - a^\dagger]. \tag{103}$$

We should note carefully that $a/a^\dagger$ *depend on* x_0. Hence all the descriptions that follow now *are valid locally*. viz. at the point x_0 on the path. To get an improved description, we induce a Bogolyubov transformation

$$b = (1-t^2)^{-1/2}(a - ta^\dagger) \tag{104a}$$

$$b^\dagger = (1-t^2)^{-1/2}(a^\dagger - ta). \tag{104b}$$

This is very similar to what was done in §3 (viz. (59)), except that we do not need to introduce the shift parameters s for the cyclical variables y. Rewriting the Hamiltonian H_{x_0} in $\xi(x_0)$ in $\tilde{D}$ normal order, the resultant expression for H_{x_0} would define an optimal "local" thermal Hartree choice if the quadratic coefficients of b and $b^\dagger$ are equated to zero. This will lead to the best mean-field descriptions at the point x_0, where the mean-field model is assumed to be a harmonic one. These conditions would determine t. The process of finding them has to be iterative, since the contractions $\{b^\dagger\}_{\tilde{D}}$ etc. would depend on the frequency of the optimized harmonic oscillator. This would then be equivalent of a *local* thermal Brillouin condition. We shall give an illustrative example of this condition by taking the case of the cubic plus quartic oscillator in §5·5.

Making use of the Gibbs–Bogolyubov inequality (Feynman 1972), we find in a manner exactly analogous to what was done in arriving at (60) that

$$\xi(x_0) \geqslant \xi^0(x_0). \tag{105}$$

Hence it is possible to define local thermal Brückner condition by demanding that we take as optimal that mean-field description which minimizes the ratio $\xi(x_0)/\xi^0(x_0)$. This condition requires for its actual implementation a cluster expansion representation of $\xi(x_0)/\xi^0(x_0)$.

Suppose we have expressed H_{x_0} in terms of operators $b/b^\dagger$ with t unspecified yet. By expanding the perturbative part of H_{x_0} as polynomials in y, writing them in $\tilde{D}$ normal order and regrouping them in terms of connected quantities, exactly analogous to what was done leading to (34), we may rewrite $\xi(x_0)/\xi^0(x_0)$ as

$$\xi(x_0)/\xi^0(x_0) = \left\langle\left\langle T\left[\exp - \int_0^\beta \left[\Sigma_{m=3}^{\infty} \frac{1}{m!} V^{(m)} y^m\right] d\tau\right]\right\rangle\right\rangle_{\tilde{D}}$$

$$= \ll \{S(\beta) + X(\beta)]\}_{\tilde{D}} \gg_{\tilde{D}}, \tag{106}$$

where $\{\exp(\cdots)\}_{\tilde{D}}$ is a symbol for $\tilde{D}$ normal-ordered exponential. $S(\beta)$ and $X(\beta)$ can be found out from a set of path-integral-based thermal cluster cumulant equations (Mandal *et al* 1994) $S(\beta)$ is a non-diagonal operator and $X(\beta)$ is a diagonal operator. For an optimal choice of the mean field leading to the minimum value of $\xi(x_0)/\xi^0(x_0)$ we can proceed in a manner exactly analogous to what was done to obtain (64) or (69).

To induce a variation in b and $b^\dagger$ involved in H_{x_0}, needed to define the mean field, we write the associated transformation as

$$b \to u^\dagger b u; \quad b^\dagger \to u^\dagger b^\dagger u \tag{10}$$

$$u^\dagger = e(\alpha/2), \quad (b^{\dagger 2} - b^2) \tag{10}$$

with α as the parameter of the variation. This is the unitary transformation analogou

to (104). The weight $\tilde{D}[y]$ used in $\xi(x_0)/\xi^0(x_0)$ up to the first-order variation gets modified then to

$$\tilde{D}[y] \to \tilde{D}[y]\frac{\alpha}{2}(b^{\dagger 2} - b^2), \tag{109}$$

where α is a first-order infinitesimal.

Hence the average gets modified as

$$\ll A \gg_{\tilde{D}} \to \ll A \gg_{\tilde{D}} + \frac{\alpha}{2} \ll b^{\dagger 2} - b^2) A \gg_{\tilde{D}}. \tag{110}$$

For an interacting bosonic Hamiltonian, we may then write, using (106),

$$\delta[\xi(x_0)/\xi^0(x_0)] = \frac{\alpha}{2} \ll (b^{\dagger 2} - b^2)\{\exp(S + X)\}_{\tilde{D}} \gg_{\tilde{D}}. \tag{111}$$

It then follows that, at the minimum of $\xi(x_0)/\xi^0(x_0)$, the components of S with the quadratic powers of b and $b^\dagger$ should be vanishing. Writing the components of S as $s_{m,n} b^{\dagger m} b^n (m \neq n)$, we then derive

$$s_{2,0} = s_{0,2} = 0. \tag{112}$$

These are the *local analogues* of the thermal Brückner condition for the path-integral-based theories of partition function for interacting bosons. We should remember that this relation would be valid *for each point on the path*, and $S(\beta)$ and $X(\beta)$ are dependent on X_0.

For the sake of completeness, let us mention that both the local Brillouin and Brückner conditions generate a potential dependent on x_0, which is to be used to generate $\xi(x_0)$ and eventually Z:

$$\begin{aligned} \xi(x_0) &= \xi^0(x_0)\left\langle\left\langle T\left[\exp - \int_0^\beta V(y)\mathrm{d}\tau\right]\right\rangle\right\rangle_{\tilde{D}} \\ &\equiv \exp[-\beta u(x_0)], \end{aligned} \tag{113}$$

which leads to

$$Z = \int_{-\infty}^{+\infty} \mathrm{d}x_0 \exp(-\beta[V(x_0) + u(x_0)])/(2\pi\beta)^{1/2}. \tag{114}$$

5.5 *Illustrative application of the local Brillouin condition: Cubic plus quartic oscillator*

Using the expression for the anharmonic oscillator of §3 (51), we generate the Hamiltonian H_{x_0},

$$H_{x_0} = \tfrac{1}{2}[\dot{y}^2 + W^2(x_0)y^2] + [\gamma + 4x_0]y^3 + \lambda y^4, \tag{115}$$

where $W(x_0) = 1 + 6x_0\gamma + 12\lambda x_0^2$. Introducing the operators $a/a^\dagger$ via (102) and (103),

we rewrite H_{x_0} as

$$H_{x_0} = W(x_0)[a^\dagger a + \tfrac{1}{2} + \gamma(x_0)/2^{3/2}(a + a^\dagger)^3 + \lambda(x_0)/4(a + a^\dagger)^4], \tag{116}$$

where

$$\gamma(x_0) = (\gamma + 4x_0)/W^{5/2}(x_0), \tag{117a}$$

$$\lambda(x_0) = (\lambda/W^3(x_0). \tag{117b}$$

This has the same form as (57) except for the scaling factor $W(x_0)$. By inducing the Bogolyubov transformation, (104), we can get an exact analogue of (60). The only difference is the explicit x_0 dependence of $\gamma(x_0)$, $\lambda(x_0)$ and hence also of $\omega \equiv \omega(x_0)$, defined as $(1-t)/(1+t)$. Also, n would have a different value.

Our discussion will be complete if we now compute the contraction $\ll b^\dagger b \gg_{\tilde{D}}$. To achieve this we first compute the value of $\xi^0(x_0)$. We note that

$$\oint D[y] \exp\left(- \int_0^\beta (1/2)[y^2 + W^2 y^2] \mathrm{d}\tau \right) = (1/2)\beta W / \mathrm{Sinh}(1/2)\beta W, \tag{118}$$

which is obtained by using the Fourier representation of y, (94), and Euler's formulae of hyperbolic functions. We can then find by a straightforward computation the value $\ll y(\tau_1) y(\tau_2) \gg_{\tilde{D}}$ by again expanding each y as a Fourier series:

$$\ll y(\tau_1) y(\tau_2) \gg_{\tilde{D}} = \mathrm{Cosh}[W|\tau_1 - \tau_2| - \beta/2]/2W \mathrm{Sinh}(1/2)\beta W - 1/\beta W^2. \tag{119}$$

We then derive, using (103), the relation

$$\ll a^\dagger a \gg_{\tilde{D}} = (1/2)\coth(1/2)\beta W - 1/\beta W - 1/2. \tag{120}$$

Since the transformation $a \rightarrow b$ changes the form of H_{x_0} only up to an additive constant $\ll H \gg$, the value of $\ll b^\dagger b \gg_D$ remains unchanged in form; the only change is the replacement of the unperturbed frequency W by the normalized frequency ω:

$$n = \ll b^\dagger b \gg_{\tilde{D}} = (1/2)\coth(1/2)\beta\omega(x_0) - 1/\beta\omega(x_0) - 1/2. \tag{121}$$

6. Concluding remarks

We have discussed in this paper ways to define certain optimal choices of mean-field and correlated descriptions of many-body systems at a fixed temperature. For this purpose, we have utilized our recently developed apparatus of thermal field theory involving concepts of thermal normal ordering and thermal Wick's expansion. The thermal normal ordering of the operators makes the attendant algebra of our thermal field theory an exact finite-temperature analgoue of the corresponding zero-temperature field theories. This algebraic homomorphy leads us to discern relations that would be hard to derive in other formulations. We have derived thermal analogues of Brillouin and Brückner conditions as conditions for a mean-field description leading respectively to the best thermally averaged energy and to the minimum value of Z/Z_0 where Z and Z_0 are exact and mean-field values of the partition function. Clearly, the latter condition leads to the best mean-field model for the free energy, in the sense of being closest to the exact free energy.

Since in the evaluating the thermal trace in the equilibrium statistical mechanics we may use correlated functions constructed from the mean-field, it is possible to use thermal Brillouin-like conditions as defining optimal descriptions of the average energy with respect to both the mean-field (i.e. the mean-field ground state) and the correlation effects superposed on the uncorrelated ground state. We have derived such conditions in our paper.

In the context of path-integral formulation of the partition function Z, it is possible to choose an auxillary potential which depends on each point on the path to enhance the performance of a perturbative or non-perturbative construction of Z. Using an appropriate generalization of the concept of normal ordering defined with respect to the measure used in the evaluation of the partition function (called $\tilde{D}$ normal ordering by us) we can derive conditions for the optimal mean-field descriptions in terms of potentials leading to the best average energy or best free energy at each point on the path. We have termed these local thermal Brillouin and Brückner conditions, respectively.

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