

# Expansion of the Gibbs potential for quantum many-body systems: General formalism with applications to the spin glass and the weakly nonideal Bose gas

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For general quantum systems the power expansion of the Gibbs potential and consequently the power expansion of the self-energy is derived in terms of the interaction strength. Employing a generalization of the projector technique, a compact representation of the general terms of the expansion results. The general aspects of the approach are discussed with special emphasis on the effects characteristic for quantum systems. The expansion is systematic and leads directly to contributions beyond the mean field of all thermodynamic quantities. These features are explicitly demonstrated and illustrated for two nontrivial systems, the infinite-range quantum spin glass and the weakly interacting Bose gas. The Onsager terms of both systems are calculated, which represent the first beyond-mean-field contributions. For the spin glass Thouless-Anderson-Palmer-like equations are presented and discussed in the paramagnetic region. The investigation of the Bose gas leads to a beyond-mean-field thermodynamic description. At the Bose-Einstein condensation temperature complete agreement is found with the results presented recently by alternative techniques.

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## I. INTRODUCTION

The problem of understanding the static properties of systems possessing large or infinite numbers of particles pervades all of theoretical physics. Apart from very rare exceptions, approximation must be employed to find the characteristic features of such many-particle systems. It is the static mean-field approximation which is usually used to find first descriptions of these many-body systems. Although this approximation leads in many cases to reasonable descriptions there are situation where beyond-mean-field approximations are needed.

More than two decades ago, the present author developed a method [1] to derive such beyond-mean-field approximations in a natural way. The approach is based on the power expansion of the Gibbs potential and was performed for the Sherrington-Kirkpatrick (SK) spin glass model [2]. The investigation confirmed the Thouless-Anderson-Palmer (TAP) equations that had been obtained previously [3]. Due to the presence of infinite-range interactions, the power expansion truncates. It is just the terms up to the second order which contribute in the thermodynamic limit.

In subsequent publications, the method of [1] was successfully applied to the infinite-ranged classical vector spin glass by Vulovic [4], to various other spin glasses [5,6] and to dynamical problems in the field of spin glasses by Biroli and Cugliandolo [7,8]. Neural networks are closely related to spin glasses [9–11]. Therefore it is natural that the Gibbs potential approach has been used for problems in this and related fields [12]. In particular the first, generally accepted TAP-like approach to the Hopfield model, worked out by Nakanishi and Takayama [13], is based on the method of [1].

The study of non-spin-glass-like problems with the Gibbs potential approach started with the contributions of Georges

and Yedidia for the ferromagnetic Ising and spherical models [14] and for the Hubbard model [15]. In addition to these investigations, further work for non-spin-glass-like problems [16] exists that uses the method developed in [1]. In general, infinite range interactions are not presumed and therefore a truncated expansion implies an approximation and higher order terms may become important. For the general Ising model, the third- and fourth-order terms were calculated first in [14] and later in [13]. Moreover, for some special Ising or spherical systems, leading terms beyond the fourth order have been presented in these papers.

Note that the majority of the systems to which the expansion of the Gibbs potential has been applied are classical systems. Exceptions are the investigations for the Hubbard model [15], the fermionic spin glass model [6], and the quantum version of the spherical  $p$  spin glass model [8]. Apart from the fact that these approaches yield interesting results, none of them is completely representative for a generalization of the Gibbs potential expansion to quantum systems. It is just the Lagrange parameter conjugate to the order parameter and the chemical potential for which the Legendre transformation is performed in [15] for the Hubbard Hamiltonian. In general, the transformation is performed for a larger set of variables. Thus the approach is very special and therefore nongeneric for quantum systems. All operators—the spin operators, the number operators, and the interaction Hamiltonian—of the fermionic spin glass model [6] commute. Again such a situation is not representative for a quantum system. Finally, the approach [8] uses very special quantum variables and it is not obvious how to generalize this work to obtain explicit results for the usual quantum spins.

Hence, it is the aim of this work to present a complete quantum version of the power expansion for the Gibbs potential. To work out the characteristic effects for quantum systems the approach should be as general as possible. Thus we start in Sec. II with an arbitrary Hamiltonian and work out all terms of the expansion up to an arbitrary order. In

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Sec. III the formal results are discussed from a general point of view.

The remaining part of this paper is reserved for two specific applications. In Sec. IV the infinite ranged quantum spin  $s=1/2$  glass is treated for nonisotropic interactions. TAP-like equations result which are discussed for isotropic interactions in the paramagnetic regime and compared to corresponding equations for classical vector spins. In Sec. V the expansion of the Gibbs potential is worked out for the weakly nonideal Bose gas up to the first beyond-mean-field contribution. The resulting equations of state are valid in the entire temperature regime. For the self-energy a complete agreement with previous and alternative approaches is found at the Bose-Einstein condensation temperature. In Sec. VI we present some concluding remarks and compare to other approaches.

Some introductory remarks should be added on the physical systems to which the general results are applied. The quantum spin  $s=1/2$  glass with infinite range interactions is the natural generalization of the SK or of the classical vector spin glass model to include quantum effects. Despite being formulated over two decades ago [17], an understanding of this spin glass model has proven elusive [18].

Although the theory of the weakly interacting Bose gas has a long history, some old problems—like the effect on the critical temperature due to such interactions—have been revived (compare [19] for an overview). In this context detailed beyond-mean-field investigations for the self-energy have recently been published [20]. As these results were derived both with Green's function methods and within the framework of Ursell operators [21], this approach is an ideal reference system to compare the Gibbs potential approach with other work.

## II. GENERAL FORMALISM

### A. Basic concepts of the Gibbs potential expansion

The many-particle system is described by the thermodynamic Hamiltonian ( $\beta=1/T$  and  $k_B=1$ )

$$\mathcal{K}_\alpha = -\beta\mathcal{H} = \sum_i \nu_\alpha^i \mathcal{A}^i + \alpha \mathcal{K}' \quad (1)$$

where the single-particle contributions and the many-particle interactions correspond to  $\sum_i \nu_\alpha^i \mathcal{A}^i$  and to  $\mathcal{K}'$ , respectively. It is assumed that the thermodynamic quantities and, in particular, all expectation values can be calculated for the free Hamiltonian  $\mathcal{K}_{\alpha=0}$  and that the problem is to find at least approximations for the interacting system.

This is a very common question and typical realizations are interacting systems of identical particles, classical or quantum spin systems, and combinations of these systems. The present approach to these problems is quite general and does not need any further requirements or assumptions.

The parameters  $\nu_\alpha^i = (\nu_\alpha^i)^*$  are real and the operators  $\mathcal{A}^i = (\mathcal{A}^i)^\dagger$  are Hermitian [22]. The variable  $\alpha$  represents an (in general complex) expansion parameter and the  $\nu_\alpha^i$  exhibit an  $\alpha$  dependence which will be specified below. The Hamiltonian of the original problem corresponds to the value

$\alpha=1$ . This implies that the values  $\nu_{\alpha=1}^i$  are given and fixed by the specific physical problem under investigation. Clearly this also implies that we have to set  $\alpha=1$  at the end of the calculation.

The index  $i$  is a shorthand index for both different particles and different operators acting in the same subspace of the individual particles. For a Hamiltonian in second quantization the  $\mathcal{A}^i$  represent products of creation and destruction operators and the index  $i$  may become a pair index.

The object is to calculate a thermodynamic potential that determines the relevant thermal mean values

$$\langle \cdots \rangle_\alpha = \text{Tr} \cdots \mathcal{R}_\alpha \quad (2)$$

where the density operator  $\mathcal{R}_\alpha$  and the partition function  $Z_\alpha$  are given by

$$\mathcal{R}_\alpha = \frac{e^{\mathcal{K}_\alpha}}{Z_\alpha} \quad \text{and by} \quad Z_\alpha = \text{Tr} e^{\mathcal{K}_\alpha}, \quad (3)$$

respectively. The usual choice for such a potential is the free energy, which is proportional to  $\ln Z_\alpha$ . This work, however, is focusing on the Gibbs potential  $G_\alpha$ , which is related to the free energy by a Legendre transformation and defined as

$$G_\alpha(A^i) = \ln Z_\alpha - \sum_i \nu_\alpha^i A^i \quad \text{with} \quad A^i = \langle \mathcal{A}^i \rangle_\alpha. \quad (4)$$

Strictly, it is the quantity  $-\beta G_\alpha(A^i)$  that represents the thermodynamic Gibbs potential. We use, however, the term for  $G_\alpha(A^i)$ , keeping in mind this difference. For systems with variable numbers of particles  $\mathcal{R}_\alpha$  and  $Z_\alpha$  represent the grand canonical density operators and the grand canonical partition function, respectively. This implies the slide modification  $\mathcal{K}_\alpha = -\beta(\mathcal{H} - \mu\mathcal{N})$  for these systems where  $\mu$  and  $\mathcal{N}$  represent the chemical potential and the number operator, respectively.

The total differential of  $G_\alpha$  is given by

$$dG_\alpha = \langle \mathcal{K}' \rangle_\alpha d\alpha - \sum_i \nu_\alpha^i dA^i. \quad (5)$$

Thus the natural variables are the expansion parameter  $\alpha$  and the variables  $A^i$  which are conjugate to the Lagrange parameters  $\nu_\alpha^i$ . Thus both the Gibbs potential and the Lagrange parameters  $\nu_\alpha^i$  are functions of  $\alpha$  and  $A^i$  and the present approach exclusively uses these natural variables as independent variables.

Next  $G_\alpha(A^i)$  is expanded around  $\alpha=0$  keeping the values  $A^i$  fixed to their thermal values. Thus the relation  $A^i = \langle \mathcal{A}^i \rangle_\alpha = \langle \mathcal{A}^i \rangle_0 = \langle \mathcal{A}^i \rangle_1$  holds. These constraints determine the functions  $\nu_\alpha^i(A^i)$  and remove the arbitrariness of the above. The Taylor expansion leads to

$$G_\alpha = S_0 + \sum_{n=1}^{\infty} \frac{\alpha^n G^{(n)}}{n!} \quad \text{with} \quad G^{(n)} = \left. \frac{\partial^n G_\alpha}{\partial \alpha^n} \right|_{\alpha=0}. \quad (6)$$

The zeroth-order term  $S_0(A^i)$  of the expansion (6) is the entropy of the noninteracting system. This is easily checked using Eq. (3), the general definition  $S_0 = -\langle \ln \mathcal{R}_0 \rangle_0$ , and

$$\mathcal{K}_0 = \sum_i \nu_0^i \mathcal{A}^i. \quad (7)$$

Considering next the first-order contribution  $G^{(1)}$  Eq. (5) yields immediately

$$G^{(1)} = \langle \mathcal{K}' \rangle_0, \quad (8)$$

which represents nothing else than the usual mean-field energy. Thus approximating the expansion (6) by the first two terms  $G_{\alpha=1} \approx S_0 + \langle \mathcal{K}' \rangle_0$  corresponds to the standard mean-field theory.

Differentiation of Eq. (6) with respect to  $A^i$  and using Eq. (5) yields for  $\alpha=0$

$$\nu_0^i(A^i) = - \frac{\partial S_0}{\partial A^i} \quad (9)$$

and for  $\alpha=1$

$$\nu_1^i = \nu_0^i + \beta \Sigma^i \quad \text{with} \quad -\beta \Sigma^i = \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial G^{(n)}}{\partial A^i}. \quad (10)$$

According to Eq. (9) the values of the Lagrange parameters  $\nu_0^i$  are determined by the derivative of the entropy of the noninteracting system that is a function of the  $A_i$ . This relation is important. Indeed, Eq. (9) is used to eliminate the dummy variables  $\nu_0^i$  that enter in the expectation values of the noninteracting system via  $\mathcal{K}_0$  [compare Eq. (7)].

Recall that the quantities  $\nu_1^i$  represent the given parameter values of the original Hamiltonian (1) and note that both terms  $\nu_0^i$  and  $\Sigma^i$  are functions of the  $A^i$ . Therefore the first equation of (10) represents a thermic equation of states from which the expectation values  $A^i$  can be determined for given values of the  $\nu_1^i$ .

The second equation of (10) represents the general definition of the self-energy  $\Sigma^i$  or for magnetic systems the general definition of the internal field. Note that this fact is well known in the theory of Green's functions where the Gibbs potential is often named the effective potential [23]. Thus the expansion of the Gibbs potential implies a systematic expansion of the self-energy that describes the effects of the interaction.

For specific examples these results are illustrated below and the reader is referred to Secs. IV A and V A for magnetic systems and for a Bose gas, respectively.

In this context it is remarked that a further differentiation of Eq. (10) with respect to  $A_j$  results in an expansion of the inverse susceptibility matrix. This quantity is of high importance as it governs the convergence of the expansion and consequently the stability of the considered system—compare [1,24] for the SK model, Eq. (83) for the quantum spin glass, and Eq. (108) for the Bose gas.

Rewriting the definition of the coefficients  $G^{(n)}$  as

$$G^{(n)} = \left. \frac{\partial^n}{\partial \alpha^n} \ln \text{Tr} \exp \left( \sum_i \nu_\alpha^i (A^i - A_i) + \alpha \mathcal{K}' \right) \right|_{\alpha=0} \quad (11)$$

it is obvious that the  $G^{(n)}$  can be interpreted as a generalization of the cumulant expectation values [25,26]. It is just the additional  $\alpha$  dependence of the Lagrange parameters  $\nu_\alpha^i$  that causes the difference from the usual cumulants.

## B. Onsager term

In this section the explicit expression for the second-order term  $G^{(2)} = \partial_{\alpha\alpha} G_{\alpha=0}$  is investigated. This term is called the Onsager term and represents the lowest beyond-mean-field contribution to the expansion.

According to Eq. (5)  $\partial_\alpha G_\alpha = \langle \mathcal{K}' \rangle_\alpha$  holds, which implies  $\partial_{\alpha\alpha} G_\alpha = \text{Tr} \mathcal{K}' \partial_\alpha \mathcal{R}_\alpha$ . Focusing therefore on the calculation of  $\partial_\alpha \mathcal{R}_\alpha$ , the definitions

$$\mathbb{E}_\alpha \{ \mathcal{U} \} = \int_0^1 \mathcal{U}(\lambda) d\lambda, \quad \mathcal{U}(\lambda) = e^{\lambda \mathcal{K}_\alpha} \mathcal{U} e^{-\lambda \mathcal{K}_\alpha}, \quad (12)$$

and

$$(\mathcal{U} | \mathcal{V})_\alpha = \langle \mathcal{U}^\dagger \mathbb{E}_\alpha \{ \mathcal{V} \} \rangle_\alpha \quad (13)$$

are introduced. The definition (13) represents the well-known Mori product [27] of the operators  $\mathcal{U}$  and  $\mathcal{V}$ . This product is a scalar product in the Liouville space, has many additional properties (compare Appendix A 1) and is physically significant in particular for the linear response theory (see [28] for a general reference).

The definition (12) permits us to represent the differential rule for exponential operators as

$$d e^{\mathcal{K}_\alpha} = \mathbb{E}_\alpha \{ d\mathcal{K}_\alpha \} e^{\mathcal{K}_\alpha}, \quad d\mathcal{K}_\alpha = \mathcal{K}' d\alpha + \sum_i \mathcal{A}^i d\nu_\alpha^i. \quad (14)$$

Due to the possibility of cyclic permutations within the trace Eq. (14) yields  $dZ_\alpha = Z_\alpha \langle d\mathcal{K}_\alpha \rangle_\alpha$ . This leads to the total differential of the density operator,

$$d\mathcal{R}_\alpha = \mathbb{E}_\alpha \{ \tilde{\mathcal{K}}' \} \mathcal{R}_\alpha d\alpha + \sum_i \mathbb{E}_\alpha \{ \tilde{\mathcal{A}}^i \} \mathcal{R}_\alpha d\nu_\alpha^i \quad (15)$$

where  $\tilde{\mathcal{U}}$  is defined by

$$\tilde{\mathcal{U}} = \mathcal{U} - \langle \mathcal{U} \rangle_\alpha. \quad (16)$$

The constraints  $A^i = \text{const}$  imply  $\text{Tr} \mathcal{A}^i d\mathcal{R}_\alpha = 0$ . This leads to

$$\partial_\alpha \nu_\alpha^j = - \sum_j \Gamma_\alpha^{ij} (\tilde{\mathcal{A}}^j | \mathcal{K}')_\alpha \quad (17)$$

using the relation (A5). The matrix  $\Gamma_\alpha^{ij}$  is the inverse of the susceptibility matrix  $\chi_\alpha^{ij}$ ,

$$\sum_k \Gamma_\alpha^{ik} \chi_\alpha^{kj} = \delta_{ij} \quad \text{where} \quad \chi_\alpha^{ij} = (\tilde{\mathcal{A}}^i | \tilde{\mathcal{A}}^j)_\alpha. \quad (18)$$

As the Mori product is a scalar product the matrix  $\chi_\alpha^{ij}$  is positive definite and thus the inverse matrix  $\Gamma_\alpha^{ij}$  exists.

For a compact notation it is convenient to introduce the projectors by  $\mathbb{P}_\alpha$  and  $\mathbb{Q}_\alpha$

$$\mathbb{P}_\alpha \mathcal{U} = (1 | \mathcal{U})_\alpha + \sum_{ij} \tilde{\mathcal{A}}^i \Gamma_\alpha^{ij} (\tilde{\mathcal{A}}^j | \mathcal{U})_\alpha, \quad \mathbb{Q}_\alpha = 1 - \mathbb{P}_\alpha. \quad (19)$$

$\mathbb{P}_\alpha$  and  $\mathbb{Q}_\alpha$  are superoperators which linearly map operators of the Hilbert space onto other operators of the Hilbert space. With the above definitions it is easy to show that the usual projector relations  $\mathbb{P}_\alpha^2 = \mathbb{P}_\alpha$ ,  $\mathbb{Q}_\alpha^2 = \mathbb{Q}_\alpha$ , and  $\mathbb{P}_\alpha \mathbb{Q}_\alpha = 0$  are satisfied. The projector  $\mathbb{P}_\alpha$  projects onto the subspace that is spanned by the elements  $\mathcal{A}^i$  and by the unit operator 1. These

basis elements are linearly independent but are in general not orthogonal.

Let us introduce some definitions. In accordance with [28] we use the term observation level for the set of operators  $\mathcal{A}^i$  spanning the subspace  $\mathbb{P}_0$  together with the unit operator. The set of all  $A^i$  and the set of all  $\nu_\alpha^i$  are called constrained and conjugate variables, respectively.

Using Eqs. (15), (17), and (19) the compact result

$$\partial_\alpha \mathcal{R}_\alpha = \mathbb{E}_\alpha \{ \mathcal{Q}_\alpha \mathcal{K}' \} \mathcal{R}_\alpha \quad (20)$$

is found, which directly leads to

$$\partial_{\alpha\alpha} G_\alpha = (\mathcal{K}' | \mathcal{Q}_\alpha \mathcal{K}' )_\alpha \quad (21)$$

and to the final expression for the Onsager term

$$G^{(2)} = (\mathcal{K}' | \mathcal{Q}_0 \mathcal{K}' )_0. \quad (22)$$

Both the Mori product and the projector  $\mathcal{Q}_0$  are related to the Hamiltonian  $\mathcal{K}_0$  of the free system. Thus  $G^{(2)}$  can explicitly be calculated. According to Eqs. (7) the conjugate variables  $\nu_0^i$  enter in this expression, which must again be eliminated with Eqs. (9) to obtain the  $A_i$  dependence of the Onsager term  $G^{(2)}$ .

### C. Cumulants for $n > 2$

From the above treatment for the Onsager term it is obvious that higher derivatives are needed to calculate the  $G^{(n)}$  for general values of  $n$ . For this purpose it is useful to generalize the definitions of  $\mathbb{E}_\alpha$ , of  $\mathbb{P}_\alpha$ , and of the Mori product.

First a commutative product  $\mathcal{B}_1 * \mathcal{B}_2 * \dots * \mathcal{B}_n$  of an arbitrary number of operators is introduced [29]. The operation  $\mathbb{E}_\alpha$  on such a  $*$  product is defined as a mapping to an (Hilbert space) operator given by

$$\begin{aligned} \mathbb{E}_\alpha \{ \mathcal{B}_1 * \mathcal{B}_2 * \dots * \mathcal{B}_n \} \\ = \int_0^1 d\lambda_1 \dots \int_0^1 d\lambda_n \mathbb{T} [ \mathcal{B}_1(\lambda_1) \mathcal{B}_2(\lambda_2) \dots \mathcal{B}_n(\lambda_n) ]. \end{aligned} \quad (23)$$

The  $\lambda_k$  dependence of the  $\mathcal{B}_k(\lambda_k)$  is given by Eq. (12) and  $\mathbb{T}$  represents the thermodynamic (or imaginary time) ordering operator. It orders the  $\mathcal{B}_k(\lambda_k)$  operators with increasing  $\lambda_k$  from the left to the right.

Next the definition of the Mori product is generalized by

$$(\nu | \mathcal{B}_1 * \dots * \mathcal{B}_n )_\alpha = (\nu^\dagger \mathbb{E}_\alpha \{ \mathcal{B}_1 * \dots * \mathcal{B}_n \} )_\alpha. \quad (24)$$

The bra must always be an ordinary operator. It is just the ket that can be an ordinary operator, a  $*$  product, or even linear combinations of these objects. Assuming in Eq. (19) that  $\mathcal{U}$  represents such an object, the generalized projectors  $\mathbb{P}_\alpha$  and  $\mathcal{Q}_\alpha$  are still defined by these equations. The characteristic projector relation  $\mathbb{P}_\alpha \mathbb{P}_\alpha = \mathbb{P}_\alpha$  remains valid, which again is easy to prove.

The above generalizations imply new properties of the modified quantities. Some of these properties are listed in Appendix A 1. Two key properties, the derivatives of  $\mathbb{E}_\alpha$  and  $\mathbb{P}_\alpha$ , are calculated in Appendixes A 2 and A 3, respectively. There we find

$$\begin{aligned} \partial_\alpha \mathbb{E}_\alpha \{ \mathcal{B}_1 * \dots * \mathcal{B}_n \} \mathcal{R}_\alpha &= \mathbb{E}_\alpha \{ (\mathcal{Q}_\alpha \mathcal{K}' ) * \mathcal{B}_1 * \dots * \mathcal{B}_n \} \mathcal{R}_\alpha \\ &+ \mathbb{E}_\alpha \{ \partial_\alpha \mathcal{B}_1 * \dots * \mathcal{B}_n \} \mathcal{R}_\alpha, \end{aligned} \quad (25)$$

where the inner derivative  $\partial_\alpha \mathcal{B}_1 * \dots * \mathcal{B}_n$  has been calculated by the usual product rule.

Introducing the shorthand notation for the  $*$  product  $\mathbf{B} = \mathcal{B}_1 * \mathcal{B}_2 * \dots * \mathcal{B}_n$  Eq. (25) and the definition (24) lead to the derivative of the generalized Mori product

$$\partial_\alpha (\mathcal{U} | \mathbf{B} )_\alpha = (\mathcal{U} | (\mathcal{Q}_\alpha \mathcal{K}' ) * \mathbf{B} )_\alpha + (\partial_\alpha \mathcal{U} | \mathbf{B} )_\alpha + (\mathcal{U} | \partial_\alpha \mathbf{B} )_\alpha. \quad (26)$$

In Appendix A 3 it is shown that the derivative of  $\mathbb{P}_\alpha$  is given by

$$\partial_\alpha \mathbb{P}_\alpha \mathbf{B} = \mathbb{P}_\alpha (\mathcal{Q}_\alpha \mathcal{K}' ) * (\mathcal{Q}_\alpha \mathbf{B} ) + \mathbb{P}_\alpha \partial_\alpha \mathbf{B}. \quad (27)$$

Both differentiation rules (26) and (27) are essential for the following. To this point it is assumed that  $\mathbf{B}$  represents an arbitrary  $*$  product. An extension, however, to linear combinations of such products is obvious. Assuming the usual addition, multiplication, and differentiation rules for these linear combinations, the above Eqs. (26) and (27) also hold for linear combinations. Thus  $\mathbf{B}$  represents in general linear combinations of  $*$  products in these equations.

With all these extensions we are well equipped to calculate the higher derivatives of  $\mathcal{R}_\alpha$  by repeated application of the above rules. With the notation

$$\mathcal{F}_1 = \mathcal{Q}_0 \mathcal{K}' \quad \text{and} \quad \mathcal{F}_n = -\frac{1}{n!} \mathbb{P}_0 \mathbf{F}^{(n)} \quad (\text{for } n \geq 2) \quad (28)$$

we find

$$(\partial_\alpha)^n \mathcal{R}_\alpha = \mathbb{E}_\alpha \{ \mathcal{Q}_\alpha \mathbf{F}^{(n)} \} \mathcal{R}_\alpha \quad (29)$$

with

$$\mathbf{F}^{(1)} = \mathcal{K}', \quad (30)$$

$$\mathbf{F}^{(2)} = \mathcal{F}_1 * \mathcal{F}_1 = \mathcal{F}_1^2, \quad (31)$$

$$\mathbf{F}^{(3)} = \mathcal{F}_1^3 + 6\mathcal{F}_1 * \mathcal{F}_2, \quad (32)$$

$$\mathbf{F}^{(4)} = \mathcal{F}_1^4 + 12\mathcal{F}_1^2 * \mathcal{F}_2 + 12\mathcal{F}_2^2 + 24\mathcal{F}_1 * \mathcal{F}_3, \quad (33)$$

$$\begin{aligned} \mathbf{F}^{(5)} &= \mathcal{F}_1^5 + 20\mathcal{F}_1^3 * \mathcal{F}_2 + 60\mathcal{F}_1 * \mathcal{F}_2^2 + 60\mathcal{F}_1^2 * \mathcal{F}_3 \\ &+ 120\mathcal{F}_2 * \mathcal{F}_3 + 120\mathcal{F}_1 * \mathcal{F}_4 \end{aligned} \quad (34)$$

for low  $n$  values. Powers of the  $*$  multiplication are denoted by bold power exponents [compare Eq. (31)].

For general values  $n \geq 1$  the  $\mathbf{F}^{(n+1)}$  are given by

$$\mathbf{F}^{(n+1)} = \sum'_{(k_1, \dots, k_n)} \frac{(n+1)!}{k_1! k_2! \dots k_n!} \mathcal{F}_1^{k_1} * \mathcal{F}_2^{k_2} \dots * \mathcal{F}_n^{k_n} \quad (35)$$

where the sum runs over all  $k_i = 0, 1, 2, \dots$  with the constraint

$$\sum_{i=0}^n ik_i = n + 1. \quad (36)$$

The general expression (35) can be proved by mathematical induction.

With these results we obtain for the cumulants

$$G^{(n+1)} = (\mathcal{K}' | Q_0 \mathbf{F}^{(n)})_0. \quad (37)$$

Note that Eqs. (28) and (35) permit a recursive determination of all the  $\mathbf{F}^{(n)}$ . Consequently this also applies to all cumulants  $G^{(n)}$ . Some examples are

$$G^{(3)} = (\mathcal{K}' | Q_0 (Q_0 \mathcal{K}')^2)_0,$$

$G^{(4)}$

$$= (\mathcal{K}' | Q_0 \{ (Q_0 \mathcal{K}')^3 - 3(Q_0 \mathcal{K}') * [P_0(Q_0 \mathcal{K}')^2] \})_0 = (\mathcal{K}' | Q_0 \{ -2(Q_0 \mathcal{K}')^3 + 3(Q_0 \mathcal{K}') * [Q_0(Q_0 \mathcal{K}')^2] \})_0, \quad (38)$$

which show a nested structure of the projectors. The different forms of the  $G^{(4)}$  result just using  $P_0 + Q_0 = \mathbf{1}$ . All the expressions are treatable as they have to be calculated with respect to the bare Hamiltonian  $\mathcal{K}_0$ . Again the dummy variables  $\nu_0^j$  enter and have to be eliminated by use of Eq. (9). Thus all terms of the expansions for the Gibbs potential (6) and for the self-energy (10) can in principle be calculated.

Even for the classical system the representation of the higher cumulants based on projectors seems to be adventurous compared to the approach based on generalized Maxwell relations [14]. Indeed, relations like Eq. (35) for general  $n$  values have not been published for the latter approach.

In this context it should be added that Eq. (38) applied to Ising systems leads to the known third- and fourth-order terms for these systems [13,14]. [For an explicit check of this claim the simplification (39) below can be used.]

### III. DISCUSSION

#### A. General remarks

The expansion of the Gibbs potential (6) and the expansion of the self-energy (10), together with the expression (8) for the coefficient  $G^{(1)}$  and the relations (37), (28), and (35), represent the most general result of this work.

According to the formal derivation the perturbation  $\mathcal{K}'$  is completely arbitrary. Moreover, no restrictions enter for the bare Hamiltonian  $\mathcal{K}_0$  or for the operators of the observation level. Thus one-particle problems as well as many-particle problems can be treated with the results presented. In the most general case the observation level may even contain many-particle operators. The work of Biroli and Cugliandolo [8] for the quantum version of the spherical  $p$  spin glass model represents such an interesting approach.

It is always possible to extend an observation level by adding arbitrary operators  $\hat{A}^i$  to the original set. With the presumption that all the corresponding Lagrange multipliers  $\hat{\nu}_\alpha^j$  satisfy the condition  $\hat{\nu}_1^j = 0$ , the physical problem is not modified. Indeed, the Hamiltonian and consequently the exact Gibbs potential do not change at all by such an extension.

The projectors  $P_0$ , however, differ, which leads to different terms of the expansions. Thus different observation levels lead to different expansions. This implies that the quality of approximations like truncations of the power series depend on the chosen observation level.

The latter conclusion is clearly illustrated by the following simple limiting case. Adding formally the interaction  $\hat{A} = \mathcal{K}'$  with  $\hat{\nu}_1 = 0$  to any observation level, Eqs. (28) and (37) yield  $\mathcal{F}_1 = 0$  and  $G^{(n \geq 2)} = 0$ , respectively. This implies that the first two terms of the expansion give the exact result whereas any truncation of the original expansion represents an approximation.

The present approach requires that the bare Hamiltonian can be represented as a linear combination of the elements of the observation level [30]. Nevertheless a reduction of the observables of the observation level is possible. This can simply be achieved by transforming just a part of the parameters of the bare Hamiltonian to conjugate variables. Again any reduction leads to different expansions.

As long as no approximations are performed all observation levels are equivalent. For specific problems this freedom can be used to choose a special observation level which leads to good or fast converging approximations. Certainly such a procedure requires in general some physical intuition for the system under consideration. Similar situations show up in all the approaches that are based on projector methods. In analogy it is generally expected that symmetry breaking operators should be included in the observation level apart from the bare Hamiltonian. For two-particle interactions the complete set of all one-particle operators should be an appropriate choice for the observation level (compare Sec. III D). Considering systems of bosons or fermions in second quantization it should usually be sufficient to span the observation level by all the occupation number operators (compare Sec. V).

#### B. Classical systems and the quasiclassical case

For *classical* systems the  $*$  product reduces to the ordinary product. All quantities commute and the Mori product (24) reduces to

$$(\mathcal{V} | \mathcal{B}_1 * \mathcal{B}_2 \cdots )_\alpha \mapsto \langle \mathcal{V}^\dagger \mathcal{B}_1 \mathcal{B}_2 \cdots \rangle_\alpha, \quad (39)$$

which usually simplifies the calculation.

For special quantum systems the situation may appear that all operators  $\mathcal{A}_i$  and the interaction  $\mathcal{K}'$  form a set of commuting operators. It is exclusively the algebra of this set which enters in the  $G^{(n)}$  and thus the replacement (39) can be used to calculate these quantities. In the following we call such situations the *quasiclassical case*.

The approach for the fermionic spin glass model by Rehner and Oppermann [6] is such a quasiclassical case. Thus it is obvious that the results of this fermionic system are very similar to the results [1,3,24] for the SK spin glass model [2]. Note that for this system a quantum treatment becomes necessary if a transverse magnetic field is added. The existing approach, however, does not contain such a treatment.

### C. High-temperature expansion

The limiting case of an empty observation level is of special interest. No variable at all is Laplace transformed. This implies a vanishing  $\mathcal{K}_0$  and a quasiclassical situation where Eq. (39) can be employed. The thermodynamic potential (4) is nothing else than the free energy  $\ln Z$  in the high-temperature approximation. The statistical operator simplifies to

$$\tilde{\mathcal{R}}_0 = \mathbf{1}/\tilde{Z}_0 \quad \text{with} \quad \tilde{Z}_0 = \text{Tr} \mathbf{1} \quad (40)$$

and the general projector reduces to  $\tilde{\mathbb{P}}_0$  which projects any  $\mathcal{U}$ ,

$$\tilde{\mathbb{P}}_0 \mathcal{U} = \langle \mathcal{U} \rangle_0, \quad (41)$$

onto the 1 direction. Setting

$$\ln Z = \sum_{n=0}^{\infty} \frac{(\ln Z)^{(n)}}{n!} \quad (42)$$

and

$$c_n = \langle (\mathcal{K}')^n \rangle_0 \quad (43)$$

we find immediately

$$(\ln Z)^{(1)} = c_1,$$

$$(\ln Z)^{(2)} = c_2 - c_1^2,$$

$$(\ln Z)^{(3)} = c_3 - 3c_2c_1 + 2c_1^3,$$

$$(\ln Z)^{(4)} = c_4 - 4c_3c_1 - 3c_2^2 + 12c_2c_1^2 - 6c_1^4, \dots \quad (44)$$

These results agree with the Ursell-Mayer expansion, a cumulant expansion of the free energy for classical or quasiclassical systems [25] and demonstrate the close relation of the present work to these former approaches.

### D. Consequences for two-particle interactions

In the typical many-body problem the interaction is a two-particle interaction. Focusing on this case the thermodynamic Hamiltonians is represented as

$$\mathcal{K}_\alpha = \sum_i \mathbf{v}_\alpha^i \cdot \mathbf{A}^i + \frac{\alpha}{2} \sum_{i,j} \mathbf{A}^i \cdot \mathbf{C}^{ij} \mathbf{A}^j \quad \text{with} \quad \mathbf{C}^{ii} = 0. \quad (45)$$

The indices  $i$  and  $j$  number the individual particles. For fixed  $i$  the components  $\mathcal{A}^{i,m}$  and  $\mathbf{v}_\alpha^{i,m}$  of the vector matrices  $\mathbf{A}^i$  and  $\mathbf{v}_\alpha^i$  represent one-particle operators and the corresponding Lagrange parameters, respectively. The elements of the square matrices  $\mathbf{C}^{ij} = \mathbf{C}^{ji}$  describe the interaction. To include the general case it is assumed that the observation level is spanned by the set of all (linear independent) single-particle operators  $\mathbf{A}^i$ .

The factorization property of the expectation values with respect to  $\mathcal{K}_0$  leads to simplifications. The mean-field contribution (8) reduces to

$$G^{(1)} = \langle \mathcal{K}' \rangle_0 = \frac{1}{2} \sum_{i,j} \langle \mathbf{A}^i \rangle \cdot \mathbf{C}^{ij} \langle \mathbf{A}^j \rangle. \quad (46)$$

Using Eq. (19) we find

$$\mathcal{F}_1 = \frac{1}{2} \sum_{i,j} \tilde{\mathbf{A}}^i \cdot \mathbf{C}^{ij} \tilde{\mathbf{A}}^j \quad \text{with} \quad \tilde{\mathbf{A}}^i = \mathbf{A}^i - \langle \mathbf{A}^i \rangle, \quad (47)$$

which leads to the Onsager term

$$G^{(2)} = \frac{1}{2} \sum_{i,j} (\tilde{\mathbf{A}}^i \cdot \mathbf{C}^{ij} \tilde{\mathbf{A}}^j | \tilde{\mathbf{A}}^i \cdot \mathbf{C}^{ij} \tilde{\mathbf{A}}^j)_0. \quad (48)$$

The latter result implies several interesting features. First of all the Onsager term is a superposition of the correlation functions which do not factorize in the general quantum case ( $i \neq j$ )

$$(\tilde{\mathcal{A}}^{i,m_i} \tilde{\mathcal{A}}^{j,m_j} | \tilde{\mathcal{A}}^{i,m'_i} \tilde{\mathcal{A}}^{j,m'_j})_0 \neq (\tilde{\mathcal{A}}^{i,m_i} | \tilde{\mathcal{A}}^{i,m'_i})_0 (\tilde{\mathcal{A}}^{j,m_j} | \tilde{\mathcal{A}}^{j,m'_j})_0. \quad (49)$$

In contrast, these correlation functions factorize for classical systems or for the quasiclassical case. The presence of these *quantum fluctuations* can be the origin of essential differences between classical and quantum systems (for an example see below).

Thermal averaging gives finite contributions to the Onsager term (48) only for such terms where each  $\tilde{\mathcal{A}}^{i,m_i}$  has at least one partner  $\tilde{\mathcal{A}}^{i,m'_i}$ . Thus the sums are double sums, and triple sums do not appear in Eq. (48). In contrast to this behavior, the second-order term of expansions of the free energy  $\ln Z$  leads to triple sums as this term is given by  $(1 | \tilde{\mathcal{K}}' * \tilde{\mathcal{K}}')_0$ , according to [25].

A similar behavior holds for the higher cumulants. In any order the number of terms of the free energy expansion extends the number of terms of the Gibbs potential approach where at maximum  $n$ -fold sums arise. This conclusion is some indication that the correlations are more efficiently treated by the Gibbs potential expansion. Note that in particular these arguments apply for systems with long ranged interactions.

In this context it is remarked that a diagrammatic interpretation of the expansion can be given, completely analogous to the classical systems [14,31]. As pointed out by these authors, the weak point of this method is that the vertex weight and the combinatorial factors cannot be calculated systematically and thus the Feynman rules are not known. Nevertheless, some conclusions are possible from these diagrammatic approaches. In particular, and relevant for this work, it is found that all diagrams are connected. Note that this can also be concluded from the general cumulant theory [25].

The last two conclusions cause the well known fact that for infinite-ranged models the expansions truncate for both nonrandom and random interactions in the thermodynamic limit.

Consider first the case that the matrix elements of  $\mathbf{C}^{ij}$  scale as  $N^{-1}$  and are nonrandom. From the discussion above it follows that all terms  $G^{(n)}$  with  $n \geq 2$  are subextensive and

can be neglected for large  $N$ . Thus the expansions Eqs. (6) and (10) reduce to the usual mean-field expressions

$$G(\langle A \rangle^i) = S_0(\langle A \rangle^i) + \frac{1}{2} \sum_{i,j} \langle A \rangle^i \cdot C^{ij} \langle A \rangle^j, \quad (50)$$

$$\nu_1^i = -\frac{\partial G}{\partial \langle A \rangle^i} \quad (\text{for } C^{ij} \sim N^{-1}), \quad (51)$$

Recall that the function  $S_0$  is the entropy of the noninteracting system. Thus Eqs. (50) and (51) completely determine all thermodynamic properties for the given parameters  $\nu_1^i$  and  $C^{ij}$  of the Hamiltonian (45).

Finally we consider random, infinite-ranged systems where the matrix elements of  $C^{ij}$  are independent random variables, or where the  $C^{ij}$  are proportional to random variables. For these cases the scaling  $C^{ij} \sim N^{-1/2}$  has to be used to get the right  $N$  dependence for the extensive quantities. All cumulants with  $n \geq 3$  are subextensive and it is just the Onsager term (48) that must be added to Eq. (50). For classical systems these conclusions are well known and for quantum systems they are in agreement with [8].

#### IV. QUANTUM SPIN GLASS ( $s=1/2$ )

##### A. General nonisotropic case

A system of  $N$  quantum spins  $s_i$  (with  $s=1/2$  and  $\hbar=1$ ) is considered in the presence of external fields  $h_i$ . The spins interact via an infinite-ranged spin-spin interaction  $J_{ij}$  and are described by the Hamiltonian

$$\mathcal{H} = -\sum_i h_i \cdot s_i - \frac{1}{2} \sum_{i,j} J_{ij} s_i \cdot \Gamma s_j, \quad (52)$$

where the dot denotes the scalar product in three-dimensional real space. The bonds  $J_{ij}=J_{ji}$  (with  $J_{ii}=0$ ) are independent random variables with zero means and standard deviations  $JN^{-1/2}$ . We consider a general spin-spin interaction and  $\Gamma$  represents an arbitrary symmetric tensor with real eigenvalues  $\gamma^\mu$  and  $\mu=x,y,z$  [32]. The norm of  $\Gamma$  is denoted by

$$\gamma^2 = (\gamma^x)^2 + (\gamma^y)^2 + (\gamma^z)^2 = \text{tr } \Gamma^2. \quad (53)$$

The complete set of all one-particle operators  $s_i^\mu$  with  $i=1, \dots, N$  and  $\mu=x,y,z$  is used as the observation level. Setting  $m_i = \langle s_i \rangle_\alpha = \langle s_i \rangle_1$  and  $m_i = |m_i|$  the entropy of the noninteracting system as a function of the  $m_i$  is well known and given by

$$S_0 = -\sum_i \left( \frac{1}{2} + m_i \right) \ln \left( \frac{1}{2} + m_i \right) + \left( \frac{1}{2} - m_i \right) \ln \left( \frac{1}{2} - m_i \right). \quad (54)$$

The operator

$$\mathcal{K}_0 = \sum_i \nu_i \cdot s_i \quad (55)$$

governs the calculation of the expectation values and the Mori products. Simplifying the notation, the variables  $\nu_0^i$  and

$\nu_1^i$  of Sec. II A are denoted by  $\nu_i$  and by  $\beta h_i$ , respectively. From Eq. (9) we find

$$\nu_i = 2 \operatorname{arctanh}(2m_i) \quad \text{and} \quad \frac{\nu_i}{\nu_i} = \frac{m_i}{m_i} = e_i. \quad (56)$$

Note that these equations have to be used to eliminate the dummy variables  $\nu_i$ . Equation (10) leads to the thermic equation of state

$$e_i 2 \operatorname{arctanh}(2m_i) = \beta(h_i - \Sigma_i). \quad (57)$$

According to Sec. III D all cumulants  $G^{(n)}$  with  $n \geq 3$  can be neglected in the thermodynamic limit. Thus the internal fields  $-\Sigma_i$  are given by

$$\beta \Sigma_i = -\frac{\partial}{\partial m_i} \left( G^{(1)} + \frac{G^{(2)}}{2} \right). \quad (58)$$

To calculate the terms  $G^{(1)}$  and  $G^{(2)}$  we note that with Eq. (52)

$$\mathcal{K}' = \frac{\beta}{2} \sum_{i,j} J_{ij} s_i \cdot \Gamma s_j \quad (59)$$

holds. All expectation values factorize, the mean-field contribution (8) becomes

$$G^{(1)} = \frac{\beta}{2} \sum_{i,j} J_{ij} m_i \cdot \Gamma m_j, \quad (60)$$

and from the definition (19)

$$Q_0 \mathcal{K}' = \frac{\beta}{2} \sum_{i,j} J_{ij} \tilde{s}_i \cdot \Gamma \tilde{s}_j \quad \text{with } \tilde{s}_i = s_i - m_i \quad (61)$$

results.

The calculation of the Onsager term is straightforward but needs some more effort. Again using the factorization property and Eq. (A7) the term (22) takes the form

$$G^{(2)} = \frac{\beta^2}{2} \sum_{i,j} J_{ij}^2 X_{ij} \quad (62)$$

with

$$X_{ij} = X_{ji} = (\tilde{s}_j \cdot \Gamma \tilde{s}_i | \tilde{s}_i \cdot \Gamma \tilde{s}_j)_0. \quad (63)$$

This Mori product is treated in Appendix A 4. The result is split into longitudinal, transverse, and mixed contributions:

$$X_{ij} = X_{ij}^{LL} + X_{ij}^{LT} + X_{ji}^{LT} + X_{ij}^{TT}, \quad (64)$$

which are given by

$$X_{ij}^{LL} = \frac{1}{\nu_i} \frac{1}{\nu_j} \Gamma_{ij}^2, \quad (65)$$

$$X_{ij}^{LT} = \frac{1}{\nu_i} \frac{m_i}{\nu_j} [(\Gamma^2)_{ii} - \Gamma_{ij}^2], \quad (66)$$

$$X_{ij}^{TT} = \frac{1}{8} \left( \frac{m_i + m_j}{\nu_i + \nu_j} - \frac{m_i - m_j}{\nu_i - \nu_j} \right) \text{tr}(\mathbf{e}_i \times) \Gamma (\mathbf{e}_j \times) \Gamma + \frac{1}{8} \left( \frac{m_i + m_j}{\nu_i + \nu_j} + \frac{m_i - m_j}{\nu_i - \nu_j} \right) [\gamma^2 - (\Gamma^2)_{ii} - (\Gamma^2)_{jj} + \Gamma_{ij}^2]. \quad (67)$$

The antisymmetric tensor associated with the cross product is denoted by  $(\mathbf{e}_i \times)$ . The quantities  $\Gamma_{ij}$  and  $(\Gamma^2)_{ii}$  are components

$$\Gamma_{ij} = \mathbf{e}_i \cdot \Gamma \mathbf{e}_j, \quad (\Gamma^2)_{ii} = \mathbf{e}_i \cdot \Gamma^2 \mathbf{e}_i \quad (68)$$

of the tensors  $\Gamma$  and  $\Gamma^2$ . To write Eqs. (66) and (67) as short as possible we have not completely eliminated the dummy variables  $\nu_i$  which, however, can easily be done with Eq. (56) and with

$$\frac{1}{\nu_i'} = \frac{\partial m_i}{\partial \nu_i} = \left( \frac{1}{4} - m_i^2 \right). \quad (69)$$

Note that the quantities  $1/\nu_i'$  and  $m_i/\nu_i$  have a physical meaning. They represent the longitudinal and the transverse susceptibilities of the bare system.

Putting things together we find finally with the usual replacement  $J_{ij}^2 \rightarrow J^2/N$

$$G = S_0 + \frac{\beta}{2} \sum_{i,j} J_{ij} \mathbf{m}_i \cdot \Gamma \mathbf{m}_j + \frac{\beta^2 J^2}{4N} \sum_{i,j} X_{ij} \quad (70)$$

and

$$\beta \mathbf{h}_i = \nu_i - \beta \sum_j J_{ij} \Gamma \mathbf{m}_j - \frac{\beta^2 J^2}{2N} \sum_j \frac{\partial X_{ij}}{\partial \mathbf{m}_j}. \quad (71)$$

For given external fields  $\mathbf{h}_i$  the magnetizations  $\mathbf{m}_i$  are determined by the equation of states (71). Provided that these solutions  $\mathbf{m}_i$  are explicitly known all other thermodynamic properties follow from the Gibbs potential (70). Recall that these equations are exact in the thermodynamic limit. They are equivalent to the TAP free energy and the TAP equations for the SK model [1,3].

To the best of the authors' knowledge such results for the quantum  $s=1/2$  spin system have not been published previously. From the analogy to the TAP equations it is expected that these equations will shed some light on the spin glass problem in quantum systems. Certainly the present results are just the basis for this purpose and additional work is needed in this direction.

Some elementary aspects are presented in the following subsections, skipping points which are interesting from the spin glass point of view. Such questions need additional efforts which are far beyond the scope of this work.

Before we go into details a general aspect of our results is pointed out. Note that the transverse contributions (67) to the Onsager term exhibit *energy denominators*. Such denominators are a characteristic feature of all expansions for quantum systems. The denominators are absent in the longitudinal and the mixed contributions given by Eqs. (65) and (66), respectively. As all operators commute this is obvious for the longitudinal part. For the mixed contributions it is a conse-

quence of the cyclic property of the trace operation.

## B. Comparison with classical models

Let us next work out the differences from the classical spin glass. For this we consider a system described again by Eq. (52) where  $\mathbf{S}_i^{\text{cl}}$  represent classical vector spins in three dimensions of length  $S_i^{\text{cl}}=1/2$ . Such a treatment leads to modified Eqs. (70) and (71). Obviously both the entropy term and the  $\nu_i$  have to be replaced by the classical expressions for  $S_0^{\text{cl}}$  and for the  $\nu_i^{\text{cl}}(m_i)$ .

As quantum fluctuations are absent the Onsager term simplifies [compare Eq. (49)]. We obtain

$$X_{ij}^{\text{cl}} = \langle (\tilde{\mathbf{S}}_j^{\text{cl}} \cdot \Gamma \tilde{\mathbf{S}}_i^{\text{cl}}) (\tilde{\mathbf{S}}_i^{\text{cl}} \cdot \Gamma \tilde{\mathbf{S}}_j^{\text{cl}}) \rangle_0 = \text{tr} \chi_i^{\text{cl}} \Gamma \chi_j^{\text{cl}} \Gamma, \quad (72)$$

where the local susceptibility tensor  $\chi_i^{\text{cl}}$  is given by

$$(\chi_i^{\text{cl}})^{\mu\bar{\mu}} = \langle (\tilde{\mathbf{S}}_i^{\text{cl}})^\mu (\tilde{\mathbf{S}}_i^{\text{cl}})^{\bar{\mu}} \rangle_0. \quad (73)$$

Writing again  $X_{ij}^{\text{cl}}$  as a sum of longitudinal, transverse, and mixed terms we find for the transverse term

$$(X_{ij}^{TT})^{\text{cl}} = \frac{m_i m_j}{\nu_i^{\text{cl}} \nu_j^{\text{cl}}} [\gamma^2 - (\Gamma^2)_{ii} - (\Gamma^2)_{jj} + \Gamma_{ij}^2], \quad (74)$$

whereas the other contributions to  $X_{ij}^{\text{cl}}$  are still given by Eqs. (65) and (66) with  $\nu_i(m_i)$  replaced by  $\nu_i^{\text{cl}}(m_i)$ .

Note that no explicit representation exists for  $\nu_i^{\text{cl}}(m_i)$ . Nevertheless this function is well defined via the inverse function

$$m_i = \frac{1}{2} \coth\left(\frac{\nu_i^{\text{cl}}}{2}\right) - \frac{1}{\nu_i^{\text{cl}}} \quad (75)$$

and can be represented by the power expansion

$$\nu_i^{\text{cl}} = 12m_i + \frac{144m_i^3}{5} + \frac{19\,008m_i^5}{175} + O(m_i^7). \quad (76)$$

It should be remarked that for the isotropic case  $\Gamma=\mathbf{1}$  all the results for the classical spins are in agreement with the previous work [4,33] where in addition the explicit expressions for the classical entropy function can be found.

## C. Paramagnetic phase for isotropic interactions

To keep the discussion as simple as possible we specialize to the isotropic case and set  $\Gamma=\mathbf{1}$ . This implies  $\gamma^2=3$ . To explore the paramagnetic limit  $m_i \rightarrow 0$  all terms have to be expanded. We find

$$\nu_i = 4m_i + \frac{16}{3}m_i^3 + O(m_i^5) \quad (77)$$

and

$$X_{ij} = \frac{3}{16} - \frac{1}{12}(5m_i^2 + 5m_j^2 + 2\mathbf{m}_i \cdot \mathbf{m}_j) + O(m_i^4). \quad (78)$$

These expansions lead to the Gibbs potential

$$G = N \ln 2 + N \frac{3}{64} \beta^2 J^2 \quad \text{for } m_i = 0 \quad (79)$$

and to the equation of states



$$\beta h_i = 4m_i - \beta \sum_j J_{ij} m_j + \frac{\beta^2 J^2}{12} \left( 5m_i + N^{-1} \sum_j m_j \right) + O(m_i^3). \quad (80)$$

Obviously the paramagnetic state (all  $m_i=0$ ) is a solution of Eq. (80) for vanishing fields  $h_i=0$ . Employing the standard relations  $U=-\partial G/\partial\beta$  and  $S=G+\beta U$  gives the internal energy  $U$  and the entropy  $S$  of this state:

$$U = -N \frac{3}{32} \beta J^2 \quad \text{and} \quad S = N \ln 2 - N \frac{3}{64} \beta^2 J^2, \quad (81)$$

respectively. For high temperatures  $\beta \rightarrow 0$  these results are expected from the high-temperature expansion according to Sec. III C. In the low-temperature regime, however, both the internal energy and the entropy are not acceptable as both quantities diverge to negative infinity. Consequently there must be a phase with solutions  $m_i \neq 0$  for low temperatures in the zero-field case.

For further analysis we focus on the singularities of the susceptibility matrix  $\chi_{ij}^{\mu\bar{\mu}} = \partial m_i^\mu / \partial h_j^{\bar{\mu}}$ . The inverse matrix is determined by

$$(\chi_{ij}^{-1})^{\mu\bar{\mu}} = \partial h_i^\mu / \partial m_j^{\bar{\mu}} = -\beta^{-1} \partial^2 G / \partial m_i^\mu \partial m_j^{\bar{\mu}}. \quad (82)$$

Reintroducing the expansion parameter  $\alpha$  we find from Eq. (80)

$$\beta (\chi_{ij}^{-1})^{\mu\bar{\mu}} = I_{ij} \delta^{\mu\bar{\mu}} \quad \text{with} \quad I_{ij}^\mu = a \delta_{ij} - b \frac{J_{ij}}{J} + \frac{c}{N} \quad (83)$$

and with the coefficients

$$a = 4 + \frac{5(\alpha\beta J)^2}{12}, \quad b = \alpha\beta J, \quad c = \frac{(\alpha\beta J)^2}{12}. \quad (84)$$

From random-matrix theory [34] the eigenvalue spectrum of the matrix  $I_{ij}$  is well known. It is a superposition of a continuous part

$$\lambda(x) = a - bx \quad \text{with} \quad -2 \leq x \leq 2 \quad (85)$$

and one discrete eigenvalue

$$\lambda_0 = a + c + \frac{b^2}{c} \quad (86)$$

which may be isolated from  $\lambda(x)$ . For the special values of the expansion parameter  $\bar{\alpha}(x)$  and  $\bar{\alpha}_0$  the eigenvalues  $\lambda(x)$  and  $\lambda_0$  vanish, respectively. These values and their absolute values are calculated as

$$\bar{\alpha}(x) = 2 \frac{3x \pm i\sqrt{60-9x^2}}{5\beta J}, \quad \bar{\alpha}_0 = \pm i \frac{4\sqrt{2}}{\beta J}, \quad (87)$$

and to

$$|\bar{\alpha}(x)|^2 = \frac{48}{5} (\beta J)^{-2}, \quad |\bar{\alpha}_0|^2 = 32 (\beta J)^{-2}, \quad (88)$$

respectively. Realize that  $\bar{\alpha}(x)$  has a finite imaginary part for the possible  $x$  values  $|x| \leq 2$ . Thus vanishing eigenvalues of the inverse of the susceptibility and singularities for the susceptibility are possible only for complex  $\bar{\alpha}$  values. In the

complex plane the singularities  $\bar{\alpha}(x)$  are located on two sectors of the circle with radius  $|\bar{\alpha}(x)|$ . As no intersections of these sectors with the real axis exist there are no singularities for real values of  $\alpha$ .

These singularities are of great importance, as already pointed out in [1], to which the reader is referred for more details. The term-by-term treatment of the approach of Sec. II can only be justified in the region of the *complex  $\alpha$  plane* in which the power expansion is convergent. The convergence criterion for a Taylor expansion is given by  $|\alpha| < \rho$  where  $\rho$  is the radius of convergence. The distance from the origin ( $\alpha=0$ ) to the nearest singular point determines this radius  $\rho$ . Thus, in the present case,  $\rho = |\bar{\alpha}(x)|$  holds [35] and the expansion for the paramagnetic solution can be justified only for temperatures  $T$  above the critical temperature

$$T_c = \sqrt{5/3} J/4. \quad (89)$$

Below  $T_c$  the expansion and consequently the paramagnetic solution breaks down and at least one new phase must exist.

For the SK model and the classical vector spin glass (see below) the singularities of the susceptibility in the complex  $\alpha$  plane show a similar behavior. For these systems the singularities are located everywhere on a circle in the complex  $\alpha$  plane. The circle intersects the positive and the negative real axes, which implies two real values of  $\alpha$ . From this point of view both the quantum spin glass and the classical models are quite similar. An important difference, however, results. For the classical models the physical staggered susceptibility diverges at  $T_c$ . Such behavior is not found for the quantum spin glass.

To complete the analysis of the paramagnetic phase we calculate the local susceptibility

$$\chi_{\text{loc}} = \frac{1}{N} \sum_i \chi_{ii}^{\mu\mu} = \beta \int_{-2}^2 \frac{\varrho(x) dx}{4 - \beta J x + 5/12 (\beta J)^2} \quad (90)$$

of the quantum spin glass. Employing the Wigner semicircle law [34] for the density  $\varrho(x) = \sqrt{(4-x^2)}/(2\pi)$  of the eigenvalues and introducing the reduced temperature

$$t = T/T_c = 4\sqrt{3/5} T/J \quad (91)$$

we find by integration

$$\chi_{\text{loc}}^2 = \frac{5(t^4 + 1) + 4t^2 - (t^2 + 1)\sqrt{25t^4 - 10t^2 + 25}}{6J^2 t^2}, \quad (92)$$

which holds for  $t > 1$ . The function  $\chi_{\text{loc}}(t)$  exhibits a maximum at the critical temperature  $t=1$  and decreases with increasing temperature from the value  $J\chi_{\text{loc}}(1) = \left[\frac{1}{3}(7 - 2\sqrt{10})\right]^{1/2} = 0.474498$ . We find  $\chi_{\text{loc}} \rightarrow \beta/4$  for  $\beta \rightarrow 0$ , in agreement with the direct high-temperature expansion.

Equations (80) and (92) give a complete thermodynamic description of the paramagnetic phase above the critical temperature given by Eq. (89). Again the author is not aware of any work that has claimed these results before.

It is of some interest to compare with the classical vector spin glass. The classical results are well known [35] but can easily be rederived. We find with Eq. (76) by expansion

$$X_{ij}^{\text{cl}} = \frac{1}{48} - \frac{1}{12}(m_i^2 + m_j^2) + O(m_i^4).$$

In contrast to Eq. (78), terms proportional to  $\mathbf{m}_i \cdot \mathbf{m}_j$  are not found. This results from the differences between  $(X_{ij}^{\text{TT}})^{\text{cl}}$  and  $X_{ij}^{\text{TT}}$ .

The remaining calculation is completely analogous to the quantum case and leads for the Gibbs potential to

$$G^{\text{cl}} = \text{const} + N(\beta J)^2/192. \quad (93)$$

The matrix  $I_{ij}^{\text{cl}}$  which governs the singularities is calculated as

$$(I_{ij}^{\text{cl}})^{\mu} = (12 + \beta^2 \alpha^2 J^2/12) \delta_{ij} - \beta \alpha J_{ij}. \quad (94)$$

The singular  $\alpha$  values are located on a circle with radius  $|\alpha| = 12(\beta J)^{-1}$ . This leads to a transition temperature of

$$T_c^{\text{cl}} = J/12 \quad (95)$$

and to a local susceptibility of

$$\chi_{\text{loc}}^{\text{cl}} = \beta/12 \quad (96)$$

for  $T \geq T_c^{\text{cl}}$ . The results for all quantities differ. These differences are exclusively caused by the different equation of states of the bare system given by Eqs. (56) and (76). The different expressions for  $X_{ij}^{\text{TT}}$  have no influence.

Obviously these conclusions are restricted to the paramagnetic phase at zero external fields. Incidentally we remark in this context that the ‘‘quantum’’ term  $c/N$  of Eq. (83) is important for systems with an additional (infinite-range) ferromagnetic interaction  $J_0/N$ . Indeed in this case an additional contribution  $-J_0/N$  has to be added to Eq. (83), leading to a competition with the term  $c/N$  due to the different signs.

The replica approaches [17,18] claim for the critical temperature of the quantum spin glass  $T_c \approx J/(4\sqrt{3})$ . These values are determined from the condition  $1 = J\chi_{\text{loc}}(T_c)$  which is a consequence of the assumption [17] that near  $T_c$  the system has a continuous behavior, like a second-order phase transition. Such a behavior, however, is not confirmed by the present work. Moreover Eq. (81) leads for a temperature of  $J/(4\sqrt{3})$  to a negative entropy value of  $S = -1.55685$ , which is impossible for a quantum system. Thus the replica theory values for  $T_c$  must be rejected.

We conclude by noting that the discussion presented in this section can be extended to the general nonisotropic case and to the low-temperature phase on the basis of the presented results. For this purpose all the tools [24,36,37], developed for the understanding of the SK model on the basis of the TAP equations, can be transferred to the quantum spin glass. Work in this direction for the quantum SK model in the presence of a transversal magnetic field will be published separately.

## V. THE WEAKLY NONIDEAL BOSE GAS

### A. The Gibbs potential in second order

The model is described by the Hamiltonian

$$\mathcal{H} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \mathcal{N}_{\mathbf{k}} + \frac{U}{2V} \sum_{\mathbf{p}, \mathbf{q}, \mathbf{k}} b_{\mathbf{p}+\mathbf{k}}^{\dagger} b_{\mathbf{q}-\mathbf{k}}^{\dagger} b_{\mathbf{p}} b_{\mathbf{q}},$$

where  $\epsilon_{\mathbf{k}} = k^2/2m$  is the free-gas spectrum,  $b_{\mathbf{k}}, b_{\mathbf{k}}^{\dagger}$  are bosonic operators,  $\mathcal{N}_{\mathbf{k}} = b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}$  are occupation number operators, and  $V$  is the volume of the gas. The interaction strength  $U$  is assumed to be momentum independent, which corresponds to a  $\delta$  function interaction in real space.

We choose the set of all operators  $\mathcal{N}_{\mathbf{k}}$  as observation level. Thus the operators  $\mathcal{K}_0$ ,  $\mathcal{K}_1$ , and  $\mathcal{K}'$  introduced in Sec. II are given by

$$\mathcal{K}_0 = \sum_{\mathbf{k}} \nu_{\mathbf{k}} \mathcal{N}_{\mathbf{k}}, \quad \mathcal{K}_1 = \sum_{\mathbf{k}} \beta(\mu - \epsilon_{\mathbf{k}}) \mathcal{N}_{\mathbf{k}} \quad (97)$$

and by

$$\mathcal{K}' = -\frac{\beta U}{2V} \sum_{\mathbf{p}, \mathbf{q}, \mathbf{k}} b_{\mathbf{p}+\mathbf{k}}^{\dagger} b_{\mathbf{q}-\mathbf{k}}^{\dagger} b_{\mathbf{p}} b_{\mathbf{q}}. \quad (98)$$

Again we simplify the notation. The variables  $\nu_0^j$  and  $\nu_1^j$  of Sec. II A are denoted by  $\nu_{\mathbf{k}}$  and by  $\beta(\mu - \epsilon_{\mathbf{k}})$ , respectively. We work with the second quantization. Thus  $G_{\alpha}$  represents the Legendre transformation of the logarithm of the grand-canonical partition function and  $\mu$  is the chemical potential.

Let us introduce the notation  $n_{\mathbf{k}} = \langle \mathcal{N}_{\mathbf{k}} \rangle_{\alpha}$ . Then the entropy  $S_0$  of the noninteracting system as function of these variables  $n_{\mathbf{k}}$  is needed and explicitly given by

$$S_0 = \sum_{\mathbf{k}} [(n_{\mathbf{k}} + 1) \ln(n_{\mathbf{k}} + 1) - n_{\mathbf{k}} \ln n_{\mathbf{k}}]. \quad (99)$$

Employing Eq. (9), this leads to

$$\nu_{\mathbf{k}} = \ln n_{\mathbf{k}} - \ln(n_{\mathbf{k}} + 1), \quad (100)$$

which has to be used to eliminate the dummy variables  $\nu_{\mathbf{k}}$ . Note that an equivalent form of the latter equation,

$$n_{\mathbf{k}} = [\exp(-\nu_{\mathbf{k}}) - 1]^{-1}, \quad (101)$$

is the Bose function.

The mean-field or Hartree-Fock contributions are given by Eq. (8) and are immediately calculated to

$$G^{(1)} = -\frac{\beta U}{V} \left( \sum_{\mathbf{p}} n_{\mathbf{p}} \right)^2, \quad (102)$$

where the relation (A36) is used. Similar to the spin glass system, the treatment of the Onsager term is more complicated and therefore is presented in some detail in Appendix A 5. Using the result Eq. (A52) together with Eqs. (99) and (102) we obtain the expansion of the Gibbs potential up to second order in  $U$ ,

$$G(\beta, n_{\mathbf{k}}) = \sum_{\mathbf{k}} [(n_{\mathbf{k}} + 1) \ln(n_{\mathbf{k}} + 1) - n_{\mathbf{k}} \ln n_{\mathbf{k}}] - \frac{\beta U}{V} \sum_{\mathbf{p}, \mathbf{q}} n_{\mathbf{p}} n_{\mathbf{q}} + \frac{\beta^2 U^2}{V^2} \sum_{\mathbf{p}, \mathbf{q}, \mathbf{k}} \frac{n_{\mathbf{p}+\mathbf{k}} n_{\mathbf{q}-\mathbf{k}} (1 + n_{\mathbf{p}} + n_{\mathbf{q}})}{\nu_{\mathbf{p}+\mathbf{k}} + \nu_{\mathbf{q}-\mathbf{k}} - \nu_{\mathbf{p}} - \nu_{\mathbf{q}}} + O(U^3), \quad (103)$$

where in principle all the  $\nu_{\mathbf{k}}$  in the denominator of the

second-order term have to be replaced according to relation (100).

The general Eqs. (9) and (10) lead immediately to the equation of states

$$\beta(\epsilon_{\mathbf{k}} - \mu) = \ln \frac{n_{\mathbf{k}} + 1}{n_{\mathbf{k}}} - \beta \Sigma_{\mathbf{k}}^{(1)} - \beta \Sigma_{\mathbf{k}}^{(2)} - \beta \tilde{\Sigma}_{\mathbf{k}}^{(2)} + O(U^3) \quad (104)$$

where  $\Sigma_{\mathbf{k}}^{(1)}$  and  $\Sigma_{\mathbf{k}}^{(2)} + \tilde{\Sigma}_{\mathbf{k}}^{(2)}$  represent the first- and the second-order contributions to the self-energy given by

$$\Sigma_{\mathbf{k}}^{(1)} = \frac{2U}{V} \sum_{\mathbf{p}} n_{\mathbf{p}}, \quad (105)$$

by

$$\Sigma_{\mathbf{k}}^{(2)} = \frac{2\beta U^2}{V^2} \sum_{\mathbf{p}\mathbf{q}} \frac{n_{\mathbf{p}+\mathbf{q}} n_{\mathbf{k}-\mathbf{q}} - n_{\mathbf{p}}(1 + n_{\mathbf{p}+\mathbf{q}} + n_{\mathbf{k}-\mathbf{q}})}{\nu_{\mathbf{k}} + \nu_{\mathbf{p}} - \nu_{\mathbf{p}+\mathbf{q}} - \nu_{\mathbf{k}-\mathbf{q}}}, \quad (106)$$

and by

$$\begin{aligned} \tilde{\Sigma}_{\mathbf{k}}^{(2)} &= \frac{2\beta U^2}{V^2} \sum_{\mathbf{p}\mathbf{q}} \frac{1}{(\nu_{\mathbf{k}} + \nu_{\mathbf{p}} - \nu_{\mathbf{p}+\mathbf{q}} - \nu_{\mathbf{k}-\mathbf{q}})^2} \\ &\times \left( \frac{n_{\mathbf{p}}(1 + n_{\mathbf{p}+\mathbf{q}})(1 + n_{\mathbf{k}-\mathbf{q}})}{(1 + n_{\mathbf{k}})} - \frac{(1 + n_{\mathbf{p}})n_{\mathbf{p}+\mathbf{q}}n_{\mathbf{k}-\mathbf{q}}}{n_{\mathbf{k}}} \right). \end{aligned} \quad (107)$$

Note that  $\tilde{\Sigma}_{\mathbf{k}}^{(2)}$  results from the application of the chain rule for differentiation to  $(\nu_{\mathbf{p}+\mathbf{k}} + \nu_{\mathbf{q}-\mathbf{k}} - \nu_{\mathbf{p}} - \nu_{\mathbf{q}})^{-1}$ .

The main part of the general results Eqs. (103)–(107) are well known in literature. Trivially this applies to the zero-order contributions. All first-order terms represent the usual Hartree-Fock expressions [19,20] for an interaction that is momentum independent. The second-order contribution  $\Sigma_{\mathbf{k}}^{(2)}$  to the self-energy looks like typical expressions calculated by the Green's function approaches [38].

Contributions like  $\tilde{\Sigma}_{\mathbf{k}}^{(2)}$  that contain the square of  $(\nu_{\mathbf{k}} + \nu_{\mathbf{p}} - \nu_{\mathbf{p}+\mathbf{q}} - \nu_{\mathbf{k}-\mathbf{q}})$  in the denominator are usually not considered or discussed by the standard Green's function treatments. In this situation some arguments are presented for the relevance of this contribution in the next section.

## B. Discussion

The first argument for the importance of the contribution  $\tilde{\Sigma}_{\mathbf{p}}^{(2)}$  is rather general. Note that this quantity enters in the susceptibility matrix that is defined as  $\chi_{\mathbf{p}\mathbf{q}} = -\partial n_{\mathbf{p}} / \partial(\epsilon_{\mathbf{q}} - \mu)$ . Indeed the inverse matrix is given by

$$\begin{aligned} \chi_{\mathbf{p}\mathbf{q}}^{-1} &= -\frac{1}{\beta} \frac{\partial^2 G}{\partial n_{\mathbf{p}} \partial n_{\mathbf{q}}} \\ &= \frac{\delta_{\mathbf{p}\mathbf{q}}}{\beta n_{\mathbf{p}}(1 + n_{\mathbf{p}})} + \frac{2U}{V} + \frac{\partial \Sigma_{\mathbf{p}}^{(2)}}{\partial n_{\mathbf{q}}} + \frac{\partial \tilde{\Sigma}_{\mathbf{p}}^{(2)}}{\partial n_{\mathbf{q}}} + O(U^3). \end{aligned} \quad (108)$$

This matrix governs the stability of the system and a funda-

mental property of this matrix is the symmetry relation  $\chi_{\mathbf{p}\mathbf{q}}^{-1} = \chi_{\mathbf{q}\mathbf{p}}^{-1}$ . Thus neglecting or modifying some terms of  $\chi_{\mathbf{q}\mathbf{p}}^{-1}$  results in general in a violation of this relation with serious consequences.

Various investigations exist for the weakly interacting Bose gas in the literature. In particular the equation of state at the critical point of the Bose-Einstein transition was recently discussed in [20]. As argued in this work, the transition

$$n_{\mathbf{q}} \gg 1 \quad (109)$$

can be used in all equations. With this approximation we find in leading order

$$\Sigma_{\mathbf{k}}^{(2)} = -\frac{2\beta U^2}{V^2} \sum_{\mathbf{p}\mathbf{q}} \frac{n_{\mathbf{p}+\mathbf{q}} n_{\mathbf{k}-\mathbf{q}} n_{\mathbf{p}} \left( \frac{n_{\mathbf{k}}}{n_{\mathbf{p}}} - \frac{n_{\mathbf{k}}}{n_{\mathbf{p}+\mathbf{q}}} - \frac{n_{\mathbf{k}}}{n_{\mathbf{k}-\mathbf{q}}} \right)}{1 + \frac{n_{\mathbf{k}}}{n_{\mathbf{p}}} - \frac{n_{\mathbf{k}}}{n_{\mathbf{p}+\mathbf{q}}} - \frac{n_{\mathbf{k}}}{n_{\mathbf{k}-\mathbf{q}}}} \quad (110)$$

and

$$\tilde{\Sigma}_{\mathbf{k}}^{(2)} = -\frac{2\beta U^2}{V^2} \sum_{\mathbf{p}\mathbf{q}} \frac{n_{\mathbf{p}+\mathbf{q}} n_{\mathbf{k}-\mathbf{q}} n_{\mathbf{p}}}{1 + \frac{n_{\mathbf{k}}}{n_{\mathbf{p}}} - \frac{n_{\mathbf{k}}}{n_{\mathbf{p}+\mathbf{q}}} - \frac{n_{\mathbf{k}}}{n_{\mathbf{k}-\mathbf{q}}}}. \quad (111)$$

Both contributions  $\Sigma_{\mathbf{k}}^{(2)}$  and  $\tilde{\Sigma}_{\mathbf{k}}^{(2)}$  to the second-order self-energy are of the same order of magnitude, which demonstrates again the relevance of  $\tilde{\Sigma}_{\mathbf{k}}^{(2)}$ .

Using  $n_{\mathbf{q}} \gg 1$  we find as approximation for the equation of states:

$$\epsilon_{\mathbf{k}} - \mu = \frac{1}{\beta n_{\mathbf{k}}} - \frac{2U}{V} \sum_{\mathbf{p}} n_{\mathbf{p}} + \frac{2\beta U^2}{V^2} \sum_{\mathbf{p}\mathbf{q}} n_{\mathbf{p}+\mathbf{q}} n_{\mathbf{k}-\mathbf{q}} n_{\mathbf{p}}, \quad (112)$$

and as approximation for the inverse of the susceptibility:

$$\chi_{\mathbf{k}\mathbf{k}'}^{-1} = \frac{\delta_{\mathbf{k}\mathbf{k}'}}{\beta n_{\mathbf{k}}^2} + \frac{2U}{V} - \frac{2\beta U^2}{V^2} \sum_{\mathbf{q}} n_{\mathbf{q}+\mathbf{k}} (2n_{\mathbf{q}+\mathbf{k}'} + n_{\mathbf{k}'-\mathbf{q}}). \quad (113)$$

By a change of the summation index it is elementary to show the symmetry of  $\chi_{\mathbf{k}\mathbf{k}'}^{-1}$ , which is not surprising as both  $\Sigma_{\mathbf{k}}^{(2)}$  and  $\tilde{\Sigma}_{\mathbf{k}}^{(2)}$  are included in Eq. (113).

All perturbations of  $\chi_{\mathbf{k}\mathbf{k}'}^{-1}$  are of the order  $V^{-1}$  and can therefore be neglected [39]. This implies that it is the  $\mathbf{k}=\mathbf{0}$  mode which becomes unstable at the critical temperature. Such a behavior was assumed in the analysis [20] without any proof and the present approach confirms this assumption.

Considering next the equation of states (112) we note that  $n_{\mathbf{q}} \gg 1$  implies the approximation [compare Eq. (101)]

$$n_{\mathbf{q}}^{-1} = -\nu_{\mathbf{q}} = \beta(\hat{\epsilon}_{\mathbf{q}} - \hat{\mu}), \quad (114)$$

where we have introduced in addition the dressed energy  $\hat{\epsilon}_{\mathbf{q}}$  and the dressed chemical potential  $\hat{\mu}$  as the  $\mathbf{q}$ -dependent and the  $\mathbf{q}$ -independent parts of  $-\nu_{\mathbf{q}}/\beta$ , respectively. Setting the average value of the density  $n = V^{-1} \sum_{\mathbf{p}} n_{\mathbf{p}}$  the equation of

states (112) can be written in terms of the dressed variables as

$$\epsilon_{\mathbf{k}} - \mu = \hat{\epsilon}_{\mathbf{k}} - \hat{\mu} - 2Un + \frac{2U^2}{\beta^2 V^2} \sum_{\mathbf{p}\mathbf{q}} \frac{1}{(\hat{\epsilon}_{\mathbf{p}+\mathbf{q}} - \hat{\mu})(\hat{\epsilon}_{\mathbf{k}-\mathbf{q}} - \hat{\mu})(\hat{\epsilon}_{\mathbf{p}} - \hat{\mu})}. \quad (115)$$

This is in complete agreement with the equation derived in [20], within the frameworks of both the Green's function and the Ursell operators. Thus we conclude that the expansion of the Gibbs potential is an alternative to other approaches for many-body systems of identical particles.

Apart from this important conclusion for the present work we remark that detailed numerical investigations of the presented result are expected to be an interesting object of further research. Indeed, a complete numerical analysis of Eqs. (103) and (104), which should include the entire temperature regime, may potentially give some new insight into the Bose-Einstein condensation for weakly interacting gases. This expectation is based on the impressive success of these equations for calculating the shift of the critical temperature of the transition [19,20].

## VI. CONCLUSIONS

In this paper we have presented a systematic power expansion of the Gibbs potential for arbitrary many-particle systems including in particular all kinds of quantum systems. By developing and employing generalized projector techniques, we were able to present explicit formulas which permit the calculation of the contributions up to an arbitrary order of the expansion for general systems. After a detailed discussion of the general results the method is applied to two nontrivial systems, the quantum spin glass with infinite-ranged interactions and the weakly interacting Bose gas. The contributions up to the Onsager terms, which are the lowest beyond-mean-field terms, have been worked out, leading to additional results or confirming recent results for these special systems.

The present method has several advantages compared to other techniques. The method can be applied for all kinds of interacting systems including, in particular, systems of identical particles, classical or quantum spin systems, and combinations of these systems. No other technique seems to have such a wide spectrum of applications.

Compared to the effort needed within the Green's function or the Ursell operator approach the expansion of the Gibbs potential is rather simple, direct, and straightforward. In particular, no partial summations are needed for the present approach to find the mean-field and the beyond-mean-field contributions to the self-energy.

As a further advantage the present approach usually gives criteria directly for the convergence of the expansion. Within the framework of other techniques additional investigations are usually needed to obtain this information.

The application of the cavity method [9] is very common for spin glasses and related problems. This method often

allows convincing interpretations of the low-order terms of formal expansions. The cavity approach was originally developed for classical systems. To treat in addition quantum spin glasses, the work [40] has been presented, which uses Trotter-Suzuki transformations and maps the quantum spin systems into classical spin models. Such treatments work only for special problems and cannot be generalized to all quantum systems. Thus the existing extensions of the cavity method to quantum systems are restricted. The present Gibbs potential approach, however, works for general quantum systems.

Summing up we conclude that the power expansion approach may potentially represent a serious alternative to the other, well-settled methods to treat the statics of many-particle systems. Certainly more applications must be worked out to confirm this possibility.

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## APPENDIX A: MATHEMATICAL DETAILS

### 1. Some properties of the Mori scalar product

Since the projector formalism is not very common, we list some elementary relations of this approach that are used in the present work. For further details and explicit proofs of these relations we refer to [28].

Apart from the general properties which are required for any scalar product the definition of the original Mori product (13) implies some additional properties. Let  $\mathcal{U}$  and  $\mathcal{V}$  be two arbitrary elements; then the relations

$$(\mathcal{U}|\mathcal{V})_{\alpha} = (\mathcal{V}^{\dagger}|\mathcal{U}^{\dagger})_{\alpha} = (\mathcal{V}|\mathcal{U})_{\alpha}^{*} = (\mathcal{U}^{\dagger}|\mathcal{V}^{\dagger})_{\alpha}^{*} \quad (A1)$$

and the Kubo identity

$$(\mathcal{U}[[\mathcal{K}_{\alpha}, \mathcal{V}]])_{\alpha} = \langle [\mathcal{V}, \mathcal{U}^{\dagger}] \rangle_{\alpha} \quad (A2)$$

can be proved from the definition and the invariance of the trace to cyclic permutations. The property (A2) implies the useful relation for special operators  $\mathcal{W}$ . If  $[\mathcal{K}_{\alpha}, \mathcal{W}] = \omega \mathcal{W}$  with  $\omega \neq 0$  is satisfied,

$$\omega(\mathcal{V}|\mathcal{W})_{\alpha} = \langle [\mathcal{W}, \mathcal{V}^{\dagger}] \rangle_{\alpha} \quad (A3)$$

results.

Equations (13) and (A1) yield for the scalar product of the unit operator 1 with an observable

$$(1|\mathcal{U})_{\alpha} = \langle \mathcal{U} \rangle_{\alpha} \quad \text{and} \quad (\mathcal{U}|1)_{\alpha} = \langle \mathcal{U}^{\dagger} \rangle_{\alpha}, \quad (A4)$$

and for fluctuations of observables  $\tilde{\mathcal{U}} = \mathcal{U} - \langle \mathcal{U} \rangle_{\alpha}$  one finds

$$(\mathcal{U}|\tilde{\mathcal{V}})_{\alpha} = (\tilde{\mathcal{U}}|\tilde{\mathcal{V}})_{\alpha} = (\tilde{\mathcal{U}}|\tilde{\mathcal{V}})_{\alpha} = (\mathcal{U}|\mathcal{V})_{\alpha} - \langle \mathcal{U}^{\dagger} \rangle_{\alpha} \langle \mathcal{V} \rangle_{\alpha}. \quad (A5)$$

The projectors  $P_{\alpha}$  and  $Q_{\alpha}$  are Hermitian in Liouville space and idempotent which implies with the definitions (19) the relations

$$(\mathcal{U}|\mathcal{P}_\alpha\mathcal{V})_\alpha = (\mathcal{P}_\alpha\mathcal{U}|\mathcal{V})_\alpha = (\mathcal{P}_\alpha\mathcal{U}|\mathcal{P}_\alpha\mathcal{V})_\alpha \quad (\text{A6})$$

and

$$(\mathcal{U}|\mathcal{Q}_\alpha\mathcal{V})_\alpha = (\mathcal{Q}_\alpha\mathcal{U}|\mathcal{V})_\alpha = (\mathcal{Q}_\alpha\mathcal{U}|\mathcal{Q}_\alpha\mathcal{V})_\alpha. \quad (\text{A7})$$

For later use it is noted that

$$(\tilde{\mathcal{A}}^k|\mathcal{Q}_\alpha\mathcal{U})_\alpha = 0 \quad (\text{A8})$$

according to Eq. (A7) and  $\mathcal{Q}_\alpha\tilde{\mathcal{A}}^k=0$ .

Let  $c$  be a complex number and let  $\mathbf{B}=\mathcal{B}_1*\mathcal{B}_2*\dots*\mathcal{B}_n$  be a  $*$  product. Then the definition (24) immediately yields

$$(\mathcal{U}|\mathbf{B}*c1)_\alpha = c(\mathcal{U}|\mathbf{B})_\alpha. \quad (\text{A9})$$

Again for later use we finally note that

$$(1|(\mathcal{Q}_\alpha\mathcal{K}')*(\mathcal{P}_\alpha\mathbf{B}))_\alpha = 0 \quad (\text{A10})$$

holds. To prove this result we recall that  $\mathcal{P}_\alpha\mathbf{B}$  represents a linear combination of the unity operator and the  $\tilde{\mathcal{A}}^k$ , whereas  $\mathcal{Q}_\alpha\mathcal{K}'$  does not contain such terms. Thus the thermal averaging eliminates all contributions.

## 2. The derivative of $\mathbf{E}_\alpha$

Let  $\mathcal{X}$  be an ordered product of  $n$  operators  $\mathcal{B}_k(\lambda_k)$ ,

$$\mathcal{X} = \mathcal{T}\mathcal{B}_1(\lambda_1)\mathcal{B}_2(\lambda_2)\dots\mathcal{B}_n(\lambda_n) \quad (\text{A11})$$

where the  $\lambda$  dependencies are given by Eq. (12). Assuming  $\lambda_1 < \lambda_2 < \dots < \lambda_n$  this product is already ordered and can be rewritten as

$$\mathcal{X} = e^{\lambda_1\mathcal{K}_\alpha}\mathcal{B}_1e^{(\lambda_2-\lambda_1)\mathcal{K}_\alpha}\mathcal{B}_2e^{(\lambda_3-\lambda_2)\mathcal{K}_\alpha}\dots\mathcal{B}_ne^{-\lambda_n\mathcal{K}_\alpha}. \quad (\text{A12})$$

From Eq. (14) one finds by elementary substitutions

$$\partial_\alpha e^{(\lambda_{k+1}-\lambda_k)\mathcal{K}_\alpha} = e^{-\lambda_k\mathcal{K}_\alpha} \int_{\lambda_k}^{\lambda_{k+1}} \frac{\partial\mathcal{K}_\alpha}{\partial\alpha}(\lambda)d\lambda e^{\lambda_{k+1}\mathcal{K}_\alpha} \quad (\text{A13})$$

and obtains

$$\begin{aligned} \partial_\alpha\mathcal{X} &= \int_0^{\lambda_1} \frac{\partial\mathcal{K}_\alpha}{\partial\alpha}(\lambda)d\lambda \mathcal{X} \\ &+ \mathcal{B}_1(\lambda_1) \int_{\lambda_1}^{\lambda_2} \frac{\partial\mathcal{K}_\alpha}{\partial\alpha}(\lambda)d\lambda \mathcal{B}_2(\lambda_2)\dots\mathcal{B}_n(\lambda_n) \\ &\vdots + \mathcal{B}_1(\lambda_1)\mathcal{B}_2(\lambda_2)\dots \int_{\lambda_{n-1}}^{\lambda_n} \frac{\partial\mathcal{K}_\alpha}{\partial\alpha}(\lambda)d\lambda \mathcal{B}_n(\lambda_n) \\ &+ \mathcal{X} \int_{\lambda_n}^0 \frac{\partial\mathcal{K}_\alpha}{\partial\alpha}(\lambda)d\lambda, \end{aligned}$$

provided that all the operators  $\mathcal{B}_k$  are independent of  $\alpha$ . The integral of the last term is rewritten with Eq. (12) as

$$\int_{\lambda_n}^0 \frac{\partial\mathcal{K}_\alpha}{\partial\alpha}(\lambda)d\lambda = \int_{\lambda_n}^1 \frac{\partial\mathcal{K}_\alpha}{\partial\alpha}(\lambda)d\lambda - \mathbb{E}_\alpha\{\partial_\alpha\mathcal{K}_\alpha\}. \quad (\text{A14})$$

Recalling the definition of the ordering operator  $\mathcal{T}$  the expression for  $\partial_\alpha\mathcal{X}$  simplifies to

$$\partial_\alpha\mathcal{X} = -\mathcal{X}\mathbb{E}_\alpha\{\partial_\alpha\mathcal{K}_\alpha\} + \int_0^1 d\lambda \mathcal{T} \frac{\partial\mathcal{K}_\alpha}{\partial\alpha}(\lambda)\mathcal{X}. \quad (\text{A15})$$

From Eqs. (14), (17), and (19)

$$\begin{aligned} \partial_\alpha\mathcal{K}_\alpha &= \mathcal{K}' + \sum_i \mathcal{A}^i \partial_\alpha \nu_\alpha^i \\ &= \mathcal{Q}_\alpha\mathcal{K}' + \langle\mathcal{K}'\rangle_\alpha + \sum_i \langle\mathcal{A}^i\rangle_\alpha \partial_\alpha \nu_\alpha^i = \mathcal{Q}_\alpha\mathcal{K}' + c \end{aligned}$$

results, where  $c$  is a number. For such numbers the relations  $\mathbb{E}_\alpha\{c\}=c$  and  $\mathcal{T}c\mathcal{X}=c\mathcal{X}$  hold. Replacing  $\partial_\alpha\mathcal{K}_\alpha$  by  $\mathcal{Q}_\alpha\mathcal{K}' + c$  in Eq. (A15) leads to

$$\partial_\alpha\mathcal{X} = -\mathcal{X}\mathbb{E}_\alpha\{\mathcal{Q}_\alpha\mathcal{K}'\} + \int_0^1 d\lambda \mathcal{T}(\mathcal{Q}_\alpha\mathcal{K}')(\lambda)\mathcal{X} \quad (\text{A16})$$

as the terms proportional to  $c$  cancel.

Note that the result (A16) does not change for any other order of the operators  $\mathcal{B}_k$  in Eq. (A11). Therefore the above restriction on the  $\lambda_k$  can be dropped and the  $\lambda_k$  integration yields finally

$$\begin{aligned} \partial_\alpha\mathbb{E}_\alpha\{\mathcal{B}_1*\dots*\mathcal{B}_n\} &= \mathbb{E}_\alpha\{\mathcal{Q}_\alpha\mathcal{K}'*\mathcal{B}_1*\dots*\mathcal{B}_n\} \\ &- \mathbb{E}_\alpha\{\mathcal{B}_1*\dots*\mathcal{B}_n\}\mathbb{E}_\alpha\{\mathcal{Q}_\alpha\mathcal{K}'\}. \end{aligned} \quad (\text{A17})$$

With Eq. (20) this result is equivalent to Eq. (25) in the text provided that all operators are independent of  $\alpha$ . If the  $\mathcal{B}_k$  depend on  $\alpha$  it is obvious that the inner derivatives have to be added and one gets the full Eq. (25).

## 3. The derivative of $\mathbf{P}_\alpha$

Let  $\mathbf{B}=\mathcal{B}_1*\mathcal{B}_2*\dots*\mathcal{B}_n$  be a  $*$  product. Then the definition (19) immediately yields

$$\begin{aligned} \partial_\alpha\mathbf{P}_\alpha\mathbf{B} &= \partial_\alpha(1|\mathbf{B})_\alpha + \sum_{ij} \tilde{\mathcal{A}}^i \Gamma_\alpha^{ij} \partial_\alpha(\tilde{\mathcal{A}}^j|\mathbf{B})_\alpha + \sum_{ij} \tilde{\mathcal{A}}^i [\partial_\alpha\Gamma_\alpha^{ij}] \\ &\times (\tilde{\mathcal{A}}^j|\mathbf{B})_\alpha. \end{aligned} \quad (\text{A18})$$

From Eq. (26) one finds

$$\partial_\alpha(1|\mathbf{B})_\alpha = (1|(\mathcal{Q}_\alpha\mathcal{K}')*\mathbf{B})_\alpha + (1|\partial_\alpha\mathbf{B})_\alpha, \quad (\text{A19})$$

and

$$\partial_\alpha(\tilde{\mathcal{A}}^i|\mathbf{B})_\alpha = (\tilde{\mathcal{A}}^i|(\mathcal{Q}_\alpha\mathcal{K}')*\mathbf{B})_\alpha + (\tilde{\mathcal{A}}^i|\partial_\alpha\mathbf{B})_\alpha. \quad (\text{A20})$$

Again with Eq. (19) these two relations permit one to rewrite the first two terms of Eq. (A18), which leads to

$$\partial_\alpha\mathbf{P}_\alpha\mathbf{B} = \mathbf{P}_\alpha(\mathcal{Q}_\alpha\mathcal{K}')*\mathbf{B} + \mathbf{P}_\alpha\partial_\alpha\mathbf{B} + \sum_{ij} \tilde{\mathcal{A}}^i [\partial_\alpha\Gamma_\alpha^{ij}](\tilde{\mathcal{A}}^j|\mathbf{B})_\alpha. \quad (\text{A21})$$

Differentiation of Eq. (18) and employing again Eq. (26) leads to

$$\partial_\alpha\Gamma_\alpha^{ij} = -\sum_{kl} \Gamma_\alpha^{ik}(\tilde{\mathcal{A}}^k|\mathcal{Q}_\alpha\mathcal{K}'*\tilde{\mathcal{A}}^l)_\alpha\Gamma_\alpha^{lj}, \quad (\text{A22})$$

and with Eq. (19) to

$$\begin{aligned} \sum_j (\partial_\alpha \Gamma_\alpha^{ij})(\tilde{\mathcal{A}}^j|\mathbf{B})_\alpha &= - \sum_k \Gamma_\alpha^{ik}(\tilde{\mathcal{A}}^k|(\mathcal{Q}_\alpha \mathcal{K}') * (\mathbb{P}_\alpha \mathbf{B}))_\alpha \\ &+ \sum_k \Gamma_\alpha^{ik}(\tilde{\mathcal{A}}^k|(\mathcal{Q}_\alpha \mathcal{K}') * (1|\mathbf{B})_\alpha)_\alpha. \end{aligned} \quad (\text{A23})$$

The Mori product in the second term of Eq. (A23) can be written as  $(1|\mathbf{B})_\alpha(\tilde{\mathcal{A}}^k|(\mathcal{Q}_\alpha \mathcal{K}'))_\alpha$  according to Eq. (A9). Due to Eq. (A8)  $(\tilde{\mathcal{A}}^k|(\mathcal{Q}_\alpha \mathcal{K}'))_\alpha=0$  holds and it is just the first term of Eq. (A23) that remains. The multiplication of Eq. (A23) with  $\tilde{\mathcal{A}}^i$  and a summation yield

$$\sum_{ij} \tilde{\mathcal{A}}^i(\partial_\alpha \Gamma_\alpha^{ij})(\tilde{\mathcal{A}}^j|\mathbf{B})_\alpha = - \mathbb{P}_\alpha(\mathcal{Q}_\alpha \mathcal{K}') * (\mathbb{P}_\alpha \mathbf{B}), \quad (\text{A24})$$

where in addition the relation (A10) was used. Equation (A24) combined with Eq. (A21) finally leads to Eq. (27) of the text.

#### 4. Calculation of $X_{ij} = \langle \tilde{s}_j \cdot \Gamma \tilde{s}_i | \tilde{s}_i \cdot \Gamma \tilde{s}_j \rangle_0$

According to the definition (13) of the Mori product we have to calculate the quantity

$$X_{ij} = \int_0^1 d\lambda \langle \tilde{s}_j \cdot \Gamma \tilde{s}_i | \tilde{s}_i(\lambda) \cdot \Gamma \tilde{s}_j(\lambda) \rangle_0. \quad (\text{A25})$$

First the  $\lambda$  dependence of  $s_i(\lambda)$  is considered. We set  $\alpha=0$  in the definition (12) and find from the rules of the spin  $s=\frac{1}{2}$  algebra

$$s_i(\lambda) = e^{\lambda \nu_i s_i} s_i e^{-\lambda \nu_i s_i} = \mathbf{\Omega}_i(\lambda) s_i, \quad (\text{A26})$$

where the tensor  $\mathbf{\Omega}_i(\lambda)$  describes a rotation of the imaginary angle  $-i\lambda \nu_i$  about the axis  $\mathbf{e}_i$

$$\mathbf{\Omega}_i(\lambda) = e^{-i\lambda(\nu_i \times)} = \mathbf{\Pi}_i + \mathbf{\Omega}_i^T(\lambda),$$

$$\mathbf{\Omega}_i^T(\lambda) = -i \sinh(\lambda \nu_i)(\mathbf{e}_i \times) - \cosh(\lambda \nu_i)(\mathbf{e}_i \times)^2 \quad (\text{A27})$$

and where  $\mathbf{\Pi}_i$  and  $\mathbf{\Omega}_i^T(\lambda)$  are the longitudinal and the transverse parts of  $\mathbf{\Omega}_i(\lambda)$ , respectively. The tensor  $\mathbf{\Pi}_i$  is the projector onto the  $\mathbf{e}_i$  direction and  $(\mathbf{e}_i \times)$  represents the antisymmetric tensor associated with the cross product of two vectors. For further use the relations

$$\mathbf{\Pi}_i = \mathbf{\Pi}_i^2 \quad (\mathbf{e}_i \times)^2 = \mathbf{\Pi}_i - \mathbf{1}, \quad \mathbf{\Omega}_i^T(\lambda) \mathbf{\Pi}_i = 0 \quad (\text{A28})$$

and

$$\mathbf{\Omega}_i^T(\lambda_1 + \lambda_2) = \mathbf{\Omega}_i^T(\lambda_1) \mathbf{\Omega}_i^T(\lambda_2), \quad \mathbf{\Omega}_i(\lambda) \mathbf{m}_i = \mathbf{m}_i,$$

$$\{\mathbf{\Omega}_i(\lambda) \mathbf{a}\} \cdot \mathbf{b} = \mathbf{a} \cdot \mathbf{\Omega}_i(-\lambda) \mathbf{b} \quad (\text{A29})$$

are noted where  $\mathbf{a}$  and  $\mathbf{b}$  are arbitrary vectors. Using these relations and Eq. (A26) the  $\lambda$ -dependent part of Eq. (A25) is rewritten as

$$\tilde{s}_i(\lambda) \cdot \Gamma \tilde{s}_j(\lambda) = [\mathbf{\Omega}_j(-\lambda) \Gamma \mathbf{\Omega}_i(\lambda) \tilde{s}_i] \cdot \tilde{s}_j. \quad (\text{A30})$$

Let  $\mathbf{a}$  and  $\mathbf{b}$  be any two vectors (or two vector operators which commute with  $s_i$ ). From the well-known identity

$$(\mathbf{s}_i \cdot \mathbf{a})(\mathbf{b} \cdot \mathbf{s}_i) = \mathbf{a} \cdot \left( \frac{1}{4} - \frac{i}{2}(\mathbf{s}_i \times) \right) \mathbf{b} \quad (\text{A31})$$

it is elementary to prove the relation

$$\langle (\tilde{s}_i \cdot \mathbf{a})(\mathbf{b} \cdot \tilde{s}_i) \rangle_0 = \mathbf{a} \cdot \mathbf{\Theta}_i(1/2) \mathbf{b} \quad (\text{A32})$$

where we have introduced

$$\mathbf{\Theta}_i(\lambda) = \frac{\mathbf{\Pi}_i}{\nu_i} + \frac{\mathbf{\Omega}_i^T(\lambda)}{4 \cosh(\nu_i/2)} \quad (\text{A33})$$

and

$$\frac{1}{\nu_i} = \frac{\partial m_i}{\partial \nu_i} = \left( \frac{1}{4} - m_i^2 \right). \quad (\text{A34})$$

Using the partial result (A30) and the relations (A28) and (A29) and applying the identity (A32) twice, we find

$$X_{ij} = \int_0^1 d\lambda \text{tr} \mathbf{\Theta}_i(1/2 - \lambda) \Gamma \mathbf{\Theta}_j(\lambda - 1/2) \Gamma \quad (\text{A35})$$

where tr stands for the trace in the three-dimensional real vector space. The  $\lambda$  dependence of  $\mathbf{\Theta}_i(\lambda)$  is explicitly known and the integration finally leads to Eqs. (64)–(67).

#### 5. Calculation of Onsager term of the Bose gas

First some elementary relations are deduced for later use. The definition  $n_{\mathbf{k}} = \langle \mathcal{N}_{\mathbf{k}} \rangle_0$  leads directly to  $dn_{\mathbf{k}}/d\nu_{\mathbf{k}} = \langle \mathcal{N}_{\mathbf{k}}^2 \rangle_0 - n_{\mathbf{k}}^2$ . From Eq. (101) we find  $dn_{\mathbf{k}}/d\nu_{\mathbf{k}} = n_{\mathbf{k}}(1 + n_{\mathbf{k}})$  and thus

$$\langle \mathcal{N}_{\mathbf{k}}^2 \rangle_0 = n_{\mathbf{k}}(1 + 2n_{\mathbf{k}}). \quad (\text{A36})$$

Generalizing this procedure to higher order we find

$$\langle \mathcal{N}_{\mathbf{k}}^3 \rangle_0 = n_{\mathbf{k}}(1 + 6n_{\mathbf{k}} + 6n_{\mathbf{k}}^2) \quad (\text{A37})$$

and

$$\langle \mathcal{N}_{\mathbf{k}}^4 \rangle_0 = n_{\mathbf{k}}(1 + 14n_{\mathbf{k}} + 36n_{\mathbf{k}}^2 + 24n_{\mathbf{k}}^3). \quad (\text{A38})$$

Equation (A36) and the factorization property lead to

$$\langle \hat{\mathcal{N}}_{\mathbf{k}} | \hat{\mathcal{N}}_{\mathbf{k}'} \rangle_0 = \delta_{\mathbf{k}\mathbf{k}'} \langle \hat{\mathcal{N}}_{\mathbf{k}}^2 \rangle_0 = \delta_{\mathbf{k}\mathbf{k}'} n_{\mathbf{k}}(1 + n_{\mathbf{k}}). \quad (\text{A39})$$

The  $\tilde{\mathcal{N}}_{\mathbf{k}}$  commute with  $\mathcal{K}_0$ . Therefore  $(\tilde{\mathcal{N}}_{\mathbf{k}} | \mathcal{U})_0 = \langle \tilde{\mathcal{N}}_{\mathbf{k}} \mathcal{U} \rangle_0$  holds. This implies that the projector  $\mathbb{P}_0$  defined by Eq. (19) simplifies to

$$\mathbb{P}_0 \mathcal{U} = \langle \mathcal{U} \rangle_0 + \sum_{\mathbf{k}} \frac{\langle \tilde{\mathcal{N}}_{\mathbf{k}} \mathcal{U} \rangle_0}{n_{\mathbf{k}}(1 + n_{\mathbf{k}})} \tilde{\mathcal{N}}_{\mathbf{k}}, \quad (\text{A40})$$

where  $\mathcal{U}$  is any Hilbert space operator.

Let us introduce a shorthand notation by

$$\mathcal{B}_{\mathbf{p}\mathbf{q}\mathbf{k}} = b_{\mathbf{p}+\mathbf{k}}^\dagger b_{\mathbf{q}-\mathbf{k}}^\dagger b_{\mathbf{p}} b_{\mathbf{q}}. \quad (\text{A41})$$

Then the interaction Hamiltonian (98) is rewritten as a sum of two contributions

$$\mathcal{K}' = - \frac{\beta U}{2V} \mathcal{Y} = - \frac{\beta U}{2V} (\mathcal{Y}^{(1)} + \mathcal{Y}^{(2)}) \quad (\text{A42})$$

with

$$\mathcal{Y}^{(1)} = 2 \sum_{\mathbf{p} \neq \mathbf{q}} \mathcal{N}_{\mathbf{p}} \mathcal{N}_{\mathbf{q}} + \sum_{\mathbf{p}} \{\mathcal{N}_{\mathbf{p}}^2 - \mathcal{N}_{\mathbf{p}}\}, \quad (\text{A43})$$

$$\mathcal{Y}^{(2)} = \sum_{\mathbf{p}\mathbf{q}\mathbf{k} \neq (0, \mathbf{q}-\mathbf{p})} \mathcal{B}_{\mathbf{p}\mathbf{q}\mathbf{k}}. \quad (\text{A44})$$

With these definitions the Onsager term (22) can be expressed as

$$G^{(2)} = \frac{\beta^2 U^2}{4V^2} \{(\mathcal{Y}|Q_0 \mathcal{Y}_1)_0 + (\mathcal{Y}|\mathcal{Y}_2)_0\}, \quad (\text{A45})$$

where we have already used that  $\langle \mathcal{Y}_2 \rangle_0 = 0$  and  $\langle \tilde{\mathcal{N}}_{\mathbf{k}} \mathcal{Y}_2 \rangle_0 = 0$  and consequently  $P_0 \mathcal{Y}_2 = 0$  holds according to Eq. (A40).

The two terms of Eq. (A45) will be treated separately. As  $Q_0 \mathcal{N}_{\mathbf{p}} \mathcal{N}_{\mathbf{q}} = \tilde{\mathcal{N}}_{\mathbf{p}} \tilde{\mathcal{N}}_{\mathbf{q}}$  results for  $\mathbf{p} \neq \mathbf{q}$  we find in consequence that the  $\mathcal{N}_{\mathbf{p}}$  commute with  $\mathcal{K}_0$ :

$$\begin{aligned} (\mathcal{Y}|Q_0 \mathcal{Y}_1)_0 &= 2 \sum_{\mathbf{p} \neq \mathbf{q}} \langle \mathcal{Y} \tilde{\mathcal{N}}_{\mathbf{p}} \tilde{\mathcal{N}}_{\mathbf{q}} \rangle_0 + \sum_{\mathbf{p}} \langle \mathcal{Y} Q_0 \mathcal{N}_{\mathbf{p}}^2 \rangle_0 \\ &= 8 \sum_{\mathbf{p} \neq \mathbf{q}} \langle \tilde{\mathcal{N}}_{\mathbf{p}}^2 \tilde{\mathcal{N}}_{\mathbf{q}}^2 \rangle_0 + \sum_{\mathbf{p}} \langle \mathcal{N}_{\mathbf{p}}^2 Q_0 \mathcal{N}_{\mathbf{p}}^2 \rangle_0 \\ &= 8 \sum_{\mathbf{p} \neq \mathbf{q}} n_{\mathbf{p}}(1+n_{\mathbf{p}})n_{\mathbf{q}}(1+n_{\mathbf{q}}) + 4 \sum_{\mathbf{p}} n_{\mathbf{p}}^2(1+n_{\mathbf{p}}^2) \end{aligned} \quad (\text{A46})$$

where in the last step Eqs. (A36)–(A38) are used.

With Eq. (A44) the second contribution to the Onsager term is written as

$$(\mathcal{Y}|\mathcal{Y}_2)_0 = \sum_{\mathbf{p}\mathbf{q}\mathbf{k} \neq (0, \mathbf{q}-\mathbf{p})} (\mathcal{Y}|\mathcal{B}_{\mathbf{p}\mathbf{q}\mathbf{k}})_0 \quad (\text{A47})$$

and we focus on the calculation of  $(\mathcal{Y}|\mathcal{B}_{\mathbf{p}\mathbf{q}\mathbf{k}})_0$  for  $\mathbf{k} \neq \mathbf{0}, \mathbf{q}-\mathbf{p}$ . Note that

$$[\mathcal{K}_0, \mathcal{B}_{\mathbf{p}\mathbf{q}\mathbf{k}}] = \sum_{\mathbf{k}} \nu_{\mathbf{k}} [\mathcal{N}_{\mathbf{k}}, b_{\mathbf{p}+\mathbf{k}}^\dagger b_{\mathbf{q}-\mathbf{k}}^\dagger b_{\mathbf{p}} b_{\mathbf{q}}] = \omega_{\mathbf{p}\mathbf{q}\mathbf{k}} \mathcal{B}_{\mathbf{p}\mathbf{q}\mathbf{k}} \quad (\text{A48})$$

with

$$\omega_{\mathbf{p}\mathbf{q}\mathbf{k}} = \nu_{\mathbf{p}+\mathbf{k}} + \nu_{\mathbf{q}-\mathbf{k}} - \nu_{\mathbf{p}} - \nu_{\mathbf{q}} \quad (\text{A49})$$

holds. Thus the relation (A3) can be employed, which yields

$$\begin{aligned} \omega_{\mathbf{p}\mathbf{q}\mathbf{k}} (\mathcal{Y}|\mathcal{B}_{\mathbf{p}\mathbf{q}\mathbf{k}})_0 &= \langle [\mathcal{B}_{\mathbf{p}\mathbf{q}\mathbf{k}}, \mathcal{Y}] \rangle_0 \\ &= 4 \langle [\mathcal{B}_{\mathbf{p}\mathbf{q}\mathbf{k}}, \mathcal{B}_{\mathbf{p}\mathbf{q}\mathbf{k}}^\dagger] \rangle_0 \\ &= 4 [n_{\mathbf{p}+\mathbf{k}} n_{\mathbf{q}-\mathbf{k}} \\ &\quad \times (1+n_{\mathbf{p}}+n_{\mathbf{q}}) - n_{\mathbf{p}} n_{\mathbf{q}} (1+n_{\mathbf{p}+\mathbf{k}}+n_{\mathbf{q}-\mathbf{k}})] \end{aligned} \quad (\text{A50})$$

where the last step, the calculation of the commutator, is tedious but straightforward.

With the definition (A49) we find for  $\mathbf{k} \neq \mathbf{0}, \mathbf{q}-\mathbf{p}$

$$(\mathcal{Y}|\mathcal{B}_{\mathbf{p}\mathbf{q}\mathbf{k}})_0 = 4 \frac{n_{\mathbf{p}+\mathbf{k}} n_{\mathbf{q}-\mathbf{k}} (1+n_{\mathbf{p}}+n_{\mathbf{q}})}{\nu_{\mathbf{p}+\mathbf{k}} + \nu_{\mathbf{q}-\mathbf{k}} - \nu_{\mathbf{p}} - \nu_{\mathbf{q}}} + 4 \frac{n_{\mathbf{p}} n_{\mathbf{q}} (1+n_{\mathbf{p}+\mathbf{k}}+n_{\mathbf{q}-\mathbf{k}})}{\nu_{\mathbf{p}} + \nu_{\mathbf{q}} - \nu_{\mathbf{p}+\mathbf{k}} - \nu_{\mathbf{q}-\mathbf{k}}} \quad (\text{A51})$$

where the  $\nu_{\mathbf{p}}$  as functions of the  $n_{\mathbf{p}}$  are given by Eq. (100). Using this dependence we can calculate the limiting behavior of  $(\mathcal{Y}|\mathcal{B}_{\mathbf{p}\mathbf{q}\mathbf{k}})_0$  for the excluded values of  $\mathbf{k}$  and we obtain

$$\lim_{\mathbf{k} \rightarrow \mathbf{0}} (\mathcal{Y}|\mathcal{B}_{\mathbf{p}\mathbf{q}\mathbf{k}})_0 = 4n_{\mathbf{p}}(1+n_{\mathbf{p}})n_{\mathbf{q}}(1+n_{\mathbf{q}}),$$

$$\lim_{\mathbf{k} \rightarrow \mathbf{q}-\mathbf{p}} (\mathcal{Y}|\mathcal{B}_{\mathbf{p}\mathbf{q}\mathbf{k}})_0 = 4n_{\mathbf{p}}(1+n_{\mathbf{p}})n_{\mathbf{q}}(1+n_{\mathbf{q}})$$

for both cases. These findings imply that just one unrestricted triple sum remains,

$$G^{(2)} = \frac{2\beta^2 U^2}{V^2} \sum_{\mathbf{p}\mathbf{q}\mathbf{k}} \frac{n_{\mathbf{p}+\mathbf{k}} n_{\mathbf{q}-\mathbf{k}} (1+n_{\mathbf{p}}+n_{\mathbf{q}})}{\nu_{\mathbf{p}+\mathbf{k}} + \nu_{\mathbf{q}-\mathbf{k}} - \nu_{\mathbf{p}} - \nu_{\mathbf{q}}}, \quad (\text{A52})$$

and all the other contributions cancel out.

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- $$\partial_\alpha G_\alpha = \frac{\beta}{2} \sum_{ij} J_{ij} \mathbf{m}_i \cdot \mathbf{m}_j + \frac{\beta}{2} \sum_{ij} J_{ij} \langle \tilde{s}_i \cdot \tilde{s}_j \rangle_\alpha$$
- holds. For classical systems the susceptibility is given by  $\chi_{ij}^{\mu\hat{\mu}} = \beta \langle \tilde{s}_i^\mu \tilde{s}_j^{\hat{\mu}} \rangle_\alpha$ , and singularities of  $\chi_{ij}^{\mu\hat{\mu}}$  imply singularities of  $\partial_\alpha G_\alpha$  and consequently of  $G_\alpha$ . For quantum systems this direct conclusion does not apply as  $\chi_{ij}^{\mu\hat{\mu}} = \beta \langle \tilde{s}_i^\mu | \tilde{s}_j^{\hat{\mu}} \rangle_\alpha$  holds, which differs from  $\beta \langle \tilde{s}_i^\mu \tilde{s}_j^{\hat{\mu}} \rangle_\alpha$ .
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