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[17]For the renormalization procedure see Ref. 12, especially Appendix III.
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[19]For the case of nonvanishing external-field wave vector $\vec{q}$, the left-hand side of (3.13) should read $i(\vec{q}\cdot\vec{v}_{kn}-\omega)\Phi_{kn}$.
[20]Note that the electron-phonon interaction enters the electron or phonon self-energy part in the form $|V_{kn,k'n'}|^2$ to the lowest order shown in Fig. 3.
[21]From (3.16) it follows that $\{|V_{kn,k'n'}|^2\}^{(s)}$ is purely imaginary. Hence $\{|V_{kn,k'n'}|^2\}^{(s)}=0$, QED.
[22]These relations were originally derived for the impurity scattering. They hold also for the electron-phonon interaction.
[23]A complication arises without this inversion symmetry. This property has also been assumed by previous authors.
[24]For more detailed discussion of this kind of approximation, see Ref. 12.
[25]In view of (2.19) we are interested only in the terms which are first order in ω. Therefore the contribution from the last two terms of (3.20) is small due to their slowly varying nature as a function of ω.
[26]Using (3.16) one has $\{V_{kn,k'n'}D_xV_{k'n',kn}\}^{(s)*}$ $=V^{(s)*}{}_{kn,k'n'}D_x\overline{V}^{*}_{k'n',kn}+\overline{V}^{*}_{kn,k'n'}D_xV^{(s)*}_{k'n',kn}$ $=-(V_{kn,k'n'}D_xV_{k'n',kn})^{(s)}$
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$S=\frac{1}{2}$, XY Model on Cubic Lattices. I. Susceptibility and Fluctuation near Critical Temperature*

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For the $S=\frac{1}{2}$, XY model of a quantum lattice fluid or a ferromagnet the conventional order parameter does not commute with the Hamiltonian. As a result, the mean-square fluctuation of the order parameter and the isothermal susceptibility are not related in the usual way the general fluctuation theorem. For the above model, arguments are here presented to support the idea that as $T\to T_c$ the quantum effect due to the noncommutation becomes masked and the two quantities have the same critical behavior. This work is consistent with the exact results of Falk and Bruch who defined a certain moment of the spectral density and used inequalities to establish that *if* the moment $\to 0$ as $T\to T_c$, then the susceptibility-fluctuation ratio becomes unity thus ensuring coinciding critical behavior. The latter result applies to a large class of models including the one considered here.

I. INTRODUCTION

The three-dimensional $S=\frac{1}{2}$, XY model defined in Sec. II is one of the simplest *quantum mechanical* cooperative models. This model is thought to be useful as an approximation for certain physical systems such as liquid helium[4] near the λ transition.[1] A few of the static properties of this model near the critical point have now been calculated and their similarity to those of other cooperative models has been observed.[2]

One unique feature of the XY model, which particularly emphasizes its quantum nature, is that its order parameter M^x (or M^y) does *not* commute with the Hamiltonian (the order parameter for the Heisenberg ferromagnet commutes with its Hamiltonian).[3] The noncommuting gives rise to two interesting related consequences. (i) The order parameter has a time-dependent behavior at all wavelengths including zero wavelength, and the system thus can *relax*. The dynamical behavior of this system has proved to be quite interesting and will be treated in a later paper. (ii) One can define the mean-square fluctuation of the order parameter Y and the zero-field static isothermal susceptibility χ which are not connected in the usual way by the general "fluctuation" theorem (we shall refer to Y and χ simply as the fluctuation and susceptibility, respectively). This paper is concerned with the nature of the distinction between the fluctuation and susceptibility whose origin is thus quantum mechanical.

While the distinction between the fluctuation and susceptibility is valid generally, one suspects that in certain physical regions such as in the critical region the dominant behavior of the susceptibility may be the same as that of the fluctuation. In particular the widely held notion of universality in critical behavior argues that both the fluctuation and susceptibility have the same critical behavior since the quantum effect of this kind is believed to be unimportant in the critical region. In this connection there is an interesting work due to Falk and Bruch[4] who have obtained the upper and lower bounds for the ratio of the susceptibility and fluctuation for rather general systems. They show that the two bounds merge provided that a certain moment of a spectral density vanishes. In their paper it is pointed out that if the moment vanishes as $T\to T_c$, then the merging of the two bounds implies that the fluctuation and susceptibility have the same critical behavior; hence, the same critical exponents.

The *XY* model represents a nontrivial case where the above ideas can be studied to gain insight into the question of how the quantum effect of the noncommutativity of M^x and $\mathcal{H}_0$ manages to become suppressed with the onset of critical fluctuations. This very interesting question is related to the question of whether the critical exponents depend on the quantum number S. Consider, for example, the *XY* model of classical spins. Here the fluctuation and susceptibility are always identical since $[M^x, \mathcal{H}_0]=0$. Thus, in the transition from $S=\frac{1}{2}$ to $S=\infty$ the effect of S on the critical exponent, say, $\gamma(S)$, must in some ways be very similar to the effect of the commutator $[M^x, \mathcal{H}_0]$ has on the difference between the fluctuation and susceptibility.

Betts *et al.*[2] and Ditzian[5] have obtained a finite number of series expansion coefficients for the fluctuation and susceptibility, respectively. Their results show a trend which indicates that both quantities (Y and χ) have the same critical behavior. The numerical work, however, sheds little light on the presumed disappearance of the quantum effect.

In this paper we shall assume the general validity of series expansions[6] and obtain an expression for an *arbitrary order* expansion coefficient for the susceptibility. By comparing this expression with that for the fluctuation we shall study the effect of the commutator $[M^x, \mathcal{H}_0]$ in the asymptotic limit. From the point of series expansions for the *XY* model, our result stands as an interpretation of the work of Falk and Bruch. Also, our formalism developed here will be found useful in obtaining the dynamic behavior of the *XY* model.

This paper is divided into three main sections. In Sec. II the basic formalism is given. Here an expression for an arbitrary order coefficient of expansion for the susceptibility is obtained via a perturbative method. This perturbative method is further described in Appendix A. In Sec. III, a numerical study is made to compare the critical behavior of the fluctuation and susceptibility and also to test the accuracy of our perturbative method. In Sec. IV the susceptibility is obtained from the closed expression for an arbitrary order expansion coefficient given in Sec. II, and contact is then made with the results of Ref. 4.

II. SUSCEPTIBILITY AND FLUCTUATION

The *XY* model of N interacting spin-$\frac{1}{2}$ particles in an external field $H^x\equiv H$ is defined by the interaction Hamiltonian

$$\mathcal{H}=-2J\sum_{\langle ij\rangle} S_i^xS_j^x+S_i^yS_j^y-H\sum_i S_i^x$$

$$\equiv -JP-HQ\ , \tag{1}$$

where the first sum is over nearest-neighbor pairs only. For $T>T_c$, the fluctuation is given by

$$Y=\sum_{r=1}^{N}\langle S_0^xS_r^x\rangle=\frac{1}{4}+\sum_{n=1}^{\infty} a_nK^n\ , \tag{2}$$

where $K=J/k_BT$ and the angular brackets denote an ensemble average in *zero* field. It has been shown that[7]

$$a_n=(n!)^{-1}\,\mathrm{Tr}Q^2P^n\ , \tag{3}$$

where the trace is taken over terms linear in N only. The zero-field static isothermal susceptibility is given by

$$\chi=\beta^{-1}\frac{\partial}{\partial H}\langle Q\rangle=\frac{1}{4}+\sum_{n=1}^{\infty}\tilde{a}_nK^n\ . \tag{4}$$

Noting that P and Q do not commute we write

$$n!\,\tilde{a}_n=\sum_{r=0}^{t_n} b_n^{(r)}B_n^{(r)}\ , \tag{5}$$

where

$$B_n^{(r)}=\mathrm{Tr}QP^rQP^{n-r}\ . \tag{6}$$

It follows directly from the definition (4) that $t_n=\frac{1}{2}n$ if n is even and $t_n=\frac{1}{2}(n-1)$ otherwise; and

$$b_n^{(r)}=2/(n+1)\equiv N_n^{-1} \tag{7}$$

for all values of r except for one value $r=t_n=\frac{1}{2}n$ (n even), for which

$$b_n^{(n/2)}=\tfrac{1}{2}N_n^{-1}\ . \tag{8}$$

Observe that if P and Q commute, $B_n^{(r)}=B_n^{(0)}$ and thus $\tilde{a}_n=a_n$.[8]

Let the commutation relation between P and Q be denoted by

$$[P,\ Q]=y\ . \tag{9}$$

From (1) and the commutation relations of spin-$\frac{1}{2}$ operators, it is easy to show that

$$y=-2i\sum_{ij} S_i^zS_j^y\ , \tag{10}$$

where now the nearest-neighbor sum includes both $i>j$ and $i<j$. With aid of the above commutator we can write

$$B_n^{(r)} = B_n^{(r-1)} - C_{n-1}^{(r-1)} , \tag{11}$$

where we shall define

$$C_n^{(r)} = \mathrm{Tr}\, y P^r Q P^{n-r} . \tag{12}$$

Using the relation (11) recursively we then obtain

$$B_n^{(r)} = B_n^{(0)} - \sum_{r'=0}^{r-1} C_{n-1}^{(r')} . \tag{13}$$

Observe that since $B_n^{(0)} = n!\, a_n$, the effect of the commutator (9) on $B_n^{(r)}$ is contained entirely in the second term.

Now the commutation relation between P and y can be obtained from (1) and (10), which we shall write as

$$[P,\ y] = qQ + \psi + \theta , \tag{14}$$

where q is the coordination number, and ψ and θ are operators given in Appendix A.

Thus, from (12) and (14) we get

$$C_n^{(r)} = C_n^{(r-1)} - qB_{n-1}^{(r-1)} - \lambda_{n-1}^{(r-1)} , \tag{15}$$

where

$$\lambda_n^{(r)} = \mathrm{Tr}(\psi + \theta) P^r Q P^{n-r} . \tag{16}$$

Using (15) recursively as before, we find that

$$\sum_{r'=0}^{r-1} C_{n-1}^{(r')} = rC_{n-1}^{(0)} - \sum_{r'=0}^{r-2} (r - r' - 1)(qB_{n-2}^{(r')} + \lambda_{n-2}^{(r')}) . \tag{17}$$

It will be assumed here that $\lambda_{n-2}^{(r')}$ is small compared with $qB_{n-2}^{(r')}$ and can thus be ignored (we shall call this step zeroth-order approximation). This approximation is numerically justified in Sec. III and further discussed in Appendix A.

Thus substituting (17) into (13) and by recursion, we obtain in *zeroth order*

$$B_n^{(r)} = \sum_{r'=0}^{l_r} q^{r'} [\binom{r}{2r'} B_{n-2r'}^{(0)} - \binom{r}{2r'+1} C_{n-2r'-1}^{(0)}] , \tag{18}$$

where $\binom{r}{r'}$ is the binomial factor and $l_r = \frac{1}{2} r$ if r is even and $l_r = \frac{1}{2}(r-1)$ otherwise. The leading term of $B_n^{(r)}$ shows the following behavior:

$$B_n^{(r)} = B_n^{(0)} - rC_{n-1}^{(0)} + \tfrac{1}{2} r(r+1) qB_{n-2}^{(0)} - \cdots . \tag{19}$$

In Appendix B it is proved that

$$C_n^{(0)} = \tfrac{1}{2}\mathrm{Tr} P^{n+1} - \mathrm{Tr} \sum_{ij} S_i^z S_j^z P^n . \tag{20}$$

Hence, within zeroth order, we have now reduced $B_n^{(r)}$ to quantities which do not explicitly depend on the commutation relation (9). For simplicity let n be an *odd* number. Then, using (18)

$$N_n n!\, \tilde{a}_n = \sum_{r=0}^{N_n-1} B_n^{(r)}$$

$$= \sum_{r=0}^{N_n-1} \sum_{r'=0}^{l_r} q^{r'} [\binom{r}{2r'} B_{n-2r'}^{(0)} - \binom{r}{2r'+1} C_{n-2r'-1}^{(0)}] . \tag{21}$$

The double sum in (21) can be reduced to a single sum by carrying out the sum over r first and then by regrouping resulting terms in powers of q. We obtain that

$$N_n n!\, \tilde{a}_n = \sum_{p=0}^{p_n} q^p (s_{2p}^{(n)} B_{n-2p}^{(0)} - s_{2p+1}^{(n)} C_{n-2p-1}^{(0)}) , \tag{22}$$

where $s_p^{(n)} = \binom{N_n}{p+1}$, and $p_n = \frac{1}{2}[\frac{1}{2}(n-1)]$ if $\frac{1}{2}(n-1)$ is even and $p_n = \frac{1}{2}[\frac{1}{2}(n-3)]$ otherwise (given that n is an odd number). Using (3) and (6), we then find for the leading behavior of $\tilde{a}_n$,

$$\tilde{a}_n = a_n - \frac{1}{2}(1 - n^{-1}) \frac{1}{2!} C_{n-1}^{(0)} \frac{1}{(n-1)!} + \left(\frac{1}{2}\right)^2 \frac{q(1-3n^{-1})}{3!} a_{n-2} - \cdots , \tag{23}$$

where the difference, $\tilde{a}_n - a_n$, can be considered as a "quantum" correction arising from the nonzero commutation relation between P and Q.

To what extent do these correction terms contribute to $\tilde{a}_n$? For n finite, we have provided a numerical answer in Sec. III. In the remainder of this section we shall study the behavior of the correction terms in the asymptotic limit $(n \to \infty)$. It was shown in Ref. 5 that $B^{(0)}$ terms consist of, in the language of graph theory,[9] open chainlike graphs, whereas $C^{(0)}$ terms consist of closed graphs. The largest graphs in the leading term of (23), $B_n^{(0)}$, for example, have lattice constants of the order $(q-1)^n$ for $q \gg 2$, while the largest graphs in the second term $C_{n-1}^{(0)}$ have lattice constants of the order $(q-1)^{n/2}$. Hence, in the large n limit (or $T \to T_c$) we can completely ignore $C^{(0)}$ terms and thus write for the leading behavior of $\tilde{a}_n$ as

$$\lim_{n\to\infty} \tilde{a}_n = a_n + \left(\frac{1}{2}\right)^2 \frac{q(1-3n^{-1})}{3!} a_{n-2} + \left(\frac{1}{2}\right)^4 \frac{q^2(1-10n^{-1})}{5!} a_{n-4} + \cdots . \tag{24}$$

Observe that for a given but large n our "quantum" correction contributes (in a quantitative sense) to critical fluctuations in the form of a decreasing order of coefficients (a_{n-2}, a_{n-4}, a_{n-6}, and so on). Is this quantum correction manifested in the critical behavior?

We shall *assume* that near the critical point both Y and χ obey a power law with exponents γ and $\tilde{\gamma}$, respectively. Then, the ratio $r_n = a_n/a_{n-1}$ for the fluctuation satisfies the well-known relation

$$\lim_{n\to\infty} r_n = K_c^{-1}[1 + (\gamma - 1)n^{-1} + O(n^{-2})] , \tag{25}$$

where K_c is the critical point. Using (24) we can obtain an expression for the ratio $\tilde{r}_n = \tilde{a}_n/\tilde{a}_{n-1}$ for

TABLE I. Expansion coefficients for the fluctuation Y from Ref. 2; exact coefficients for the susceptibility χ from Ref. 5; and coefficients for the zeroth-order susceptibility $\chi^{(0)}$ calculated from Eq. (22).

n	$2Y$	2χ	$2\chi^{(0)}$
0	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
1	3	3	3
2	16.5	16	16
3	82	80.75	80.75
4	397.875	396.15	398.625
5	1914.8125	1911.962	1926.7625
6	9141.270833	9131.062	9241.315477
7	43 322.59747	43283.731	43 820.45862
8	204 151.3777	⋯	207 016.1153
9	957 786.7005	⋯	971 655.1863

the susceptibility

$$\lim_{n\to\infty}\tilde{r}_n/r_n = \frac{1+qs_2^{(n)}[n(n-1)s_0^{(n)}]^{-1}a_{n-2}/a_n+\cdots}{1+qs_2^{(n-1)}[(n-1)(n-2)s_0^{(n-1)}]^{-1}a_{n-3}/a_{n-1}+\cdots} . \tag{26}$$

The ratios such as a_{n-2}/a_n can be further replaced by using (25) and we obtain

$$\lim_{n\to\infty}\tilde{r}_n/r_n = 1+O(n^{-2}) . \tag{27}$$

The meaning of (27) can be readily seen from (25). That both Y and χ have the same critical temperature needs no further comment as it is intuitively obvious. The absence of a term linear in n^{-1} in (27) clearly implies that $\tilde{\gamma}=\gamma$. Our result suggests that while the quantum correction persists in all temperatures, as $T\to T_c$ it becomes masked and does not influence critical fluctuations. Our result further suggests that critical exponents are independent of the spin quantum number S (as is generally believed) in a manner analogous to our situation here regarding the susceptibility and fluctuation.

While our result (27) is valid strictly for zeroth order, we show in Appendix A that the same conclusion still holds in higher orders.

III. NUMERICAL RESULTS

Although our result (27) is asymptotically exact in zeroth order (strictly speaking, the series expansion has a meaning only asymptotically), it would nevertheless be interesting to see whether one could predict $\tilde{\gamma}=\gamma$ from a finite number of expansion coefficients. It is also desirable to see the accuracy of our zeroth-order approximation.

Betts *et al.*[2] have obtained the first nine coefficients of the fluctuation series Y [see Eq. (2)] for cubic lattices. In the second column of Table I the coefficients a_n for the fcc lattice are listed. In the third column of Table I we list the coefficients $\tilde{a}_n$ of the susceptibility series obtained by Ditzian[5] from (5) using a technique developed by Betts *et al.* The coefficients $\tilde{a}_n$ of the zeroth-order susceptibility series, which we shall denote as $\chi^{(0)}$, can be directly obtained by (22) using the values for $B_n^{(0)}$ and $C_n^{(0)}$. These are listed in the fourth column of Table I.

As may be seen by comparing the last two columns of Table I, the coefficients of $\chi^{(0)}$ look to be a reasonably good approximation for the coefficients of χ, differing at most about 1%. The validity of the zeroth-order approximation and the procedure of introducing higher approximations are further discussed in Appendix A.

In Table II we have compared the values of $B_n^{(0)}$ and $C_{n-1}^{(0)}$. From the table it is clear that even for n finite the $C^{(0)}$ terms contribute only negligibly. With an increasing n, the contribution of $C^{(0)}$ terms becomes less and less important.

In Fig. 1 we have shown a familiar ratio plot of ratios of coefficients for Y and $\chi^{(0)}$ (ratios of coefficients for χ are not shown here since these values fall very near those of $\chi^{(0)}$). As may be observed from the figure, one would conclude that within an acceptable error limit $\tilde{\gamma}=\gamma$.

IV. DISCUSSION

It was shown in Sec. II that in zeroth order the leading "quantum" correction to the susceptibility coefficient $\tilde{a}_n$ are those of lower order fluctuation coefficients a_{n-2}, a_{n-4}, a_{n-6}, etc. We have concluded that the weight of these lower order terms is not large enough (compared with that of the principal term a_n) to be manifested in the critical behavior.

It is desirable here to relate our result to the work of Falk and Bruch. In obtaining our asymptotic expression (27) we have argued that the contribution from $C^{(0)}$ is negligible compared with that of $B^{(0)}$. We have shown in Appendix B that the second moment of the spectral density ν_2 is given by

TABLE II. Reduced coefficients $B_n^{(0)}$ and the second moment coefficients $C_n^{(0)}$ obtained from Refs. 2 and 11.

n	$2B_n^{(0)}/n!$	$2C_{n-1}^{(0)}/(n-1)!$
0	$\frac{1}{2}$	⋯
1	3	⋯
2	16.5	3
3	83	7.5
4	397.875	12.75
5	1914.8125	22.25
6	9141.270833	62.775
7	43 322.59747	208.135
8	204 151.3777	730.77264
9	957 786.7005	2645.2201

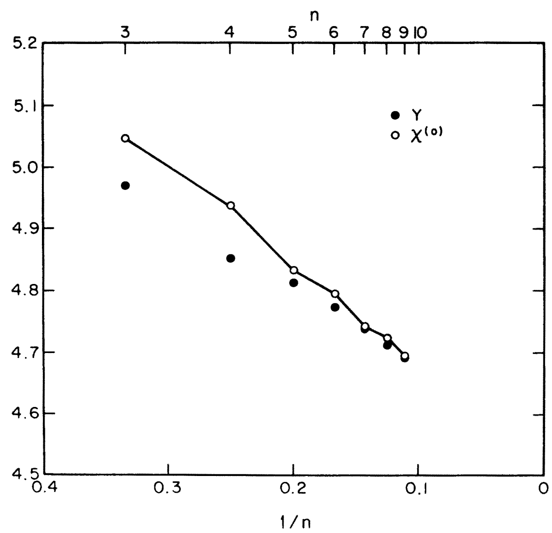

FIG. 1. Ratios of coefficients for the fluctuation and the zeroth-order susceptibility (both on the fcc lattice).

$$\nu_2/-J=\langle[Q,[P,Q]]\rangle=-2\sum_{n=0}^{\infty}K^nC_n^{(0)}/n!\ . \tag{28}$$

Now using (4) and (22) we can obtain the susceptibility in terms of reduced quantities [those not explicitly depending on the commutator (9)]

$$\chi=\sum_{n=0}^{\infty}\tilde{a}_nK^n$$
$$=\sum_{n=0}^{\infty}\frac{K^n}{N_n n!}\sum_{p=0}^{p_n}q^p\left[s_{2p}^{(n)}B_{n-2p}^{(0)}-s_{2p+1}^{(n)}C_{n-2p-1}^{(0)}\right]\ . \tag{29}$$

For n even, the above expression requires a slight modification.[10] We observe that, for a given p, the sum over n for each $B_{n-2p}^{(0)}$ produces a term proportional to Y and similarly for each $C_{n-2p-1}^{(0)}$ a term proportional to ν_2. Hence, first enumerating the p sum in (29), we obtain after some rearrangement with (2) and (28)

$$\chi^{(0)}=fY+g\nu_2\ , \tag{30}$$

where

$$f=\sinh\sqrt{q}K/\sqrt{q}K\ , \tag{31}$$

$$g=(1-\cosh\sqrt{q}K)/2(\sqrt{q}K)^2\ . \tag{32}$$

The above result can be more directly obtained by another method.[11] Now observe that if $Y\gg\nu_2$ as $T\rightarrow T_c$, then $\chi^{(0)}$ and Y have a similar critical behavior since $f(T)$ and $g(T)$ are analytic at $T=Tc$. This is consistent with the general result of Falk and Bruch.

As $T\rightarrow T_c$, $Y\gg\nu_2$ follows from our earlier argument that their coefficients of expansion satisfy $B_n^{(0)}\gg C_n^{(0)}$ as $n\rightarrow\infty$. We shall also show in a subsequent paper[12] that in the critical region the second moment is nondivergent ($\nu_2\sim\Delta T^{-\alpha+1}$), whereas the fluctuation as we know is strongly singular ($Y\sim\Delta T^{-\gamma}$).[13] The best present estimates available for the exponents for cubic lattices are $\alpha\approx 0$ and $\gamma\approx\frac{4}{3}$.[2]

If we proceed beyond zeroth order, we obtain essentially the same form for χ as for $\chi^{(0)}$ except that now the two functions f and g are replaced by more complicated functions which are nevertheless still analytic at $T=T_c$ (see Appendix A). Thus our conclusion of zeroth order still holds.

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APPENDIX A: HIGHER-ORDER CORRECTION

The commutation relation between P and y was denoted in the form [see (14)]

$$[P,y]=qQ+\psi+\theta\ . \tag{A1}$$

Using (1) and (10) we identify

$$\psi=4J^2\sum S_{r_1}^zS_{r_2}^zS_{r_3}^x\equiv U^{(1)}Q \tag{A2}$$

and

$$\theta=4J^2\sum S_{r_1}^y(S_{r_2}^xS_{r_3}^y-S_{r_2}^yS_{r_3}^x)\ , \tag{A3}$$

where the lattice sum is now restricted to that of a linear chain of two units of the nearest-neighbor distance in the sequence $r_1r_2r_3$. Equations (13) and (15) then provide the recursion relation

$$B_n^{(r)}=B_n^{(0)}-rC_{n-1}^{(0)}+\sum_{r'=0}^{r-2}(r-r'-1)(qB_{n-2}^{(r')}+\lambda_{n-2}^{(r')})\ , \tag{A4}$$

where $\lambda_n^{(r)}$ is defined by (16). The *zeroth-order* approximation results if we neglect the last term in (A4) by assuming that $qB_{n-2}^{(r')}\gg\lambda_{n-2}^{(r')}$. Inclusion of the last term leads to the following recursion relation:

$$B_n^{(r)}=[B_n^{(r)}]^{(0)}+\sum_{n'=1}^{t_n}q^{n'-1}\prod_{R=1}^{n'}\sum_{r_R=0}^{r_{R-1}-2}(r_{R-1}-r_R-1)\lambda_{n-2R}^{(r_R)}, \tag{A5}$$

where the first term in (A5) represents our zeroth-order result (18) and $r_0\equiv r$.

Now $\lambda_n^{(r)}$ may be evaluated as follows. Consider, first, the leading term ($r=0$),

$$\lambda_n^{(0)}=\mathrm{Tr}(\psi+\theta)QP^n\ . \tag{A6}$$

From the definition of θ we see that as n becomes large, the small difference between the two terms arising from the restricted sum becomes less and less important.[14] In fact, it may be seen that as $n\rightarrow\infty$, $\mathrm{Tr}\theta QP^n\rightarrow 0$. [Also note that if the restriction on the sum r_1 in (A3) is relaxed, $\mathrm{Tr}\theta QP^n=0$ for all n.] As our *first*-order approximation, we shall therefore ignore the contribution of $\mathrm{Tr}\theta QP^n$ in (A6) and write, with (A2),

$$\lambda_{n(1)}^{(r)} = \mathrm{Tr}(U^{(1)}Q)P^r QP^{n-r} + O(\theta)\,. \tag{A7}$$

It is now straightforward to develop a recursion relation for $\lambda_{n(1)}^{(r)}$. First, we obtain the commutation relation between P and $U^{(1)}Q$ in first order,

$$[P, U^{(1)}Q] = q_1 y + U^{(1)}y + O(\theta)\ , \tag{A8}$$

where $q_1 = q_0 - 1$, with $q_0 \equiv q$,[15] and $U^{(1)}y$ is defined analogously to $U^{(1)}Q$,

$$U^{(1)}y = \sum \mathrm{Tr} S_{r_1}^z S_{r_2}^z S_{r_3}^z S_{r_4}^y\ , \tag{A8a}$$

where the lattice sum is restricted to that of a linear chain of three units in the above numerical sequence. With aid of (A8) we get from (A7) in first order

$$\lambda_{n(1)}^{(r)} = \lambda_{n(1)}^{(0)} - \sum_{r'=0}^{r-1} (q_1 C_{n-1}^{(r')} + \kappa_{n-1(1)}^{(r')})\ , \tag{A9}$$

where

$$\kappa_{n(1)}^{(r)} = \mathrm{Tr}(U^{(1)}y)P^r QP^{n-r}\ . \tag{A10}$$

Similarly the commutation relation between P and $U^{(1)}y$ can be defined as

$$[P, U^{(1)}y] = q_2 U^{(1)}Q + U^{(2)}Q + O(\theta)\ , \tag{A11}$$

where q_2 denotes the free end sum of a linear chain of three units (see Ref. 15), and

$$U^{(2)}Q = (4J^2)^2 \sum S_{r_1}^z S_{r_2}^z S_{r_3}^z S_{r_4}^z S_{r_5}^x\ , \tag{A12}$$

where the lattice sum is restricted to that of a linear chain of four units in the sequence from r_1 to r_5. Hence, by recursion,

$$\kappa_{n(1)}^{(r)} = \kappa_{n(1)}^{(0)} - \sum_{r'=0}^{r-1} (q_2 \lambda_{n-1(1)}^{(r')} + \lambda_{n-1(2)}^{(r')})\ , \tag{A13}$$

where

$$\lambda_{n(2)}^{(r)} = \mathrm{Tr}(U^{(2)}Q)P^r QP^{n-r}\ . \tag{A14}$$

Using (A9) and (A13) we can eliminate $\kappa_{n(1)}^{(r)}$ entirely and obtain the following expression:

$$\lambda_{n(1)}^{(r)} = \lambda_{n(1)}^{(0)} - q_1 r C_{n-1}^{(0)} - r\kappa_{n-1(1)}^{(0)} + \sum_{r'=0}^{r-1} (r - r' - 1)[q_0 q_1 B_{n-2}^{(r')} + (q_1 + q_2)\lambda_{n-2(1)}^{(r')} + \lambda_{n-2(2)}^{(r')}]\ . \tag{A15}$$

This procedure may be further continued to give a complete hierarchy of recursion relations in terms of reduced quantities. One can however considerably simplify the procedure by using the method of a continued-fraction representation of Mori.[16] In a subsequent paper we will apply the method of Mori to our perturbation approach and obtain in a much more simple form the hierarchy of recursion relations.

The numerical work shown in Sec. III provides a measure of accuracy of our zeroth-order approximation. Now for our principal result (27) to be valid beyond zeroth order, it is only necessary that, for a given $B_n^{(r)}$, the first-order correction $\lambda_{n-2}^{(r)}$ be of the order equal to, or less than, the zeroth-order correction $qB_{n-2}^{(r)}$ [see (A4)]. This follows since $qB_{n-2}^{(0)}$, while not negligible compared with $B_n^{(0)}$, was shown nevertheless *not* to influence the critical behavior which is solely determined by the leading term $B_n^{(0)}$. We shall briefly sketch here a proof that $\lambda_n^{(r)}$ is of the order less than $qB_n^{(r)}$. A more detailed proof is found in the second paper of our series[12] together with other related proofs.

For our purpose it is sufficient to compare $\lambda_n^{(0)}$ and $qB_n^{(0)}$ for large n. Using (A2) we have (setting $2J = 1$)

$$\lambda_n^{(0)} = \sum \mathrm{Tr} S_{r_3}^z S_{r_2}^z S_{r_1}^x S_{r_j}^x P^n\ , \tag{A16}$$

where the lattice sum is over $(r_1 r_2 r_3)$, which are constrained to be a linear chain, and r_j which is unrestricted. It is convenient to divide (A16) into two parts,

$$\lambda_n^{(0)} = (\tfrac{1}{4} q_2) \sum \mathrm{Tr} S_r^x S_{r'}^x P^n + \sum{}' \mathrm{Tr} S_{r_3}^z S_{r_2}^z S_{r_1}^x S_{r_j}^x P^n\ , \tag{A17}$$

where by the prime we mean $r_j \neq r_1$. The first term in (A17), which is proportional to $C_n^{(0)}$, can therefore be neglected for large n (see Sec. II and Appendix B). Now in terms of the raising and lowering operators $S^{\pm} = S^x \pm iS^y$, we can rewrite (A17) in the following form:

$$\lambda_n^{(0)} = \tfrac{1}{2} \sum{}' \mathrm{Tr} S_{r_3}^z S_{r_2}^z [S_{r_1}^+ S_{r_j}^- + S_{r_1}^- S_{r_j}^+](S_p^+ S_{p'}^-) \times (S_q^+ S_{q'}^-)(S_r^+ S_{r'}^-) \cdots\ , \tag{A18}$$

where, in addition to the restricted lattice sum, a sum over nearest-neighbor pairs pp', qq', rr', ... is implied. Now since S^z is itself a traceless operator, the above expression vanishes identically unless r_2 and r_3 are both degenerate with some r in $\{S_r^{\pm}\}$. Then, by using the well-known relation

$$S^z S^{\pm} = \pm \tfrac{1}{2} S^{\pm}\ , \tag{A19}$$

S^z operators can be replaced by their eigenvalues, leaving behind only the lattice restriction. Now if r_2 or $r_3 = r_j$, we only get a term proportional to $C_n^{(0)}$. Thus, the largest contribution from (A18) arises when the lattice restriction on r_2 and r_3 coincides with some particular configuration of a nonzero combination of $\{S_r^{\pm}\}$ (then the restriction on r_2 and r_3 becomes redundant). Consider the first term in (A18). Let r_1 be singly degenerate: $r_1 = p'$ (an arbitrary choice). Then by our argument we must have $r_2 = p$. For r_3, it has two possibilities $r_3 = q$ or q', each of which however cancels out the other exactly by (A19). The same applies to the second term in (A18). One can obtain nonzero combinations only when r_1 is at least triply degenerate, e.g., $r_1=p'=q=r'$. An elaboration of this kind of argument leads to the conclusion that

$$\max[\mathrm{Tr}(U^{(1)}Q)QP^n]\sim \mathrm{Tr}Q^2P^{n-1}=B_{n-1}^{(0)} . \quad (A20)$$

Now since $B_n^{(0)}>B_{n-1}^{(0)}$, where $B_n^{(0)}\sim(q-1)^n$, we arrive at the desired conclusion that

$$qB_n^{(0)}>|\lambda_n^{(0)}| . \quad (A21)$$

In view of (A20) and (A21) we now understand the extreme accuracy of our zeroth-order approximation indicated in Sec. III. It is also evident that since $\lambda_n^{(r)}$ produces terms of $C_n^{(0)}$ and $B_{n-1}^{(0)}$, a first-order correction to the susceptibility (30) can bring about a change only in the analytic functions f and g.

APPENDIX B: SECOND MOMENT

The second moment of a spectral density function[17] is defined by

$$\nu_2/-J=\langle[Q,[P,Q]]\rangle$$
$$=-2i\sum_k\sum_{ij}\langle[S_k^x,S_i^zS_j^y]\rangle , \quad (B1)$$

where the second line follows from (1), (9), and (10). Hence,

$$\nu_2/-J=-2\sum_{ij}\langle S_i^yS_j^y\rangle+2\sum_{ij}\langle S_i^zS_j^z\rangle . \quad (B2)$$

Now observing that (B2) is invariant under rotation $x\leftrightarrow y$ we obtain

$$\nu_2/-J=-\sum_{ij}\langle S_i^xS_j^x+S_i^yS_j^y\rangle+2\sum\langle S_i^zS_j^z\rangle$$
$$=-\langle P\rangle+2\sum_{ij}\langle S_i^zS_j^z\rangle . \quad (B3)$$

If we expand (B3) in powers of temperature, we get

$$\nu_2/-J=-\sum_n(K^n/n!)\,\mathrm{Tr}P^{n+1}$$
$$+2\sum_n(K^n/n!)\,\mathrm{Tr}\sum_{ij}S_i^zS_j^zP^n . \quad (B4)$$

Now we have defined (12),

$$C_n^{(0)}=\mathrm{Tr}yQP^n \;=-2i\sum_k\sum_{ij}\mathrm{Tr}S_i^zS_j^yS_k^xP^n , \quad (B5)$$

where the second line follows from (1) and (10). It can be seen that since the angular-momentum operators $\vec{s}=(S^x, S^y, S^z)$ are all traceless, the only nonzero terms result when $k=i$ and $k=j$. Hence,

$$C_n^{(0)}=\sum_{ij}\mathrm{Tr}(S_i^yS_j^y-S_i^zS_j^z)P^n$$
$$=\tfrac{1}{2}\,\mathrm{Tr}P^{n+1}-\sum_{ij}\mathrm{Tr}S_i^zS_j^zP^n . \quad (B6)$$

Comparing it with (B4) we see that

$$\nu_2/-J=-2\sum_n(K^n/n!)C_n^{(0)} . \quad (B7)$$

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[1]T. Matsubara and H. Matsuda, Prog. Theor. Phys. 16, 416 (1956); P. R. Zilsel, Phys. Rev. Lett. 15, 476 (1965); D. D. Betts and M. H. Lee, Phys. Rev. Lett. 20, 1507 (1968).

[2]D. D. Betts, C. J. Elliott, and M. H. Lee, Can. J. Phys. 48, 1566 (1970).

[3]R. B. Griffiths, Phys. Rev. 152, 240 (1967).

[4]H. Falk and L. W. Bruch, Phys. Rev. 180, 442 (1969); L. W. Bruch, Phys. Rev. B 2, 721 (1970).

[5]R. V. Ditzian, Ph.D. thesis (University of Alberta, 1970) (unpublished). The author is grateful to Dr. Ditzian for providing him with her numerical results and other related information.

[6]This is tantamount to assuming that the critical temperature exists and that the critical behavior is of a power-law form. Because of our use of this assumption (albeit widely held), our result contained herein does not constitute a proof in the sense of Ref. 4.

[7]M. H. Lee, J. Math. & Phys. 12, 61 (1971).

[8]Observe that a_n [see Eq. (3)] does not explicitly depend on the commutation relation between P and Q. (That is, P and Q are not mixed, which we shall call "reduced.") Thus, it may be readily evaluated for n up to ~ 10 (see Ref. 7). On the other hand, to evaluate $\tilde{a}_n$ [see Eqs. (5) and (6)] one must explicitly take into account the commutation relation. As a result, it is much more difficult to evaluate $\tilde{a}_n$ than a_n.

[9]See, for example, C. Domb, Adv. Phys. 9, 149 (1960).

[10]The expression (29) requires a slight modification for the case of n even. The correction is however straightforward. Write $\chi=\Sigma\tilde{a}_{2n+1}K^{2n+1}+\Sigma\tilde{a}_{2n}K^{2n}$. For $\tilde{a}_{2n+1}$ use (21) as in (29). A similar expression for a_{2n} can be obtained by noting that $N_{2n}(2n)!\,\tilde{a}_{2n}=\Sigma^n{}_{r=0}\,B_{2n}^{(r)}-\frac{1}{2}B_{2n}^{(n)}$.

[11]M. H. Lee, Phys. Rev. B (to be published).

[12]M. H. Lee, Phys. Rev. B (to be published).

[13]The technique of N. D. Mermin and H. Wagner [Phys. Rev. Lett. 17, 1133 (1966)] enables one to rigorously bound ν_2 for the XY model (see footnote 1 of Ref. 4); and the divergence of Y for $T\to T_c$ guarantees the merging of Falk and Bruch's bounds. That establishes that the isothermal susceptibility and the fluctuation have coinciding critical behavior for this model.

[14]This may be more apparent if one considers $\mathrm{Tr}\dot{\theta}QP^n$ in terms of diagrams. For $n\to\infty$, the principal diagrams associated with $\Sigma\mathrm{Tr}\,S_1^yS_2^xS_3^yQP^n$ and $\Sigma\mathrm{Tr}\,S_1^yS_2^yS_3^xQP^n$ are each asymptotically large so that the small restriction imposed on $r_1r_2r_3$ becomes unimportant. Hence the two terms will largely cancel out.

[15]Consider a linear chain of two units of the nearest-neighbor distance. The first lattice sum produces N, the second sum the coordination number q_0, and the third sum q_0-1 which we define as q_1. In a linear chain of n units, according to our system, the last sum then gives q_{n-1}.

[16]H. Mori, Prog. Theor. Phys. 33, 423 (1965).

[17]See, for example, W. Marshall and R. D. Lowde, Rep. Prog. Phys. 31, 705 (1968); and L. W. Bruch (Ref. 4). 4).