Renormalization and Statistical Mechanics in Many-Particle Systems. II. Statistical Perturbation Method*

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A general nonperturbation problem, described by the Hamiltonian $\mathcal{H}$, is considered. Approximate creation operators $\theta_i^\dagger$ are defined as operators which satisfy the Hamiltonian commutator equations $[\mathcal{H},\theta_i^\dagger]=\omega_i\theta_i^\dagger+R_i^\dagger$, where ω_i are the creation energies, and the remainder operators $R_i^\dagger$ are small in the sense that statistical averages involving the $R_i^\dagger$ are small. A zeroth approximation is to neglect the $R_i^\dagger$. In this case, a straightforward derivation provides general relations between statistical averages such as $\langle\theta_i^\dagger\Omega\rangle$ and $\langle\theta_i^\dagger\Omega\pm\Omega\theta_i^\dagger\rangle$, where Ω is any operator. The usual boson and fermion occupation numbers are a trivial result of these zeroth-order relations. Corrections to the general zeroth-order relations arise from the $R_i^\dagger$; such corrections are considered in the spirit of perturbation theory. An explicit first-order correction is obtained for the averages $\langle\theta_i^\dagger\theta_i\rangle$, and this correction is related to a self-consistent energy-renormalization procedure. The present method is similar to the method of thermodynamic Green's functions in that the derivations given here do not require evaluation of any state vectors or of the partition function. The general results are applied to the Heisenberg ferromagnet problem. At low temperatures, the zeroth-order relations give the Bloch spin-wave results, and an approximate evaluation of the first-order contribution gives the leading term in Dyson's T^4 correction to the spontaneous magnetization. For arbitrary temperatures, the zeroth-order relations give the Tyablikov equations for $\langle S^z\rangle$, and Callen's results are obtained from the first-order corrections. These examples illustrate the simplicity of calculating statistical averages of functions of the $\theta_i^\dagger$, θ_i operators by the present method.

I. INTRODUCTION

We consider a general nonperturbation problem described by the Hermitian Hamiltonian $\mathcal{H}$. The object is to define creation operators for $\mathcal{H}$, in terms of the commutators of these operators with $\mathcal{H}$, and then to derive expressions relating statistical averages of functions of the creation operators. These expressions can then be used to calculate the statistical average of any Hermitian operator representing an observable of the problem.

To begin with, assume that we can find one or more approximate creation operators $\theta_i^\dagger$ which satisfy the Hamiltonian commutator equation

$$[\mathcal{H},\theta_i^\dagger]=\omega_i\theta_i^\dagger+R_i^\dagger\,, \quad (1.1)$$

where ω_i are real, positive numbers and $R_i^\dagger$ are "small" operators. Several comments about (1.1) are in order. Firstly, the $\theta_i^\dagger$, θ_i need not be good boson or fermion operators, i.e., we need not be concerned about the commutators or anticommutators among these operators. The index i represents any labeling appropriate to the satisfaction of (1.1). Secondly, we require $\omega_i>0$; if $\omega_i\neq0$, this can always be satisfied since the Hermitian conjugate of (1.1) is

$$[\mathcal{H},\theta_i]=-\omega_i\theta_i-R_i\,. \quad (1.2)$$

Finally, the definition of small for the operators $R_i^\dagger$ is that any statistical average involving $R_i^\dagger$ should be small. Denoting statistical averages by $\langle\ \rangle$, we require

$$\langle R_i^\dagger\Omega\rangle=\text{small}\,, \quad (1.3)$$

where Ω is any operator. Obviously the condition (1.3) will depend on Ω and also on the values of the thermodynamic variables, such as the temperature. As an example, one might consider the operator $(A-\langle A\rangle)$ as small, for any A, and use this as a basis to define suitably small $R_i^\dagger$. In practice, our procedure is to treat the effects of the $R_i^\dagger$ as a perturbation, and then make an *a posteriori* check to see if the $R_i^\dagger$ do indeed give small contributions to the statistical average which is to be calculated.

In Sec. I of the preceding paper (this paper is referred to as I in the following), we noted three circumstances which keep the Hamiltonian commutator equations (1.1) from providing a complete solution of the problem. These difficulties were avoided in I by relying heavily on the spirit of perturbation theory. These circumstances also give no difficulty in the present theory; the essential reason is that we deal here with operator equations without requiring their evaluation in a particular representation. This is discussed more fully at the end of Sec. II.

A powerful modern method for treating nonperturbation problems is the method of thermodynamic Green's functions.[1–4] In application of this method it is generally necessary to carry out infinite self-energy sums, or else to decouple the Dyson equation by means of an approximation. In the present method, the counterpart of decoupling is the identification of the $R_i^\dagger$ of (1.1) as being small. We wish to stress, however, that this identification is not strictly analogous to decoupling; indeed,

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we are able to make use of the remainders $R_i^\dagger$ to calculate corrections to the zeroth approximations.

In Sec. II we develop the basic equation which relates statistical averages of functions of the $\theta_i^\dagger$, θ_i operators, and then derive a perturbation term based on the $R_i^\dagger$. The usual boson and fermion occupation numbers are a trivial result of the zeroth-order equation. The method is illustrated by an application to the Heisenberg ferromagnet in Sec. III, where the appropriate approximations are found to lead directly to Bloch spin waves, the Tyablikov result, and the Callen result, respectively. Some concluding remarks are presented in Sec. IV.

II. GENERAL THEORY

A. Zeroth Order

Basic Equation

Let us first see what we can learn about the $\theta_i^\dagger$ operators in the case that the $R_i^\dagger$ may be neglected. Then we write, in place of (1.1),[5]

$$[\mathcal{H},\theta_i^\dagger]_-=\omega_i\theta_i^\dagger\,,\quad \omega_i>0\,. \tag{2.1}$$

Equation (2.1) represents all the information we have about the $\theta_i^\dagger$ operators. For the present discussion, it is of no consequence whether (2.1) is an exact equality, representing an exactly solvable problem, or whether (2.1) is an approximation.

The commutator of $\theta_i^\dagger$ with $\exp(\alpha\mathcal{H})$, where α is a number, may be calculated directly with the aid of (2.1). The first step is to prove the relation

$$\mathcal{H}^n\theta_i^\dagger=\theta_i^\dagger(\mathcal{H}+\omega_i)^n\,,\quad n=0,\,1,\,2,\,\cdots; \tag{2.2}$$

this follows by induction for any $n>1$. Then, with the aid of (2.2) and the power series for $\exp(\alpha\mathcal{H})$, we find

$$\exp(\alpha\mathcal{H})\theta_i^\dagger=\exp(\alpha\omega_i)\theta_i^\dagger\exp(\alpha\mathcal{H})\,. \tag{2.3}$$

Now the basic equation is obtained simply by calculating the statistical average $\langle\theta_i^\dagger\Omega\rangle$ for any operator Ω. The partition function Z is

$$Z=\mathrm{Tr}\exp(-\beta\mathcal{H})\,;\quad \beta=(KT)^{-1}\,. \tag{2.4}$$

With the aid of (2.3) and the cyclic-permutation theorem for traces, we have

$$\begin{aligned}\langle\theta_i^\dagger\Omega\rangle&=Z^{-1}\,\mathrm{Tr}\theta_i^\dagger\Omega\exp(-\beta\mathcal{H})\,,\\&=Z^{-1}\,\mathrm{Tr}\Omega\exp(-\beta\mathcal{H})\theta_i^\dagger\,,\\&=\exp(-\beta\omega_i)Z^{-1}\,\mathrm{Tr}\Omega\theta_i^\dagger\exp(-\beta\mathcal{H})\,.\end{aligned} \tag{2.5}$$

From (2.1), the same derivation also holds with $\theta_i^\dagger$ replaced by θ_i, and ω_i replaced by $-\omega_i$. All of these results are stated in the compact form

$$\langle\theta_i^\dagger\Omega\rangle=\exp(-\beta\omega_i)\langle\Omega\theta_i^\dagger\rangle\,, \tag{2.6a}$$

$$\langle\Omega\theta_i\rangle=\exp(-\beta\omega_i)\langle\theta_i\Omega\rangle\,. \tag{2.6b}$$

[5] In Sec. II only we use the customary notation $[A,B]_\pm=AB\pm BA$. In other sections we deal only with commutators, and omit the $\pm$ subscript.

It is useful to cast (2.6) into forms involving commutators and anticommutators. For this purpose, (2.6a) can be rewritten in the form

$$[\exp(\beta\omega_i)\pm1]\langle\theta_i^\dagger\Omega\rangle=\langle\Omega\theta_i^\dagger\pm\theta_i^\dagger\Omega\rangle\,. \tag{2.7}$$

We introduce the notation

$$\phi_i(\pm)=[\exp(\beta\omega_i)\pm1]^{-1}\,. \tag{2.8}$$

Then (2.7), and its counterpart for θ_i, become

$$\langle\theta_i^\dagger\Omega\rangle=\phi_i(\pm)\langle[\Omega,\theta_i^\dagger]_\pm\rangle\,, \tag{2.9a}$$

$$\langle\Omega\theta_i\rangle=\phi_i(\pm)\langle[\theta_i,\Omega]_\pm\rangle\,. \tag{2.9b}$$

Equations (2.6) and (2.9) are forms of the zeroth-order basic equation of our theory. Note that the pair (2.9), as well as the pair (2.6), are not necessarily Hermitian conjugates of one another, since Ω is not necessarily Hermitian.

Bosons and Fermions

Let the operators $\theta_i^\dagger$, θ_i satisfy, in addition to (2.1), the boson commutators

$$[\theta_i,\theta_{i'}]_-=0\,;\quad [\theta_i,\theta_{i'}^\dagger]_-=\delta_{ii'}\,. \tag{2.10}$$

Then (2.9), with $\Omega=\theta_{i'}$, gives the usual boson results

$$\langle\theta_i^\dagger\theta_{i'}\rangle=\phi_i(-)\delta_{ii'}\,, \tag{2.11a}$$

$$\langle\theta_i\theta_{i'}\rangle=0\,. \tag{2.11b}$$

In particular, (2.11a) gives the boson statistical-average occupation number

$$\langle\theta_i^\dagger\theta_i\rangle=[\exp(\beta\omega_i)-1]^{-1}\,. \tag{2.12}$$

In principle, the basic equation can be used to calculate the statistical average of any function of the $\theta_i^\dagger$, θ_i operators. As a further example, use (2.9a) with $\Omega=\theta_{i'}^\dagger\theta_{i''}\theta_{i'''}$ to obtain

$$\langle\theta_i^\dagger\theta_{i'}^\dagger\theta_{i''}\theta_{i'''}\rangle=\phi_i(-)\langle[\theta_{i'}^\dagger\theta_{i''}\theta_{i'''},\theta_i^\dagger]\rangle\,. \tag{2.13}$$

From the commutators (2.10), the right-hand side is evaluated to give

$$\langle\theta_i^\dagger\theta_{i'}^\dagger\theta_{i''}\theta_{i'''}\rangle=\phi_i(-)\phi_{i'}(-)\times[\delta_{ii''}\delta_{i'i'''}+\delta_{ii'''}\delta_{i'i''}]\,. \tag{2.14}$$

The usual derivation of statistical averages such as (2.11) and (2.14) for bosons is based on a knowledge of how the boson operators transform the wave functions; here we have required only the boson commutators.

Let us now suppose the $\theta_i^\dagger$, θ_i are fermion operators; that is, they satisfy, in addition to (2.1), the fermion anticommutators

$$[\theta_i,\theta_{i'}]_+=0\,;\quad [\theta_i,\theta_{i'}^\dagger]_+=\delta_{ii'}\,. \tag{2.15}$$

Then (2.9), with $\Omega=\theta_{i'}$, gives the usual fermion results

$$\langle\theta_i^\dagger\theta_{i'}\rangle=\phi_i(+)\delta_{ii'}\,, \tag{2.16a}$$

$$\langle\theta_i\theta_{i'}\rangle=0\,. \tag{2.16b}$$

In particular, the fermion statistical-average occupation is

$$\langle\theta_i^\dagger\theta_i\rangle=[\exp(\beta\omega_i)+1]^{-1}. \quad (2.17)$$

In order to evaluate a four-operator statistical average, it is convenient to start with (2.6a) for $\theta_i^\dagger$ with $\Omega=\theta_{i'}^\dagger\theta_{i''}\theta_{i'''}$. The right-hand side is easily evaluated with the aid of the anticommutators (2.15), to get back the four-operator average plus some two-operator averages. The two-operator averages are evaluated with (2.16a), and the result is

$$\langle\theta_i^\dagger\theta_{i'}^\dagger\theta_{i''}\theta_{i'''}\rangle=\phi_i(+)\phi_{i'}(+)\times[\delta_{ii'''}\delta_{i'i''}-\delta_{ii''}\delta_{i'i'''}]. \quad (2.18)$$

Again, we have not required the evaluation of operators in any representation in calculating the fermion statistical averages (2.16) and (2.18).

The above calculations hold for systems composed of bosons, fermions, or both. In addition these calculations hold for a grand canonical ensemble simply by replacing ω_i by $\omega_i-\mu$, where μ is a chemical potential. To show this for a system of bosons, for example, let N_b be the total number of bosons, given by

$$N_b=\Sigma_i\theta_i^\dagger\theta_i. \quad (2.19)$$

Then with the aid of (2.1) and the boson commutators (2.10), we have

$$[\mathcal{H}-\mu_bN_b,\ \theta_i^\dagger]_-=(\omega_i-\mu_b)\theta_i^\dagger. \quad (2.20)$$

Similarly for fermions, with N_f given by an expression analogous to (2.19) and with the aid of (2.1) and (2.15),

$$[\mathcal{H}-\mu_fN_f,\ \theta_i^\dagger]_-=(\omega_i-\mu_f)\theta_i^\dagger. \quad (2.21)$$

Thus for a grand canonical ensemble, when $\mathcal{H}$ is replaced by $\mathcal{H}-\mu N$, the basic equations (2.6) and (2.9) hold with ω_i replaced by $\omega_i-\mu$. In order for (2.20) and (2.21) to hold for a system of bosons plus fermions, the boson operators must commute with N_f and the fermion operators must commute with N_b.

Time-Dependent Correlation Functions

The object here is to express time-dependent correlation functions in terms of statistical averages of zero-time commutators. In the Heisenberg picture, with $\hbar=1$ and $\mathcal{H}$ independent of time,

$$\theta_i^\dagger(t)=\exp(i\mathcal{H}t)\theta_i^\dagger\exp(-i\mathcal{H}t), \quad (2.22)$$

where $\theta_i^\dagger=\theta_i^\dagger(0)$. Since the $\theta_i^\dagger$ satisfy (2.1), then (2.3) gives

$$\theta_i^\dagger(t)=\exp(i\omega_it)\theta_i^\dagger. \quad (2.23)$$

Now for any operators A and B,

$$\langle A(t)B(t')\rangle=\langle A(t-t')B\rangle,$$

so it is sufficiently general to calculate the single-time functions $\langle\theta_i^\dagger(t)\Omega\rangle$ and $\langle\Omega\theta_i(t)\rangle$. From (2.9), and with the aid of (2.23) and its Hermitian conjugate, these correlation functions are given by

$$\langle\theta_i^\dagger(t)\Omega\rangle=\exp(i\omega_it)\phi_i(\pm)\langle[\Omega,\theta_i^\dagger]_\pm\rangle, \quad (2.24a)$$

$$\langle\Omega\theta_i(t)\rangle=\exp(-i\omega_it)\phi_i(\pm)\langle[\theta_i,\Omega]_\pm\rangle. \quad (2.24b)$$

Here Ω is any operator, and these equations are not necessarily Hermitian conjugates of one another.

B. Statistical Perturbation

Basic Equation

We now consider the remainder terms in the Hamiltonian commutator equations (1.1).

$$[\mathcal{H},\theta_i^\dagger]=\omega_i\theta_i^\dagger+R_i^\dagger,\quad \omega_i>0. \quad (2.25)$$

This equation can be written in the form

$$\mathcal{H}\theta_i^\dagger=\theta_i^\dagger(\mathcal{H}+\omega_i)+R_i^\dagger, \quad (2.26)$$

and by induction it is easy to prove

$$\mathcal{H}^n\theta_i^\dagger=\theta_i^\dagger(\mathcal{H}+\omega_i)^n+\sum_{p=0}^{n-1}\mathcal{H}^pR_i^\dagger(\mathcal{H}+\omega_i)^{n-p-1},\quad n=1,2,\cdots. \quad (2.27)$$

With the aid of the power series for $\exp(-\beta\mathcal{H})$, (2.27) gives directly

$$\exp(-\beta\mathcal{H})\theta_i^\dagger=\exp(-\beta\omega_i)\theta_i^\dagger\exp(-\beta\mathcal{H})+\sum_{n=1}^{\infty}(1/n!)(-\beta)^n\sum_{p=0}^{n-1}\mathcal{H}^pR_i^\dagger(\mathcal{H}+\omega_i)^{n-p-1}. \quad (2.28)$$

Finally, we calculate the statistical average $\langle\theta_i^\dagger\Omega\rangle$, for any operator Ω, just as in the derivation of (2.6) above. The result is

$$\langle\theta_i^\dagger\Omega\rangle=\exp(-\beta\omega_i)\langle\Omega\theta_i^\dagger\rangle+Z^{-1}\,\mathrm{Tr}\Omega\sum_{n=1}^{\infty}(1/n!)(-\beta)^n\times\sum_{p=0}^{n-1}\mathcal{H}^pR_i^\dagger(\mathcal{H}+\omega_i)^{n-p-1}. \quad (2.29)$$

Equation (2.29) is still exact, and is a primitive form of the basic equation with the remainders $R_i^\dagger$ included. The second term on the right-hand side would be difficult to evaluate in general. However, to the extent that the $R_i^\dagger$ are small, this term is small and can be evaluated by a zeroth-order approximation. A useful form of the basic equation (2.29) is obtained for the special case $\Omega=\theta_i$. An approximate evaluation of the second term on the right, henceforth called the perturbation term, is then carried out with the aid of the Hermitian conjugate of (2.27):

$$\theta_i\mathcal{H}^n=(\mathcal{H}+\omega_i)^n\theta_i+0(R_i). \quad (2.30)$$

With the aid of (2.30) and the cyclic permutation theorem for traces, the zeroth-order evaluation of the perturbation term is as follows:

$$Z^{-1}\,\mathrm{Tr}\theta_i \sum_{n=1}^{\infty}(1/n!)(-\beta)^n \sum_{p=0}^{n-1} \mathcal{H}^p R_i^\dagger(\mathcal{H}+\omega_i)^{n-p-1}$$

$$=Z^{-1}\,\mathrm{Tr}\sum_{n=1}^{\infty}(1/n!)(-\beta)^n \sum_{p=0}^{n-1} \mathcal{H}^p R_i^\dagger(\mathcal{H}+\omega_i)^{n-p-1}\theta_i$$

$$=Z^{-1}\,\mathrm{Tr}\sum_{n=1}^{\infty}(1/n!)(-\beta)^n \sum_{p=0}^{n-1} \mathcal{H}^p R_i^\dagger\theta_i\mathcal{H}^{n-p-1} +0(R_i^\dagger R_i)$$

$$=Z^{-1}\,\mathrm{Tr}\sum_{n=1}^{\infty}(1/n!)(-\beta)^n \sum_{p=0}^{n-1} R_i^\dagger\theta_i\mathcal{H}^{n-1}+0(R_i^\dagger R_i)$$

$$=-\beta Z^{-1}\,\mathrm{Tr}R_i^\dagger\theta_i\exp(-\beta\mathcal{H})+0(R_i^\dagger R_i). \quad (2.31)$$

The basic equation (2.29) finally becomes

$$\langle\theta_i^\dagger\theta_i\rangle=\exp(-\beta\omega_i)\langle\theta_i\theta_i^\dagger\rangle-\beta\langle R_i^\dagger\theta_i\rangle+0(R_i^\dagger R_i). \quad (2.32)$$

The perturbation aspect of (2.32) is evident. If we can consider $R_i^\dagger$ as being of order ϵ, where ϵ is a number small compared to 1, then the perturbation term in (2.32) is of order ϵ, while the error is of order ϵ^2. Furthermore, in the spirit of perturbation theory, we can use the zeroth-order basic equation (2.6) or (2.9), with $\Omega=R_i^\dagger$, to evaluate the perturbation term. Such procedure gives the right-hand side of (2.32) correct to order ϵ.

It is useful to cast (2.32) into a form containing commutators and anticommutators. This is done exactly as in the derivation of (2.9); the result is

$$\langle\theta_i^\dagger\theta_i\rangle=\phi_i(\pm)\langle[\theta_i,\theta_i^\dagger]_\pm\rangle\pm\beta[\phi_i(\pm)\mp1]\langle R_i^\dagger\theta_i\rangle +0(R_i^\dagger R_i). \quad (2.33)$$

The Hermitian conjugate of (2.33) is the same equation to zeroth order. To first order, we then expect $\langle R_i^\dagger\theta_i\rangle=\langle\theta_i^\dagger R_i\rangle$.

Energy Renormalization

In the treatment of perturbation problems in I, we developed the idea of renormalizing the creation operators and particle energies so as to satisfy the Hamiltonian commutator equations to a higher order. There we found that we could calculate particle energies to one order higher than the creation operators were determined. An analogous calculation can be carried out in the present theory to get first-order energy corrections ω_{1i}. To do this, rewrite the Hamiltonian commutator equations (1.1) in the form

$$[\mathcal{H},\theta_i^\dagger]=(\omega_i+\omega_{1i})\theta_i^\dagger+(R_i^\dagger-\omega_{1i}\theta_i^\dagger);\ \omega_i+\omega_{1i}>0. \quad (2.34)$$

In view of (2.34), the above derivations of various forms of the basic equation can all be carried out with ω_i replaced by $\omega_i+\omega_{1i}$ and $R_i^\dagger$ replaced by $R_i^\dagger-\omega_{1i}\theta_i^\dagger$. In particular, dropping terms of order $R_i^\dagger R_i$ in (2.33), that equation becomes

$$\langle\theta_i^\dagger\theta_i\rangle=\phi_{1i}(\pm)\langle[\theta_i,\theta_i^\dagger]_\pm\rangle\pm\beta[\phi_{1i}(\pm)\mp1] \times\langle(R_i^\dagger-\omega_{1i}\theta_i^\dagger)\theta_i\rangle, \quad (2.35)$$

where

$$\phi_{1i}(\pm)=\{\exp[\beta(\omega_i+\omega_{1i})]\pm1\}^{-1}. \quad (2.36)$$

Now we determine ω_{1i} so that the perturbation term in (2.35) vanishes. This condition is

$$\langle(R_i^\dagger-\omega_{1i}\theta_i^\dagger)\theta_i\rangle=0, \quad (2.37)$$

or solving for ω_{1i},

$$\omega_{1i}=\langle R_i^\dagger\theta_i\rangle/\langle\theta_i^\dagger\theta_i\rangle. \quad (2.38)$$

Thus, with ω_{1i} given by (2.38), the first-order basic equation for $\langle\theta_i^\dagger\theta_i\rangle$ reduces to a zeroth-order basic equation with renormalized energies:

$$\langle\theta_i^\dagger\theta_i\rangle=\phi_{1i}(\pm)\langle[\theta_i,\theta_i^\dagger]_\pm\rangle. \quad (2.39)$$

In principle, the coupled equations (2.38) and (2.39) must be solved simultaneously. The self-consistent results for $\langle\theta_i^\dagger\theta_i\rangle$ must still be regarded as of first order, however, since terms of second and higher orders in $R_i^\dagger$, R_i have been dropped from (2.33). In practice, therefore, the use of (2.39) to calculate $\langle\theta_i^\dagger\theta_i\rangle$ is justified if ω_{1i} is small compared to ω_i; in this case, it is reasonable to evaluate (2.38) in zeroth order. We stress the point that ω_{1i} has been designed to take care of first-order terms in the particular average $\langle\theta_i^\dagger\theta_i\rangle$; in order to remove first-order terms in $\langle\theta_i^\dagger\Omega\rangle$, for any Ω, ω_{1i} is, in general, a function of Ω.

Comments

The basic premiss of the present method is that, while the Hamiltonian may not provide a convenient expansion parameter, we can nevertheless manufacture a statistical perturbation parameter in the sense that statistical averages involving $R_i^\dagger$, R_i are small. Such a procedure will depend intimately on the problem to be treated, on the values of thermodynamic variables, and perhaps even on the particular operator for which one desires to compute the statistical average.

In I, we noted the following circumstances which keep the creation operators $\theta_i^\dagger$ alone, which are found to satisfy (1.1), from providing a complete solution to $\mathcal{H}$.

(i) We need at least one eigenfunction to start with.

(ii) There is no obvious way of finding all the $\theta_i^\dagger$, and hence getting the complete set of eigenfunctions.

(iii) $\theta_i^\dagger\psi$ does not have to be an eigenfunction of $\mathcal{H}$ just because ψ is; $\theta_i^\dagger\psi$ can be zero.

In the above derivations we have made no reference to wave functions. Thus the present method allows the calculation of statistical averages without any knowledge of the eigenfunctions of $\mathcal{H}$. In addition, we have worked entirely with operator equations, so the circumstance $\theta_i^\dagger\psi=0$, which might arise for some function ψ, causes no difficulty. This takes care of any problems due to (i) or (iii) above. Finally, the basic equations hold for any number of $\theta_i^\dagger$ which might be found to satisfy the Hamiltonian commutator equations. In practice, however, the method will be most useful if a sufficient number of $\theta_i^\dagger$ are found to span the space of $\mathcal{H}$, so that any desired operator can be represented as a function of the $\theta_i^\dagger$, θ_i, and the statistical average of the operator may be calculated from the basic equation. This requirement is not difficult to satisfy in practice; doing so removes any problems due to (ii) above.

We now proceed to demonstrate the application of this method by a treatment of the Heisenberg ferromagnet in the following section.

III. APPLICATION TO THE HEISENBERG FERROMAGNET

A. Definition of the Problem

The Heisenberg Hamiltonian for a ferromagnetic monatomic lattice with isotropic nearest-neighbor exchange is

$$\mathcal{H}=-g\mu H\Sigma_n S_n{}^z - J\Sigma'_{nn'}\mathbf{S}_n\cdot\mathbf{S}_{n'}. \tag{3.1}$$

Here g is the spectroscopic splitting factor for the localized spins, μ is the Bohr magneton, H is the magnitude of the external field, the index n labels the spin sites in the lattice, $\mathbf{S}_n$ is the spin vector at site n (in units of $\hbar$), $S_n{}^z$ is the z component of $\mathbf{S}_n$, and J is the nearest-neighbor exchange constant. We take $J>0$, H in the z direction with $H>0$ when in the $+z$ direction, and $\Sigma'_{nn'}$ goes over all n but only over n' which are nearest neighbors to n. This Hamiltonian is the same as that used by Dyson,[6] except that his H is in the $-z$ direction and his J is twice the present J. The definition of the problem is completed by the spin commutators

$$[S_n{}^+,S_{n'}{}^-]=2S_n{}^z\delta_{nn'}, \tag{3.2a}$$

$$[S_n{}^\pm,S_{n'}{}^z]=\mp S_n{}^\pm\delta_{nn'}, \tag{3.2b}$$

$$[S_n{}^+,S_{n'}{}^+]=[S_n{}^z,S_{n'}{}^z]=0. \tag{3.2c}$$

It is convenient for all the following calculations to work with Fourier transforms of the spin operators. These are defined by

$$A_\mathbf{k}{}^\dagger=N^{-\frac{1}{2}}(2S)^{-1/2}\Sigma_n S_n{}^-\exp(i\mathbf{k}\cdot\mathbf{r}_n), \tag{3.3}$$

$$A_\mathbf{k}=N^{-\frac{1}{2}}(2S)^{-1/2}\Sigma_n S_n{}^+\exp(-i\mathbf{k}\cdot\mathbf{r}_n), \tag{3.4}$$

$$B_\mathbf{k}=N^{-1}\Sigma_n S_n{}^z\exp(-i\mathbf{k}\cdot\mathbf{r}_n), \tag{3.5}$$

where $\mathbf{r}_n$ is the position vector of the site n, $\mathbf{k}$ is a wave vector, N is the number of spins in the crystal, and S is the magnitude of the spin vectors. We also define the functions $J_\mathbf{k}$ by

$$J_\mathbf{k}=J\Sigma'_n\exp(i\mathbf{k}\cdot\mathbf{r}_n), \tag{3.6}$$

where Σ'_n is over $\mathbf{r}_n$ which are nearest-neighbors to the origin (the origin is $\mathbf{r}_n=0$). Then we have

$$J_\mathbf{k}=J_{-\mathbf{k}},\quad J_0=\mathfrak{z}J, \tag{3.7}$$

$$\Sigma_\mathbf{k}J_\mathbf{k}=0, \tag{3.8}$$

where $\mathfrak{z}$ is the number of nearest neighbors.

In terms of the transformed operators, the definition of the problem becomes

$$\mathcal{H}=-g\mu HNB_0-\Sigma_\mathbf{k}J_\mathbf{k}(NB_\mathbf{k}B_{-\mathbf{k}}+2SA_\mathbf{k}{}^\dagger A_\mathbf{k}); \tag{3.9}$$

$$[A_\mathbf{k},A_{\mathbf{k}'}{}^\dagger]=S^{-1}B_{\mathbf{k}-\mathbf{k}'}; \tag{3.10a}$$

$$[A_\mathbf{k},B_{\mathbf{k}'}]=-N^{-1}A_{\mathbf{k}+\mathbf{k}'},\ [A_\mathbf{k}{}^\dagger,B_{\mathbf{k}'}]=N^{-1}A_{\mathbf{k}-\mathbf{k}'}{}^\dagger; \tag{3.10b}$$

$$[A_\mathbf{k},A_{\mathbf{k}'}]=[B_\mathbf{k},B_{\mathbf{k}'}]=0. \tag{3.10c}$$

A useful equation for $S=\frac{1}{2}$ is

$$S_n{}^z=S-S_n{}^-S_n{}^+,\quad S=\tfrac{1}{2}. \tag{3.11}$$

Transforming (3.11) gives

$$B_\mathbf{k}=S\delta(\mathbf{k})-N^{-1}\Sigma_{\mathbf{k}'}A_{\mathbf{k}'-\mathbf{k}}{}^\dagger A_{\mathbf{k}'},\quad S=\tfrac{1}{2}. \tag{3.12}$$

Finally, from (3.9) and (3.10) we derive an equation which is the starting point for our calculations:

$$[\mathcal{H},A_\mathbf{k}{}^\dagger]=g\mu HA_\mathbf{k}{}^\dagger+2\Sigma_{\mathbf{k}'}(J_{\mathbf{k}'-\mathbf{k}}-J_{\mathbf{k}'})A_{\mathbf{k}'}{}^\dagger B_{\mathbf{k}'-\mathbf{k}}. \tag{3.13}$$

The $A_\mathbf{k}{}^\dagger$ are of course the Bloch-spin-wave creation operators; the Hamiltonian commutator equation (3.13) suggests than an approximation to their energies is $g\mu H$. The "remainder" in (3.13) is large, however, and in all the following approximate calculations the zeroth-order energies are taken to include part of the diagonal terms in this remainder.

B. Approximations for Low Temperature

Convergence Factor

The low-temperature convergence factor is $\phi_\mathbf{k}$, defined by (3.20) below. Each independent sum over $\phi_\mathbf{k}$ contributes a factor proportional to $T^{3/2}$, so we say $\phi_\mathbf{k}$ is of order $T^{3/2}$. From this, we can use the zeroth-order basic equation repeatedly to conclude that a statistical average involving n creation operators and n annihilation operators, in normal order, is of order $T^{3n/2}$. A much more detailed study indicates that this is true for $n\ll N$ as long as there are no low-lying statistically important bound states.

An operator power series for $S_n{}^z$ for arbitrary S is[7]

$$S_n{}^z=S-S_n{}^-S_n{}^+-\cdots; \tag{3.14}$$

the transform of (3.14) is

$$B_\mathbf{k}=S\delta(\mathbf{k})-N^{-1}\Sigma_{\mathbf{k}'}A_{\mathbf{k}'-\mathbf{k}}{}^\dagger A_{\mathbf{k}'}-\cdots. \tag{3.15}$$

Here and in the following the notation $+\cdots$ means higher order operator terms, and hence terms which contribute of higher order in $\phi_\mathbf{k}$ to the statistical averages. Equation (3.15) is an appropriate "low-tempera-

[6] F. J. Dyson, Phys. Rev. **102**, 1217 (1956); **102**, 1230 (1956).

[7] T. Morita and T. Tanaka, Phys. Rev. **138**, A1395 (1965).

ture" expansion; the leading term is just the ground-state value ($S_n^z=S$). For $S=\frac{1}{2}$, the higher order terms in (3.14) and (3.15) vanish. With (3.15), the Hamiltonian commutator equation (3.13) is transformed to a low-temperature expansion.

$$[\mathcal{H},A_{\mathbf{k}}^\dagger]=\omega_{\mathbf{k}}A_{\mathbf{k}}^\dagger+2N^{-1}\Sigma_{\mathbf{k}'\mathbf{k}''}(J_{\mathbf{k}'}-J_{\mathbf{k}'-\mathbf{k}})\times A_{\mathbf{k}'}^\dagger A_{\mathbf{k}''-\mathbf{k}'+\mathbf{k}}^\dagger A_{\mathbf{k}''}+\cdots; \quad (3.16)$$

$$\omega_{\mathbf{k}}=g\mu H+2S(J_0-J_{\mathbf{k}}). \quad (3.17)$$

Bloch Spin Waves

The zeroth approximation for low temperature is to take the leading term in (3.16) and use the zeroth-order basic equation (2.9). This gives

$$[\mathcal{H},A_{\mathbf{k}}^\dagger]=\omega_{\mathbf{k}}A_{\mathbf{k}}^\dagger, \quad (3.18)$$

$$\langle A_{\mathbf{k}}^\dagger A_{\mathbf{k}}\rangle=\phi_{\mathbf{k}}\langle[A_{\mathbf{k}},A_{\mathbf{k}}^\dagger]\rangle, \quad (3.19)$$

where we use the simplified notation

$$\phi_{\mathbf{k}}=[\exp(\beta\omega_{\mathbf{k}})-1]^{-1}. \quad (3.20)$$

From the commutators (3.10a) and the expansion (3.15), $[A_{\mathbf{k}},A_{\mathbf{k}}^\dagger]=1-\cdots$, so to zeroth order (3.19) gives

$$\langle A_{\mathbf{k}}^\dagger A_{\mathbf{k}}\rangle=\phi_{\mathbf{k}}. \quad (3.21)$$

We now multiply (3.21) by $N^{-1}\Sigma_{\mathbf{k}}$, and use (3.15) to get the leading term for the left-hand side, with the result

$$S-\langle B_0\rangle=N^{-1}\Sigma_{\mathbf{k}}\phi_{\mathbf{k}}. \quad (3.22)$$

Noting that $\langle B_0\rangle=\langle S^z\rangle$, the statistical-average z component of spin per atom, (3.22) may be written

$$\langle S^z\rangle=S-\Phi, \quad (3.23)$$

$$\Phi=N^{-1}\Sigma_{\mathbf{k}}\phi_{\mathbf{k}}. \quad (3.24)$$

Equations (3.23) and (3.24) are the Bloch result,[8] as corrected by Dyson[6] for terms of higher order than $T^{3/2}$, for the low-temperature magnetization. Evaluation of the integral for primitive cubic lattices gives

$$\Phi=Z_{3/2}\theta^{3/2}+\tfrac{3}{4}\pi\nu Z_{5/2}\theta^{5/2}+\pi^2\nu^2\omega Z_{7/2}\theta^{7/2}+\cdots, \quad (3.25)$$

where we have used Dyson's[6] notation. In particular, ν and ω are dimensionless parameters which depend on the lattice structure, and

$$\theta=(3KT/4\pi\nu JS\mathfrak{z});\quad Z_q=\sum_{m=1}^{\infty}m^{-q}e^{-mg\mu H/KT}. \quad (3.26)$$

It is of interest now to examine the contribution of terms which have been neglected in this calculation.

Statistical Perturbation for Bloch Spin Waves

The remainder operators of (3.16) are given by

$$R_{\mathbf{k}}^\dagger=2N^{-1}\Sigma_{\mathbf{k}'\mathbf{k}''}(J_{\mathbf{k}'}-J_{\mathbf{k}'-\mathbf{k}})A_{\mathbf{k}'}^\dagger A_{\mathbf{k}''-\mathbf{k}'+\mathbf{k}}^\dagger A_{\mathbf{k}''}; \quad (3.27)$$

[8] F. Bloch, Z. Physik **61**, 206 (1930); **74**, 295 (1932).

the neglected higher order terms (i.e., five-operator terms in $R_{\mathbf{k}}^\dagger$) contribute to $\langle S^z\rangle$ of order higher than T^4. The first-order basic equation (2.33) can be written for $\langle A_{\mathbf{k}}^\dagger A_{\mathbf{k}}\rangle$ and summed over $\mathbf{k}$ to give

$$N^{-1}\Sigma_{\mathbf{k}}\langle A_{\mathbf{k}}^\dagger A_{\mathbf{k}}\rangle=N^{-1}\Sigma_{\mathbf{k}}\phi_{\mathbf{k}}\langle[A_{\mathbf{k}},A_{\mathbf{k}}^\dagger]\rangle -\beta N^{-1}\Sigma_{\mathbf{k}}(\phi_{\mathbf{k}}+1)\langle R_{\mathbf{k}}^\dagger A_{\mathbf{k}}\rangle. \quad (3.28)$$

The perturbation term on the right-hand side of (3.28) contains four-operator statistical averages which are difficult to evaluate accurately. An *approximate* evaluation, which is satisfactory for the present purposes, is obtained by using the zeroth-order basic equation (2.9) to write

$$\langle R_{\mathbf{k}}^\dagger A_{\mathbf{k}}\rangle=\phi_{\mathbf{k}}\langle[A_{\mathbf{k}},R_{\mathbf{k}}^\dagger]\rangle. \quad (3.29)$$

This evaluation gives the correct order of T for $\langle R_{\mathbf{k}}^\dagger A_{\mathbf{k}}\rangle$, but not the correct coefficient; see the discussion at the end of the present Sec. IIIB. Carrying out the commutator in (3.29), commuting the spin-wave operators to normal order, and dropping terms higher than quadratic in the operators (since the commutator is already multiplied by $\phi_{\mathbf{k}}$), gives

$$\langle R_{\mathbf{k}}^\dagger A_{\mathbf{k}}\rangle=2\phi_{\mathbf{k}}N^{-1}\Sigma_{\mathbf{k}'\mathbf{k}''}(J_{\mathbf{k}'}-J_{\mathbf{k}'-\mathbf{k}})\langle A_{\mathbf{k}''}^\dagger A_{\mathbf{k}''}\rangle \times[\delta(\mathbf{k}'-\mathbf{k})+\delta(\mathbf{k}'-\mathbf{k}'')-N^{-1}S^{-1}]. \quad (3.30)$$

According to (3.21), the zeroth-order evaluation of $\langle A_{\mathbf{k}''}^\dagger A_{\mathbf{k}''}\rangle$ is $\phi_{\mathbf{k}''}$. The remaining double integral in the perturbation term is evaluated as follows:

$$\begin{aligned}-\beta N^{-1}\Sigma_{\mathbf{k}}(\phi_{\mathbf{k}}+1)\langle R_{\mathbf{k}}^\dagger A_{\mathbf{k}}\rangle &=-2\beta N^{-2}\Sigma_{\mathbf{k}\mathbf{k}'}(\phi_{\mathbf{k}}^2+\phi_{\mathbf{k}})\phi_{\mathbf{k}'}(J_{\mathbf{k}}+J_{\mathbf{k}'}-J_{\mathbf{k}'-\mathbf{k}}-J_0)\\ &=(\tfrac{3}{2}\pi\nu S^{-1})Z_{3/2}Z_{5,2}\theta^4.\end{aligned} \quad (3.31)$$

Referring now to the commutator term in (3.28), it is no longer consistent to keep only the leading term. For with the aid of (3.15), we find

$$\begin{aligned}\langle[A_{\mathbf{k}},A_{\mathbf{k}}^\dagger]\rangle=S^{-1}\langle B_0\rangle&=1-S^{-1}N^{-1}\Sigma_{\mathbf{k}'}\langle A_{\mathbf{k}'}^\dagger A_{\mathbf{k}'}\rangle-\cdots\\ &=1-S^{-1}\Phi-\cdots.\end{aligned} \quad (3.32)$$

The commutator term then becomes

$$N^{-1}\Sigma_{\mathbf{k}}\phi_{\mathbf{k}}\langle[A_{\mathbf{k}},A_{\mathbf{k}}^\dagger]\rangle=\Phi-S^{-1}\Phi^2-\cdots. \quad (3.33)$$

The higher order terms here are zero for $S=\frac{1}{2}$, and of order $T^{9/2}$ for $S>\frac{1}{2}$.

Let us now take $S=\frac{1}{2}$ for simplicity; the left-hand side of (3.28) is then $S-\langle S^z\rangle$. If $S>\frac{1}{2}$, the left-hand side contains additional terms of lowest order T^3. Gathering up the terms evaluated above, (3.28) yields

$$\langle S^z\rangle=S-\Phi+S^{-1}\Phi^2-(\tfrac{3}{2}\pi\nu S^{-1})Z_{3/2}Z_{5/2}\theta^4,\quad S=\tfrac{1}{2}. \quad (3.34)$$

This result is quite instructive and is discussed below.

Interpretation

The correction to $\langle S^z\rangle$ due to the perturbation term is similar to Dyson's[6] accurate result [his Q is approximated by 1 in (3.34)], and is the same as the leading term of the perturbation expansion in S^{-1}, as obtained by Oguchi.[9] However, the commutator term in the basic equation contributes a spurious term of lowest order T^3, namely, the term $S^{-1}\Phi^2$. This is the famous Green's function T^3 term.[10,11] The above derivation clearly shows that the physical origin of the spurious term is the departure of the Bloch spin waves from good bosons, i.e., the failure of the boson commutators for the $A_{\mathbf{k}}^\dagger$, $A_{\mathbf{k}}$ operators. This failure of the boson commutators is just the kinematical interaction.[6]

From this comment, it might be expected that if we assume the Bloch spin waves are good bosons, and use boson statistics together with a perturbation based on the Hamiltonian, then the Φ^2 term will go away. This procedure is justified by Dyson's[6] proof that kinematical effects are negligible at low temperatures. Thus one can treat $\mathcal{H}-\Sigma_{\mathbf{k}}\omega_{\mathbf{k}}A_{\mathbf{k}}^\dagger A_{\mathbf{k}}$ as a perturbation and use ordinary perturbation theory for bosons, or treat the $R_{\mathbf{k}}^\dagger$ of (3.27) as a perturbation and use the Hamiltonian perturbation theory of I for bosons. In either case, the Φ^2 term does not appear, as expected. This is essentially the procedure used by Keffer and Loudon[12] and by Tahir-Kheli and ter Haar[13] in arriving at the perturbation term in (3.34), without having the Φ^2 term show up.

In this connection, we have carried out a straightforward renormalization of the spin-wave operators, by the method of undetermined coefficients as developed in I. These renormalized operators are independent bosons, to the order required to compute $\langle S^z\rangle$ correct to order T^4. This calculation is beyond the scope of the present paper, and will be presented later.

A final remark is in order regarding the evaluation of four-operator statistical averages at low temperature. In (3.29) a sum of four-operator terms is expressed as a sum of the indicated commutators. A representative four-operator term is thus evaluated as follows:

$$\begin{aligned}\langle A_{\mathbf{k}'}^\dagger A_{\mathbf{k}''-\mathbf{k}'+\mathbf{k}}^\dagger A_{\mathbf{k}''}A_{\mathbf{k}}\rangle &= \phi_{\mathbf{k}}\langle[A_{\mathbf{k}},A_{\mathbf{k}'}^\dagger A_{\mathbf{k}''-\mathbf{k}'+\mathbf{k}}^\dagger A_{\mathbf{k}''}]\rangle \\ &= \phi_{\mathbf{k}}\phi_{\mathbf{k}'}[\delta(\mathbf{k}'-\mathbf{k})+\delta(\mathbf{k}'-\mathbf{k}'')-N^{-1}S^{-1}]. \end{aligned} \tag{3.35}$$

We have made a detailed study of this procedure and conclude that it gives only the correct order of T for the four-operator average. The right-hand side of (3.35) is a zeroth-order evaluation; the appropriate perturbation term contributes of the same order, the error in the perturbation term is of the same order, and so forth. The evaluation (3.35) is better than a strictly boson evaluation, such as given by (2.14) above for exact bosons, because of the term $N^{-1}S^{-1}$ in (3.35). For example, this term, which results from commuting the spin-wave operators to normal order, makes the average $\langle S_n^-S_n^-S_n^+S_n^+\rangle$ vanish for $S=\frac{1}{2}$, as it must.

[9] T. Oguchi, Phys. Rev. **117**, 117 (1960).
[10] S. V. Tyablikov, Ukr. Math. Zh. **11**, 287 (1959).
[11] R. A. Tahir-Kheli and D. ter Haar, Phys. Rev. **127**, 88 (1962).
[12] F. Keffer and R. Loudon, J. Appl. Phys. **32**, 2S (1961).
[13] R. A. Tahir-Kheli and D. ter Haar, Phys. Rev. **127**, 95 (1962).

We wish to go no further into the problems associated with Bloch spin-wave operators, since these difficulties are easily avoided with the renormalized operators mentioned above.

C. Approximations for Arbitrary Temperature

Tyablikov Approximation

Tyablikov's[10] decoupling of the higher order Green's function amounts to replacing S_n^z by $\langle S^z\rangle$ in certain four-operator statistical averages. We introduce the same approximation into our operator equations by writing

$$S_n^z=\langle S^z\rangle+[S_n^z-\langle S^z\rangle], \tag{3.36}$$

and considering the $[S_n^z-\langle S^z\rangle]$ as small operators. This is analogous to the low-temperature approximations, where $S_n^z\approx S$ was used. In view of the definition (3.5) for $B_{\mathbf{k}}$, (3.36) gives directly

$$B_{\mathbf{k}}=\langle S^z\rangle\delta(\mathbf{k})+[B_{\mathbf{k}}-\langle S^z\rangle\delta(\mathbf{k})]. \tag{3.37}$$

Now with (3.37) the Hamiltonian commutator equations (3.13) become

$$[\mathcal{H},A_{\mathbf{k}}^\dagger]=\epsilon_{\mathbf{k}}A_{\mathbf{k}}^\dagger+P_{\mathbf{k}}^\dagger, \tag{3.38}$$

where

$$\epsilon_{\mathbf{k}}=g\mu H+2\langle S^z\rangle(J_0-J_{\mathbf{k}}), \tag{3.39}$$

$$P_{\mathbf{k}}^\dagger=2\Sigma_{\mathbf{k}'}(J_{\mathbf{k}'-\mathbf{k}}-J_{\mathbf{k}'})A_{\mathbf{k}'}^\dagger[B_{\mathbf{k}'-\mathbf{k}}-\langle S^z\rangle\delta(\mathbf{k}'-\mathbf{k})]. \tag{3.40}$$

We first carry out a zeroth-order calculation by neglecting the remainder operators $P_{\mathbf{k}}^\dagger$. The zeroth-order basic equation for $\langle A_{\mathbf{k}}^\dagger A_{\mathbf{k}}\rangle$ is

$$\langle A_{\mathbf{k}}^\dagger A_{\mathbf{k}}\rangle=\psi_{\mathbf{k}}\langle[A_{\mathbf{k}},A_{\mathbf{k}}^\dagger]\rangle; \tag{3.41}$$

$$\psi_{\mathbf{k}}=[\exp(\beta\epsilon_{\mathbf{k}})-1]^{-1}. \tag{3.42}$$

The commutator term in (3.41) can be evaluated exactly in terms of $\langle B_0\rangle=\langle S^z\rangle$ to give

$$\langle A_{\mathbf{k}}^\dagger A_{\mathbf{k}}\rangle=S^{-1}\langle S^z\rangle\psi_{\mathbf{k}}. \tag{3.43}$$

Let us first take $S=\frac{1}{2}$. Multiplying (3.43) by $N^{-1}\Sigma_{\mathbf{k}}$, using (3.12) for B_0, and rearranging terms gives

$$\langle S^z\rangle(1+S^{-1}\Psi)=S, \quad \text{for} \quad S=\tfrac{1}{2}; \tag{3.44}$$

$$\Psi=N^{-1}\Sigma_{\mathbf{k}}\psi_{\mathbf{k}}. \tag{3.45}$$

Equations (3.44) and (3.45), together with (3.42) and (3.39), are just the Tyablikov coupled equations for $\langle S^z\rangle$ for $S=\frac{1}{2}$.

Tahir-Kheli and ter Haar[11] have extended the Tyablikov approximation to higher spins. We wish to demonstrate the generality of the present method by deriving their implicit equations for $\langle S^z\rangle$. For arbitrary S we want to compute $\langle(S_n^-)^p(S_n^+)^p\rangle$, for any power $p\geq 1$. Define Ω_n by

$$\Omega_n=(S_n^-)^p(S_n^+)^{p-1}, \tag{3.46}$$

so that

$$\langle (S_n^-)^p (S_n^+)^p \rangle = \langle \Omega_n S_n^+ \rangle . \qquad (3.47)$$

In view of (3.38), we can use the zeroth-order basic equation (2.9) for an arbitrary operator $\Omega = \Omega_n$ to write

$$\langle \Omega_n A_{\mathbf{k}} \rangle = \psi_{\mathbf{k}} \langle [A_{\mathbf{k}}, \Omega_n] \rangle , \qquad (3.48)$$

where $\psi_{\mathbf{k}}$ is given by (3.42). With the definition (3.4) of $A_{\mathbf{k}}$, it follows that

$$[A_{\mathbf{k}}, \Omega_n] = N^{-1/2}(2S)^{-1/2}[S_n^+, \Omega_n] \exp(-i\mathbf{k}\cdot\mathbf{r}_n) , \qquad (3.49)$$

since the general commutator $[S_{n'}^+, \Omega_n]$ contains a $\delta_{nn'}$. Multiplying (3.48) by $N^{-1/2}(2S)^{1/2} \exp(i\mathbf{k}\cdot\mathbf{r}_n)$ and summing over $\mathbf{k}$, with the aid of (3.49) and the inverse of (3.4), gives

$$\langle \Omega_n S_n^+ \rangle = \Psi \langle [S_n^+, \Omega_n] \rangle , \qquad (3.50)$$

where, according to (3.45) and (3.42),

$$\Psi = N^{-1}\Sigma_{\mathbf{k}}[\exp(\beta\epsilon_{\mathbf{k}}) - 1]^{-1} . \qquad (3.51)$$

Equations (3.50) and (3.51), together with (3.39) for $\epsilon_{\mathbf{k}}$, is the set of equations for $\langle S^z \rangle$ which were obtained by Tahir-Kheli and ter Haar[11] by the Green's-function method (their Eqs. (3.11), (3.13), and (3.14), together with their (2.8) for $[S_n^+, \Omega_n]$). We should like to emphasize the simplicity of the present derivations.

We can now show how the Tyablikov decoupling approximation leads to a vanishing energy correction $\epsilon_{1\mathbf{k}}$. According to (2.38), the energy renormalization is given by

$$\epsilon_{1\mathbf{k}} = \langle P_{\mathbf{k}}^\dagger A_{\mathbf{k}} \rangle \langle A_{\mathbf{k}}^\dagger A_{\mathbf{k}} \rangle^{-1} . \qquad (3.52)$$

From (3.40), $\langle P_{\mathbf{k}}^\dagger A_{\mathbf{k}} \rangle$ contains a sum of factors of the form

$$\langle A_{\mathbf{k}'}^\dagger B_{\mathbf{k}'-\mathbf{k}} A_{\mathbf{k}} \rangle - \langle S^z \rangle \delta(\mathbf{k}'-\mathbf{k}) \langle A_{\mathbf{k}'}^\dagger A_{\mathbf{k}} \rangle . \qquad (3.53)$$

For the first term in (3.53) the Tyablikov approximation is

$$\langle A_{\mathbf{k}'}^\dagger B_{\mathbf{k}'-\mathbf{k}} A_{\mathbf{k}} \rangle \approx \langle B_{\mathbf{k}'-\mathbf{k}} \rangle \langle A_{\mathbf{k}'}^\dagger A_{\mathbf{k}} \rangle = \langle S^z \rangle \delta(\mathbf{k}'-\mathbf{k}) \times \langle A_{\mathbf{k}'}^\dagger A_{\mathbf{k}} \rangle . \qquad (3.54)$$

Thus all terms like (3.53) vanish when (3.54) is used, and hence $\langle P_{\mathbf{k}}^\dagger A_{\mathbf{k}} \rangle$ vanishes and so does $\epsilon_{1\mathbf{k}}$.

Callen Approximation

Callen[14] has observed that (in the language of the present paper) alternate approximations for $\langle P_{\mathbf{k}}^\dagger A_{\mathbf{k}} \rangle$ lead to different results for $\epsilon_{1\mathbf{k}}$. We will take $S=\frac{1}{2}$ for simplicity. For renormalized energies, the basic equation (2.39) gives

$$\langle A_{\mathbf{k}}^\dagger A_{\mathbf{k}} \rangle = \psi_{1\mathbf{k}} \langle [A_{\mathbf{k}}, A_{\mathbf{k}}^\dagger] \rangle ; \qquad (3.55)$$

$$\psi_{1\mathbf{k}} = \{\exp[\beta(\epsilon_{\mathbf{k}} + \epsilon_{1\mathbf{k}})] - 1\}^{-1} . \qquad (3.56)$$

Just as in the derivation of (3.43)–(3.45) above, we find

$$\langle A_{\mathbf{k}}^\dagger A_{\mathbf{k}} \rangle = S^{-1} \langle S^z \rangle \psi_{1\mathbf{k}} ; \qquad (3.57)$$

$$\langle S^z \rangle (1 + S^{-1}\Psi_1) = S , \quad \text{for} \quad S = \tfrac{1}{2} ; \qquad (3.58)$$

$$\Psi_1 = N^{-1}\Sigma_{\mathbf{k}} \psi_{1\mathbf{k}} . \qquad (3.59)$$

We now turn to the evaluation of $\epsilon_{1\mathbf{k}}$, as given by (3.52) along with (3.40) for $P_{\mathbf{k}}^\dagger$. For $S=\frac{1}{2}$, $B_{\mathbf{k}}$ is given by (3.12); with this expression for $B_{\mathbf{k}'-\mathbf{k}}$, (3.40) becomes

$$P_{\mathbf{k}}^\dagger = 2(S - \langle S^z \rangle)(J_0 - J_{\mathbf{k}})A_{\mathbf{k}}^\dagger + 2N^{-1}\Sigma_{\mathbf{k}'\mathbf{k}''}(J_{\mathbf{k}'} - J_{\mathbf{k}'-\mathbf{k}}) + A_{\mathbf{k}'}^\dagger A_{\mathbf{k}''-\mathbf{k}'+\mathbf{k}}^\dagger A_{\mathbf{k}''} . \qquad (3.60)$$

In calculating $\langle P_{\mathbf{k}}^\dagger A_{\mathbf{k}} \rangle$ we are again faced with four-operator statistical averages; our procedure is to use a zeroth-order basic equation for the case of renormalized energies:

$$\langle P_{\mathbf{k}}^\dagger A_{\mathbf{k}} \rangle = \psi_{1\mathbf{k}} \langle [A_{\mathbf{k}}, P_{\mathbf{k}}^\dagger] \rangle . \qquad (3.61)$$

A representative four-operator term is then evaluated as follows:

$$\begin{aligned} &\langle A_{\mathbf{k}'}^\dagger A_{\mathbf{k}''-\mathbf{k}'+\mathbf{k}}^\dagger A_{\mathbf{k}''} A_{\mathbf{k}} \rangle \\ &= \psi_{1\mathbf{k}} \langle [A_{\mathbf{k}}, A_{\mathbf{k}'}^\dagger A_{\mathbf{k}''-\mathbf{k}'+\mathbf{k}}^\dagger A_{\mathbf{k}''}] \rangle \\ &= \psi_{1\mathbf{k}} S^{-1} \langle A_{\mathbf{k}''-\mathbf{k}'+\mathbf{k}}^\dagger B_{\mathbf{k}-\mathbf{k}'} A_{\mathbf{k}''} + A_{\mathbf{k}'}^\dagger B_{\mathbf{k}'-\mathbf{k}''} A_{\mathbf{k}''} \\ &\qquad - N^{-1} A_{\mathbf{k}''}^\dagger A_{\mathbf{k}''} \rangle \\ &\approx \psi_{1\mathbf{k}} S^{-1} \langle S^z \rangle \langle A_{\mathbf{k}''}^\dagger A_{\mathbf{k}''} \rangle [\delta(\mathbf{k}'-\mathbf{k}) + \delta(\mathbf{k}'-\mathbf{k}'') \\ &\qquad - N^{-1} \langle S^z \rangle^{-1}] , \end{aligned} \qquad (3.62)$$

where the last line follows from the Tyablikov-type approximation (3.54). With (3.62) and (3.57), the right-hand side of (3.61) is easily evaluated and is then simplified with the aid of (3.58). The result for $\epsilon_{1\mathbf{k}}$ is nonzero; we denote this value by $\tilde{\epsilon}_{1\mathbf{k}}$, where

$$\tilde{\epsilon}_{1\mathbf{k}} = 2S^{-1} \langle S^z \rangle N^{-1} \Sigma_{\mathbf{k}'} (J_{\mathbf{k}'} - J_{\mathbf{k}'-\mathbf{k}}) \psi_{1\mathbf{k}'} . \qquad (3.63)$$

Equation (3.63) can be obtained more simply from (3.61) by leaving $P_{\mathbf{k}}^\dagger$ in the form (3.40), instead of transforming to (3.60), and then approximating averages of the form $\langle B_{\mathbf{k}} B_{-\mathbf{k}} \rangle$; we have given the above derivation since the correspondence with Callen's work is more easily seen.

The approximate calculation of $\tilde{\epsilon}_{1\mathbf{k}}$ is equivalent to Callen's treatment for the case when his parameter $\alpha = 1$.[14] On the other hand, the calculation discussed in (3.52)–(3.54) corresponds to $\alpha = 0$. More specifically, since $B_{\mathbf{k}}$ is given by (3.12) for $S=\frac{1}{2}$, we can write

$$B_{\mathbf{k}} = \alpha [S\delta(\mathbf{k}) - N^{-1}\Sigma_{\mathbf{k}'} A_{\mathbf{k}'-\mathbf{k}}^\dagger A_{\mathbf{k}'}] + (1-\alpha) B_{\mathbf{k}} , \qquad (3.64)$$

where α is any number. This expression is analogous to Eq. (12) of Callen[14] for S_n^z. If we now use (3.64) for $B_{\mathbf{k}'-\mathbf{k}}$ in (3.40) and go through the above derivations, the result for $\epsilon_{1\mathbf{k}}$ is obviously

$$\epsilon_{1\mathbf{k}} = \alpha \tilde{\epsilon}_{1\mathbf{k}} . \qquad (3.65)$$

Callen has presented arguments for choosing $\alpha = S^{-1}\langle S^z \rangle$ for $S=\frac{1}{2}$. For this case, the complete energies are

$$\epsilon_{\mathbf{k}} + \epsilon_{1\mathbf{k}} = g\mu H + 2\langle S^z \rangle (J_0 - J_{\mathbf{k}}) + 2[S^{-1}\langle S^z \rangle]^2 \times N^{-1}\Sigma_{\mathbf{k}'} (J_{\mathbf{k}'} - J_{\mathbf{k}'-\mathbf{k}}) \psi_{1\mathbf{k}'} . \qquad (3.66)$$

[14] H. B. Callen, Phys. Rev. **130**, 890 (1963).

Equations (3.58) and (3.59), together with (3.56) and (3.66), are the same as Callen's[14] Eqs. (49)–(52) for the case $S=\frac{1}{2}$.

It is interesting to note that $\tilde{\epsilon}_{1\mathbf{k}}$ of (3.63) is small compared to $\epsilon_{\mathbf{k}}$ at low temperatures, but not at high temperatures. To show the failure at high T, assume first that $\tilde{\epsilon}_{1\mathbf{k}} \ll \epsilon_{\mathbf{k}}$, so that $\psi_{1\mathbf{k}} \approx \psi_{\mathbf{k}}$. Now as $H \rightarrow 0$, $\langle S^z \rangle \rightarrow 0$ and hence $\epsilon_{\mathbf{k}} \rightarrow 0$ along with $\langle S^z \rangle$. However, in order to satisfy (3.58) under these conditions, we find that $\psi_{\mathbf{k}} \rightarrow \infty$ in such a way that $\langle S^z \rangle \psi_{\mathbf{k}}$ remains finite. Then replacing $\psi_{1\mathbf{k}'}$ by $\psi_{\mathbf{k}'}$ in (3.63), it is seen that $\tilde{\epsilon}_{1\mathbf{k}}$ remains finite, and hence $\tilde{\epsilon}_{1\mathbf{k}} \ll \epsilon_{\mathbf{k}}$ cannot hold. We further conclude that if α is taken to be proportional to $[S^{-1}\langle S^z \rangle]^n$, then $\epsilon_{1\mathbf{k}} = \alpha \tilde{\epsilon}_{1\mathbf{k}}$ will approach zero at least as fast as $\langle S^z \rangle$ for $n \geq 1$. The perturbation treatment is thus justified for $n \geq 1$, at least within the framework of the approximations made in evaluating $\langle P_{\mathbf{k}}^\dagger A_{\mathbf{k}} \rangle$.

IV. CONCLUDING REMARKS

The utility of the present method will depend on two factors. First, the remainder operators $R_i^\dagger$ of the Hamiltonian commutator equations must be small enough to be reasonably treated as a statistical perturbation. Second, in order to calculate the statistical average of any operator corresponding to an observable of the problem, a sufficient number of creation and annihilation operators $\theta_i^\dagger$, θ_i must be found to represent the observable. This latter requirement is not difficult to satisfy in practice; note that one has the same requirement in applying the Green's-function method to calculating observables.

The statistical perturbation theory which we have derived bears a great resemblance to the method of thermodynamic Green's functions[1–4] in actual application. We believe that the present method has two advantages. In the first place, for a given problem, one makes an obvious approximation in saying that the $R_i^\dagger$ operators are small, and hence gains more physical insight than is offered by the decoupling of higher order Green's functions. In the second place, the perturbation term in the basic equation can be evaluated to give an estimate of the accuracy of the zeroth-order results; further, if this term is indeed small, it can be considered as a correction to the zeroth-order results.

Referring to the general derivation of Sec. II, and particularly to the derivation of the perturbation equation (2.32), there are two obvious possibilities for trying to improve the zeroth- and first-order approximations of this theory. These are (a) develop the perturbation term of (2.29), which is still exact, into a power series in the $R_i^\dagger$, R_i operators by repeated commutation of these operators with $\mathcal{H}$, and (b) renormalize the $\theta_i^\dagger$ operators so as to make the $R_i^\dagger$ even smaller, especially for those $R_i^\dagger$ which contribute most to the statistical mechanics. The first possibility is represented by the basic equations (2.32) and (2.33), where the perturbation term is just the leading term in a power-series expansion. However, the second possibility seems to offer the most promise. In the low-temperature Heisenberg-ferromagnet problem, for example, the development of the perturbation term for Bloch spin-wave operators leads to an infinite series of contributions which appear to be all of the same order, while the operator renormalization removes all of such contributions in a one-step procedure.

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