Dynamic Behavior of $S = 1/2$ XY Model on Cubic Lattices. I. Molecular-Field Approximation

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The time behavior of the spin operator $S_{\vec{k}}^{x}(t)$ in the XY model is studied by a perturbative method. The zeroth order, which truncates a certain zero-time commutator, is shown to be equivalent to a molecular-field approximation. An analytic expression for the dynamic form factor is then obtained which satisfies basic sum rules. Through the fluctuation-dissipation theorem the dynamic susceptibility and other related physical quantities are also given. Within this zeroth-order approximation there exists a high-frequency collective mode at $q^{1/2}J$. This mode is undamped and is similar to the plasmon.

I. INTRODUCTION

Present theoretical attempts to understand dynamic behavior of lattice models of spin-exchange systems such as the Heisenberg paramagnet are largely semiphenomenological.[1] They are more or less limited to relating the fluctuation spectrum to the first two moments of the spectral shape function which can be exactly calculated at $T=\infty$. Recently, new methods have been proposed by which these calculations can be extended to finite temperatures.[2]

Dynamic behavior is usually looked at in low- and high-frequency regimes. In the low-frequency regime (or hydrodynamic regime as is often referred to) the dominant behavior is believed to be a diffusion process. Central to this notion is that the total spin is a constant of motion, as it is for the Heisenberg paramagnet, for example.[3] Most of current theoretical and experimental works such as those concerning dynamic scaling laws fall in this regime. In the high-frequency regime or collisionless regime there seems to be no comparable progress being made.

We remarked in an earlier paper[4] that the $S=\frac{1}{2}$ XY paramagnet serves as an interesting model for studying dynamic behavior since the total spin (M^x or M^y) is *not* a constant of motion. It appears, therefore, that the dynamics of the XY paramagnet may prove to be considerably different from that of the Heisenberg paramagnet. In particular in the low-frequency regime the dominant process may not be diffusionlike. Also, since the total spin is not conserved at long wavelengths, one can distinguish in the XY paramagnet what is purely kinematic from what is dynamic.

The principal quantity which we seek to obtain is the dynamic form factor defined in Sec. III which is fundamental to all dynamic processes. The dynamic form factor satisfies certain well-known basic sum rules. The difficulty in obtaining an analytic expression for the dynamic form factor is that the time-dependence of the operator $S_{\vec{k}}^{x}(t)$ cannot easily be reduced to a tractable form. Thus, this direct approach is normally avoided.

We introduce here in this paper (Sec. IV) a procedure by which the time dependence of $S_{\vec{k}}^{x}(t)$ can be obtained approximately. Given in the Heisenberg representation, $S_{\vec{k}}^{x}(t)$ can be expanded in terms of successive zero-time commutators. Our procedure is to consider the commutator $[\mathcal{H}_0, S_{\vec{k}}^{x}]$ in a perturbative way such that in zeroth order it represents a certain truncation of the commutator. In succeeding orders the truncated portion is then systematically included.

In this paper we explore in some detail the consequence of the zeroth-order approximation which is found to be equivalent to a molecular-field approximation. Within zeroth order we find that an analytic expression for $S_{\vec{k}}^{x}(t)$ can be easily given. The result is then used to obtain the dynamic form factor and, with aid of the fluctuation-dissipation theorem, the dynamic susceptibility. Our result for the dynamic susceptibility is found to be exact in the high-frequency limit. In our second paper[5] we shall consider the truncated portion of the commutator as a correction to zeroth order and study the physical basis of our truncation procedure.

II. XY PARAMAGNET

The XY paramagnet is described by the XY Hamiltonian

$$\mathcal{H}_0 = -2J \sum_{(rr')} (S_r^x S_{r'}^x + S_r^y S_{r'}^y), \tag{1}$$

where S_r^α is a spin operator ($S=\frac{1}{2}$) at site r with $\alpha = x, y, z$, the sum is over nearest-neighbor pairs (rr'), and J is the exchange integral. The XY Hamiltonian is believed to be a useful model for

liquid helium-4 near the λ transition and for certain ferro- and antiferromagnets.[6] Some of the static critical properties of this model are already found.[7]

Since the Hamiltonian does not have spin exchange in the longitudinal direction, the transverse total spin $M^x = -m\sum S_r^x$ and the longitudinal spin $M^z = -m\sum S_r^z$ have considerably different dynamical and static behavior. For example, the XY Hamiltonian does not commute with M^x but it commutes with M^z. Hence, $S_{\vec{k}}^x(t)$ has dynamic behavior at all values of $\vec{k}$, whereas $S_{\vec{k}}^z(t)$ ceases to be dynamical at $\vec{k} = 0$.[8] On the other hand, it is the mean-square fluctuation $\langle (M^x)^2 \rangle$ which has a divergent behavior as $T \to T_{c+}$ (with an exponent whose three-dimensional value is about $\frac{4}{5}$). The mean-square fluctuation $\langle (M^z)^2 \rangle$ is nondivergent[9] and its most "singular" part behaves as $\Delta T^{-\alpha+1}$. Thus, the order parameter for the XY model is M^x and not M^z. In this paper we shall be concerned primarily with the time-dependent behavior of the transverse spin component $S_{\vec{k}}^x(t)$.

III. DYNAMIC FORM FACTOR AND SUM RULES

The dynamic form factor or spectral density function, which is a fundamental quantity in both theory and experiment, is defined[1] as

$$\mathcal{S}^{\alpha\alpha}(\vec{k}\omega) = \int_{-\infty}^{\infty} dt\, e^{-i\omega t}\, \mathcal{S}^{\alpha\alpha}(\vec{k}t)\,, \tag{2}$$

with

$$\mathcal{S}^{\alpha\alpha}(\vec{k}t) = \langle S_{-\vec{k}}^{\alpha}(0) S_{\vec{k}}^{\alpha}(t) \rangle\,, \tag{3}$$

where in the usual way we have

$$S_{\vec{k}}^{\alpha}(t) = e^{i\mathcal{H}_0 t} S_{\vec{k}}^{\alpha} e^{-i\mathcal{H}_0 t} \tag{4}$$

and

$$S_{\vec{k}}^{\alpha} = \sum_r e^{i\vec{k}\cdot\vec{r}} S_r^{\alpha}. \tag{5}$$

The importance of the dynamic form factor derives from its relation to the partial differential cross section

$$\frac{d^2\sigma}{d\Omega\, d\omega} = A(\vec{k}\vec{k}') \sum_{\alpha} (1 - \hat{k}_{\alpha}^2)\, \mathcal{S}^{\alpha\alpha}(\vec{k} - \vec{k}', \omega), \tag{6}$$

where $A(kk')$ is the neutron scattering form factor. Our system, which has only exchange coupling, has no off-diagonal terms in (6). With an appropriate choice of the incident momentum $(\vec{k})$, one can restrict the cross section to transverse components (xx and yy).

We recall here the three well-known sum rules for the dynamic form factor[10] which will be found useful in our consideration.

(i) Static form factor sum rule.

$$\int_{-\infty}^{\infty} d\omega\; \mathcal{S}^{\alpha\alpha}(\vec{k}\omega) = Y^{\alpha\alpha}(\vec{k}), \tag{7}$$

where

$$Y^{\alpha\alpha}(\vec{k}) = \langle S_{-\vec{k}}^{\alpha} S_{\vec{k}}^{\alpha} \rangle - \langle S_{-\vec{k}}^{\alpha} \rangle \langle S_{\vec{k}}^{\alpha} \rangle\,. \tag{8}$$

The second term of (8) vanishes since we are considering $T > T_c$ only.

(ii) f-sum rule.

$$\int_{-\infty}^{\infty} d\omega\; \omega\, \mathcal{S}^{\alpha\alpha}(\vec{k}\omega) = \tfrac{1}{2} \nu_2^{\alpha\alpha}(\vec{k}), \tag{9}$$

where

$$\nu_2^{\alpha\alpha}(\vec{k}) = \langle [S_{-\vec{k}}^{\alpha}, [\mathcal{H}_0, S_{\vec{k}}^{\alpha}]] \rangle\,. \tag{10}$$

(iii) Compressibility sum rule.

$$\int_{-\infty}^{\infty} d\omega\, \frac{1 - e^{-\beta\omega}}{\omega}\; \mathcal{S}^{\alpha\alpha}(\vec{k}\omega) = \chi^{\alpha\alpha}(\vec{k}), \tag{11}$$

where $\chi^{\alpha\alpha}(\vec{k})$ is the static susceptibility. In an earlier paper[4] we have described the distinction between $Y^{\alpha\alpha}(\vec{k})$ and $\chi^{\alpha\alpha}(\vec{k})$. It follows from (11) that the dynamic form factor is required to satisfy the symmetry relation

$$\mathcal{S}^{\alpha\alpha}(\vec{k}, -\omega) = e^{-\beta\omega}\, \mathcal{S}^{\alpha\alpha}(\vec{k}\omega)\,. \tag{12}$$

IV. TRUNCATION OF COMMUTATORS AND ZEROTH-ORDER APPROXIMATION

Since $S_{\vec{k}}^x$ does not commute with $\mathcal{H}_0$ at any value of $\vec{k}$, it is not a trivial matter to deduce the time behavior of $S_{\vec{k}}^x(t)$. We introduce here a procedure by which an approximate expression for the time behavior can be obtained. From (4) one can write $S_{\vec{k}}^x(t)$ in the following expansion form:

$$\begin{aligned} S_{\vec{k}}^x(t) &= S_{\vec{k}}^x + it\,[\mathcal{H}_0, S_{\vec{k}}^x] + \frac{(it)^2}{2}\,[\mathcal{H}_0, [\mathcal{H}_0, S_{\vec{k}}^x]] \\ &\quad + \frac{(it)^3}{3!}\,[\mathcal{H}_0, [\mathcal{H}_0, [\mathcal{H}_0, S_{\vec{k}}^x]]] + \cdots \\ &\equiv \sum_n \frac{(it)^n}{n!}\, c_n\,. \end{aligned} \tag{13}$$

If c_1 is defined by

$$[\mathcal{H}_0, S_{\vec{k}}^x] = y_{\vec{k}}^x \tag{14}$$

by working out the commutator it can be shown that

$$y_{\vec{k}}^x = i\sum J_{rr'}\, e^{i\vec{k}\cdot\vec{r}} S_r^z S_{r'}^y\,, \tag{15}$$

where $J_{rr'} = 2J\delta_{\vec{r}-\vec{r}',\vec{\delta}}$ with $\vec{\delta}$ being the nearest-neighbor vector. Using the above result, we find for c_2 that

$$[\mathcal{H}_0, y_{\vec{k}}^x] = qJ^2 S_{\vec{k}}^x + \psi_{\vec{k}} + \theta_{\vec{k}}, \tag{16}$$

where q is the coordination number and

$$\psi_{\vec{k}} = \sum J_{rr'} J_{r'r''}\, e^{i\vec{k}\cdot\vec{r}} S_r^z S_{r'}^z S_{r''}^x\,, \tag{17}$$

$$\theta_{\vec{k}} = \sum J_{rr'} J_{r'r''}\, e^{i\vec{k}\cdot\vec{r}'} S_r^y (S_{r'}^x S_{r''}^y - S_{r'}^y S_{r''}^x). \tag{18}$$

Observe in (16) that apart from the constant factor qJ^2 the first term of c_2 is exactly c_0. The second term $\psi_{\vec{k}}$ contains essentially the z-spin pair correlation which in the XY model is weak compared with the x-spin pair correlation.[9] Insofar as c_2 is concerned, one can thus regard $\psi_{\vec{k}}$ as a

kind of perturbation to the first term. If the restriction on the lattice sum (rr') is slightly relaxed, the third term $\theta_{\vec{k}}$ is identically zero. When one calculates the dynamic form factor, it enters into the calculation in the form $\mathrm{Tr}\theta\mathcal{H}_0^n$ which becomes very small in the limit $n \to \infty$.

Now consider the next order c_3. The first term of c_2 reproduces c_1 exactly. Hence, if (16) is truncated keeping only the first term qJ^2S^x, it leads to a simple summable series for the expansion (16). We shall call this step our *zeroth-order* approximation. It will be shown later (see Sec. XIV and Appendix D) that the zeroth-order approximation is equivalent to a molecular-field approximation. As to the truncated portion $\psi_{\vec{k}}$ and $\theta_{\vec{k}}$, $[\mathcal{H}_0, \theta_{\vec{k}}]$ produces terms which are all proportional to $\theta_{\vec{k}}$. Thus, as a start it seems reasonable to neglect the contribution of $\theta_{\vec{k}}$ in all orders of expansion (13). In contrast, $[\mathcal{H}_0, \psi_{\vec{k}}]$ generates nonlinear terms, which evidently make the contribution of $\psi_{\vec{k}}$ to the expansion very complex to handle. Nevertheless, by regarding $\psi_{\vec{k}}$ formally as a perturbation to $S^x_{\vec{k}}$, one can in principle make the expansion (13) summable.[4a] As we shall see, the summability is directly related to some interesting dynamical properties of the system. We shall call this step [i.e., inclusion of $\psi_{\vec{k}}$ in Eq. (13) and neglecting terms proportional to $\theta_{\vec{k}}$] our *first-order* approximation. Finally, the contribution of $\theta_{\vec{k}}$ is considered as a still-higher-order correction.

In this paper we shall explore the consequence of our zeroth-order or molecular-field approximation in some detail. In a subsequent paper[5] the first-order approximation is taken up as a leading correction to the zeroth-order result. The physical nature of our approximation will not be fully apparent until the first-order correction is introduced. In Sec. XIV, a physical basis for the truncation is discussed in a limited way.

In *zeroth order* then we truncate the commutator (16) and write

$$[\mathcal{H}_0, y^x_{\vec{k}}]^{(0)} = \omega_0^2 S^x_{\vec{k}}, \tag{19}$$

where $\omega_0 = \sqrt{q}\,J$. Then, using (14) and (19) we can evaluate the successive commutators for $S^x_{\vec{k}}(t)$ to *all* orders of expansion and directly obtain

$$[S^x_{\vec{k}}(t)]^{(0)} = S^x_{\vec{k}} \cos\omega_0 t + iy^x_{\vec{k}}(\sin\omega_0 t)/\omega_0. \tag{20}$$

V. DYNAMIC FORM FACTOR

We can now readily obtain an analytic expression for the zeroth-order dynamic form factor using (20) in the definition (3);

$$[\mathcal{S}^{xx}(\vec{k}t)]^{(0)} = Y^{xx}(\vec{k})\cos\omega_0 t + i\nu_2^{xx}(\vec{k})(\sin\omega_0 t)/\omega_0, \tag{21}$$

where we have used the relation that

$$\langle S^x_{-\vec{k}}\, y^x_{\vec{k}}\rangle = \tfrac{1}{2}\nu_2^{xx}(\vec{k}), \tag{22}$$

which is derived in Appendix A. It should be pointed out that Y^{xx} and ν_2^{xx}, given, respectively, by (8) and (10), do not depend on the truncation and are therefore exact. After a trivial time integration, we obtain

$$[\mathcal{S}^{xx}(\vec{k}\omega)]^{(0)} = [\tfrac{1}{2}Y^{xx}(\vec{k}) + \nu_2^{xx}(\vec{k})/4\omega] \times [\delta(\omega-\omega_0)+\delta(\omega+\omega_0)]. \tag{23}$$

The zeroth-order dynamic form factor (23) satisfies the first two sum rules [(i) and (ii)] trivially. It also satisfies the compressibility sum rule (iii) as we shall see. Substituting (23) into (11) we get for the static susceptibility

$$[\chi^{xx}(\vec{k})]^{(0)} = Y^{xx}(\vec{k})\frac{\sinh\beta\omega_0}{\omega_0} + \frac{\nu_2^{xx}(\vec{k})}{2\omega_0^2}(1-\cosh\beta\omega_0). \tag{24}$$

It will be shown in Sec. VI that the above expression does indeed correspond to the zeroth-order static susceptibility. Although it is somewhat less obvious at this stage, the expression for the dynamic form factor (23) also satisfies the symmetry relation (12). This is proved in Appendix B.

It is perhaps not so surprising that our zeroth-order dynamic form factor should satisfy the sum rules. What is to be remembered is that truncation still leaves a principal portion of the commutator (16) intact. The exact expression for the dynamic form factor is thus expected to contain our zeroth-order result (23) as a leading term.

If we investigate the scattering with an incident momentum $\vec{k}$ in the [001] direction, the diffuse cross section (for $T > T_c$) follows from (6) and (23);

$$\left(\frac{d^2\sigma(001)}{d\Omega\, d\omega}\right)^{(0)} = A(\vec{k}\vec{k}')[Y^{xx}(\vec{k}-\vec{k}') + \nu_2^{xx}(\vec{k}-\vec{k}')/2\omega] \times [\delta(\omega-\omega_0)+\delta(\omega+\omega_0)]. \tag{25}$$

The cross section is sharply peaked at $\omega = \pm\omega_0$ and it has no central peak.[11] This is in contrast to the cross section for the Heisenberg paramagnet which is commonly taken to be a Lorentzian about $\omega = 0$.[12] The absence of a central peak already suggests a different kind of low-frequency dynamical behavior for the XY model.

Using (23) we can obtain expression for a variety of other physical quantities of interest such as the relaxation function, spectral shape function and its moments, dynamic susceptibility, etc. These are given in Secs. VI–XII.

VI. STATIC SUSCEPTIBILITY

The static susceptibility, which we have already introduced through the compressibility sum rule, is given formally by[1]

$$\chi^{\alpha\alpha}(\vec{k}) = \{S^\alpha_{-\vec{k}}, S^\alpha_{\vec{k}}\}, \tag{26}$$

where the inner product means that

$$\{A, B\} = \int_0^\beta d\lambda \langle e^{\lambda \mathcal{H}_0} A e^{-\lambda \mathcal{H}_0} B\rangle - \beta \langle A\rangle \langle B\rangle . \quad (27)$$

From (20) it follows that

$$[e^{\lambda \mathcal{H}_0} S_{\vec{k}}^x e^{-\lambda \mathcal{H}_0}]^{(0)} = S_{\vec{k}}^x \cosh\omega_0\lambda + y_{\vec{k}}^x (\sinh\omega_0\lambda)/\omega_0 . \quad (28)$$

Using (28) and our earlier result (22), we obtain after a trivial integration the result previously obtained through the sum rule (iii):

$$[\chi^{xx}(\vec{k})]^{(0)} = Y^{xx}(\vec{k}) \frac{\sinh\beta\omega_0}{\omega_0} + \frac{\nu_2^{xx}(\vec{k})}{2\omega_0^2} (1 - \cosh\beta\omega_0) \quad (29)$$

In the high-temperature limit ($\beta \to 0$), the susceptibility and the fluctuation become, as is expected, identically the same:

$$\beta^{-1}[\chi^{xx}(\vec{k})]^{(0)} = Y^{xx}(\vec{k}) + O(\beta) . \quad (30)$$

We have previously shown that the susceptibility and fluctuation have the same critical behavior.[4] That is, both diverge near the critical point with the same critical exponent γ_x.

VII. DYNAMIC FORM FACTOR AND RELAXATION FUNCTION

The relaxation function $R^{\alpha\alpha}(\vec{k}\omega)$ is defined as

$$R^{\alpha\alpha}(\vec{k}\omega) = \int_{-\infty}^{\infty} dt\, e^{-i\omega t} R^{\alpha\alpha}(\vec{k}t) , \quad (31)$$

where

$$R^{\alpha\alpha}(\vec{k}t) = \{S_{-\vec{k}}^\alpha(0), S_{\vec{k}}^\alpha(t)\} . \quad (32)$$

In terms of the relaxation function, the spectral shape function is given by

$$F^{\alpha\alpha}(\vec{k}t) = R^{\alpha\alpha}(\vec{k}t)/\chi^{\alpha\alpha}(\vec{k}) . \quad (33)$$

With our result (20) we can obtain an analytic expression for $[R^{xx}(\vec{k}\omega)]^{(0)}$ from the definition (33) and hence also for $[F^{xx}(\vec{k}\omega)]^{(0)}$. However, it is somewhat more instructive, first, to utilize the relation[1]

$$R^{\alpha\alpha}(\vec{k}\omega) = \frac{1 - e^{-\beta\omega}}{\omega} \mathcal{S}^{\alpha\alpha}(\vec{k}\omega) . \quad (34)$$

Then, it follows from (23) and (34) that

$$[R^{xx}(\vec{k}\omega)]^{(0)} = (1 - e^{-\beta\omega_0}) \left[\frac{Y^{xx}(\vec{k})}{2\omega_0} + \frac{\nu_2^{xx}(\vec{k})}{4\omega_0^2}\right] \delta(\omega - \omega_0) - (1 - e^{\beta\omega_0}) \left[\frac{Y^{xx}(\vec{k})}{2\omega_0} - \frac{\nu_2^{xx}(\vec{k})}{4\omega_0^2}\right] \delta(\omega + \omega_0) . \quad (35)$$

The spectral shape function $[F^{xx}(\vec{k}\omega)]^{(0)}$ is thus given by (33) and (34).

VIII. DYNAMIC FORM FACTOR AND DYNAMIC SUSCEPTIBILITY

The dynamic susceptibility is defined by

$$\chi^{\alpha\alpha}(\vec{k}\omega) = \lim_{\mu \to 0} [-i \int_0^\infty dt\, e^{-i(\omega - i\mu)t} \chi^{\alpha\alpha}(\vec{k}t)] , \quad (36)$$

where the response function $\chi^{\alpha\alpha}(\vec{k}t)$ is given by

$$\chi^{\alpha\alpha}(\vec{k}t) = \tfrac{1}{2} \langle [S_{-\vec{k}}^\alpha(0), S_{\vec{k}}^\alpha(t)] + [S_{-\vec{k}}^\alpha(t), S_{\vec{k}}^\alpha(0)] \rangle . \quad (37)$$

Again, one can obtain the dynamic susceptibility using our result (20). However, we shall defer this to Sec. IX and here exploit the fluctuation dissipation theorem[1,10]

$$-\pi \mathcal{S}^{\alpha\alpha}(\vec{k}\omega) = (1 - e^{-\beta\omega})^{-1} \operatorname{Im} \chi^{\alpha\alpha}(\vec{k}\omega) ; \quad (38)$$

hence,

$$\operatorname{Im}[\chi^{xx}(\vec{k}\omega)]^{(0)} = -\pi(1 - e^{-\beta\omega})[\tfrac{1}{2} Y^{xx}(\vec{k}) + \nu_2^{xx}(\vec{k})/4\omega] \times [\delta(\omega - \omega_0) + \delta(\omega + \omega_0)] . \quad (39)$$

Now the real and imaginary parts of the dynamic susceptibility are related by a Kramers-Kronig relation,[10]

$$\operatorname{Re}\chi^{\alpha\alpha}(\vec{k}\omega) = \frac{\mathcal{P}}{\pi} \int_{-\infty}^{\infty} d\omega' \frac{\omega'}{\omega^2 - \omega'^2} \operatorname{Im}\chi^{\alpha\alpha}(\vec{k}\omega') , \quad (40)$$

where $\mathcal{P}$ denotes the principal value of the integral.

Thus, with (39) we obtain

$$\operatorname{Re}[\chi^{xx}(\vec{k}\omega)]^{(0)} = -\frac{\omega_0^2}{\omega^2 - \omega_0^2} \left(Y^{xx}(\vec{k}) \frac{\sinh\beta\omega_0}{\omega_0} + \frac{\nu_2^{xx}(\vec{k})}{2\omega_0^2} (1 - \cosh\beta\omega_0) \right) . \quad (41)$$

From (29) and (41) we see that

$$\operatorname{Re}[\chi^{xx}(\vec{k}\omega \to 0)]^{(0)} = \chi^{xx}(\vec{k}) + O(\omega^2) \quad (42)$$

and

$$\operatorname{Re}[\chi^{xx}(\vec{k}\omega \to \infty)]^{(0)} = -\frac{\omega_0^2 \chi^{xx}(\vec{k})}{\omega^2} + O(\omega^{-4}) . \quad (43)$$

The above result is valid for all values of $\vec{k}$ including $\vec{k} = 0$. Thus, (42) implies that in the long-time limit ($\omega \to 0$) the zeroth-order dynamic (Kubo or isolated) susceptibility becomes identical to the isothermal susceptibility. It is perhaps worth pointing out that the longitudinal component does not satisfy this relation. That is, $\operatorname{Re}\chi^{zz}(\vec{k}\omega \to 0) = 0$ at $\vec{k} = 0$, whereas the isothermal susceptibility $\chi^{zz}(\vec{k} = 0) \neq 0$.[13]

From (41) we observe that $\operatorname{Re}\chi^{xx}(\vec{k}\omega)$ has two real poles at $\omega = \pm\omega_0$. When the first-order terms are introduced, the poles can become complex whose imaginary part is then related to the width in the cross section (25).

IX. DYNAMIC SUSCEPTIBILITY

It follows from the definition (36) that the real part of the dynamic susceptibility can be expanded

in the form

$$\mathrm{Re}\chi^{\alpha\alpha}(\vec{k}\omega) = -\nu_2^{\alpha\alpha}(\vec{k})/\omega^2 - \nu_4^{\alpha\alpha}(\vec{k})/\omega^4 - \cdots , \quad (44)$$

where

$$\nu_{2n}^{\alpha\alpha}(\vec{k}) = (-i)^{2n-1}\left\langle\left[S_{-\vec{k}}^{\alpha}, \frac{\partial^{2n-1}}{\partial t^{2n-1}} S_{\vec{k}}^{\alpha}(t=0)\right]\right\rangle,$$

$$n = 1, 2, 3, \ldots . \quad (45)$$

Thus, one can calculate the dynamic susceptibility directly through the zero-time commutators of (44)[14] or through the response function $\chi^{\alpha\alpha}(\vec{k}t)$ using (40). We shall follow the latter procedure here, and in Sec. XI the former procedure (44).

Using (20) in (37), we have the response function

$$[\chi^{xx}(\vec{k}t)]^{(0)} = \nu_2^{xx}(\vec{k})(\sin\omega_0 t)/\omega_0; \quad (46)$$

hence, from (36) and (46)

$$\mathrm{Re}[\chi^{xx}(\vec{k}\omega)]^{(0)} = -\nu_2^{xx}(\vec{k})/(\omega^2 - \omega_0^2) \quad (47)$$

and

$$\mathrm{Im}[\chi^{xx}(\vec{k}\omega)]^{(0)} = \frac{\pi\nu_2^{xx}(\vec{k})}{2\omega}[\delta(\omega-\omega_0)+\delta(\omega+\omega_0)] . \quad (48)$$

The real and imaginary parts of the dynamic susceptibility [(47) and (48)] satisfy the Kramers-Kronig relations exactly. Observe that in the high-frequency limit ($\omega \to \infty$) our result (47) becomes exact to the order ω^{-2} [see (44)]. Now comparing (47) with our previous result obtained using the fluctuation-dissipation theorem [(41)] we see that if the two results are to be consistent, we must have

$$\omega_0^2[\chi^{xx}(\vec{k})]^{(0)} = \nu_2^{xx}(\vec{k}) . \quad (49)$$

This result (49) follows directly from (47) if we recall the relation

$$\chi^{\alpha\alpha}(\vec{k}) = \mathrm{Re}\chi^{\alpha\alpha}(\vec{k}\omega = 0) . \quad (50)$$

It also follows from (48) and the Kramers-Kronig relation (40) with ω set at zero,

$$\mathrm{Re}\chi^{xx}(\vec{k}0) = -\frac{1}{\pi}\int_{-\infty}^{\infty} d\omega \frac{\mathrm{Im}\chi^{xx}(\vec{k}\omega)}{\omega} . \quad (40a)$$

It is worth noting that for low frequencies our zeroth-order expression (50) appears to be a very poor approximation for the true dynamic susceptibility, since at $T = T_c$ and at long wavelengths $\chi^{xx}(\vec{k}\omega \approx 0)$ is expected to be strongly singular whereas, according to (49), $[\chi^{xx}(\vec{k}\omega \approx 0)]^{(0)}$ is finite or at most weakly singular. In fact the two results [(29) and (49)] for $[\chi^{xx}(\vec{k})]^{(0)}$ seem to be inconsistent. This arises from the fact that in obtaining the response function through the definition (37), $S_{\vec{k}}^{x}(t)$ enters into the problem only through the commutator $[S_{-\vec{k}}^{x}(0), S_{\vec{k}}^{x}(t)]$. Thus, that component of $S_{\vec{k}}^{x}(t)$, whose time behavior is of the form $f(t)S_{\vec{k}}^{x}$, can never contribute to the above commutator. The response function obtained through the dynamic form factor, however, contains precisely this piece of information which is divergent at $T = T_c$ and at long wavelengths. In first order, $S_{\vec{k}}^{x}(t)$ will contain this lost piece in some other form through which the apparent inconsistency will be repaired.

If we combine (29) and (49), we obtain

$$\frac{[\chi^{xx}(\vec{k})]^{(0)}}{\beta Y^{xx}(\vec{k})} = \frac{\tanh\frac{1}{2}\beta\omega_0}{\frac{1}{2}\beta\omega_0} . \quad (51)$$

Interestingly, the above expression is formally similar to an exact equation due to Falk and Bruch[15]

$$\chi^{\alpha\alpha}(\vec{k})/\beta Y^{\alpha\alpha}(\vec{k}) = (\tanh z_{\vec{k}})/z_{\vec{k}}, \quad (52)$$

where

$$z_{\vec{k}}\tanh z_{\vec{k}} = \beta\nu_2^{\alpha\alpha}(\vec{k})/2Y^{\alpha\alpha}(\vec{k}) . \quad (53)$$

X. RELAXATION FUNCTION

As was pointed out in Sec. VII, the relaxation function can be directly obtained from the definitions (31) and (32). Using (20) and (28) in (32) we obtain after a trivial integration

$$[R^{xx}(\vec{k}t)]^{(0)} = \cos\omega_0 t\left(Y^{xx}(\vec{k})\frac{\sinh\beta\omega_0}{\omega_0} + \frac{\nu_2^{xx}(\vec{k})}{2\omega_0^2}(1-\cosh\beta\omega_0)\right) + i\frac{\sin\omega_0 t}{\omega_0} \times\left(\frac{\nu_2^{xx}(\vec{k})}{2}\frac{\sinh\beta\omega_0}{\omega_0} - \frac{\Lambda^{xx}(\vec{k})}{\omega_0^2}(1-\cosh\beta\omega_0)\right), \quad (54)$$

where

$$\Lambda^{xx}(\vec{k}) = \langle y_{-\vec{k}}^{x} y_{\vec{k}}^{x}\rangle . \quad (55)$$

The imaginary part of (54) actually vanishes as is required from physical consideration (also see our previous result in Sec. XII). This can be seen as follows: From the definition of y_k^x, we can write

$$\Lambda^{xx}(\vec{k}) = -\frac{d}{dt}\langle \dot{S}_{-\vec{k}}^{x} S_{\vec{k}}^{x}(t=0)\rangle . \quad (56)$$

With the aid of (4) we have

$$\Lambda^{xx}(\vec{k}) = \langle \ddot{S}_{-\vec{k}}^{x} S_{\vec{k}}^{x}\rangle . \quad (57)$$

Hence, using (20) we get within the zeroth-order approximation

$$[\Lambda^{xx}(\vec{k})]^{(0)} = -\omega_0^2 Y^{xx}(\vec{k}) . \quad (58)$$

Now with (51) and (58) we can easily show that to zeroth order the imaginary part of (54) vanishes and with (29)

$$[R^{xx}(\vec{k}t)]^{(0)} = \cos\omega_0 t[\chi^{xx}(\vec{k})]^{(0)} . \quad (59)$$

Observe that the relaxation function (59) satisfies the required relations[1]

$$R^{\alpha\alpha}(\vec{k}t=0)=\chi^{\alpha\alpha}(\vec{k}) \tag{60}$$

and

$$\frac{\partial}{\partial t}R^{\alpha\alpha}(\vec{k}t)=-\chi^{\alpha\alpha}(\vec{k}t). \tag{61}$$

By calculating $\Lambda^{xx}(\vec{k})$ directly from (57) one can actually obtain a measure of accuracy of the zeroth-order approximation (58).

XI. SPECTRAL SHAPE FUNCTION

With the aid of a theorem due to Kubo, [1] one can write the spectral shape function (33) as

$$F^{\alpha\alpha}(\vec{k}t)=1+\frac{i}{\chi^{\alpha\alpha}(\vec{k})}\int_0^t dt'\,\langle[S^{\alpha}_{-\vec{k}}(0),\ S^{\alpha}_{\vec{k}}(t')]\rangle. \tag{62}$$

Hence, using (20) we obtain

$$[F^{xx}(\vec{k}t)]^{(0)}=1-\frac{\nu_2^{xx}(\vec{k})}{\omega_0^2\chi^{xx}(\vec{k})}(1-\cos\omega_0 t). \tag{63}$$

We observe that $[\dot{F}^{xx}(\vec{k}t=0)]^{(0)}=0$ as is required. In the short-time limit the spectral shape function (63) can be approximated as

$$\lim_{t\to 0}[F^{xx}(\vec{k}t)]^{(0)}=1-(gt)^2/2+\cdots\approx e^{-(gt)^2/2}, \tag{64}$$

where

$$g=[\nu_2^{xx}(\vec{k})/\chi^{xx}(\vec{k})]^{1/2}. \tag{65}$$

Thus in the short-time limit we obtain a Gaussian form for the spectral shape function with the decay rate g, which according to (49) is $[g]^{(0)}=\omega_0$. From the definition of the relaxation function, it follows that

$$[R^{xx}(\vec{k}t)]^{(0)}=\chi^{xx}(\vec{k})-[\nu_2^{xx}(\vec{k})/\omega_0^2](1-\cos\omega_0 t). \tag{66}$$

Now using (63) we obtain

$$[F^{xx}(\vec{k}\omega)]^{(0)}=\left(1-\frac{\nu_2^{xx}(\vec{k})}{\omega_0^2\chi^{xx}(\vec{k})}\right)\delta(\omega)+\frac{\nu_2^{xx}(\vec{k})}{2\omega_0^2\chi^{xx}(\vec{k})}[\delta(\omega-\omega_0)+\delta(\omega+\omega_0)]. \tag{67}$$

Thus, the spectral shape function is a peaked function, peaked at $\omega=0$ and $\omega=\pm\omega_0$. The central peak is to zeroth-order spurious, however, since the coefficient of $\delta(\omega)$ vanishes according to (49). For the Heisenberg paramagnet it is commonly assumed that $F^{\alpha\alpha}(\vec{k}\omega)$ is a Lorentzian function up to some cutoff frequency proportional to $[\nu_2^{\alpha\alpha}(\vec{k})/\chi^{\alpha\alpha}(\vec{k})]^{1/2}$ and zero beyond the cutoff. [3] The necessity of the cutoff arises because all frequency moments of the spectral shape function must exist.

Using (14) and (19) repeatedly we obtain zeroth-order frequency moments for all n (derived in Appendix C):

$$[\nu_{2n}^{xx}(\vec{k})]^{(0)}=\omega_0^{2(n-1)}\nu_2^{xx}(\vec{k}) \tag{68}$$

with $[\nu_2^{xx}]^{(0)}\equiv\nu_2^{xx}$. This result may be used to check our previously obtained expressions for F^{xx} and χ^{xx}.

Marshall[16] has shown that

$$F^{\alpha\alpha}(\vec{k}\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dt\,e^{-i\omega t}\left(1-\frac{t^2}{2}F_2^{\alpha\alpha}(\vec{k})+\frac{t^4}{4!}F_4^{\alpha\alpha}(\vec{k})-\cdots\right), \tag{69}$$

where

$$F_{2n}^{\alpha\alpha}(\vec{k})=\int_{-\infty}^{\infty}d\omega\,\omega^{2n}F^{\alpha\alpha}(\vec{k}\omega). \tag{70}$$

Now it can be easily seen that

$$F_{2n}^{\alpha\alpha}(\vec{k})=\nu_{2n}^{\alpha\alpha}(\vec{k})/\chi^{\alpha\alpha}(\vec{k}). \tag{71}$$

Substituting (68) and (71) into (69) we recover the previous zeroth-order result (67). Similarly, using (68) in (44) we obtain the real part of the dynamic susceptibility (47) quite easily.

XII. CORRELATION FUNCTIONS

Within zeroth order it is a simple matter to obtain expressions for various correlation functions, some of which are shown below.

(a) $\langle S^x_{-\vec{k}}(0)S^x_{\vec{k}}(t)\rangle$: This correlation, which is the dynamic form factor $s^{xx}(\vec{k}t)$, has already been obtained (see Sec. V). If we define the spin correlation function in the coordinate space as

$$s^{\alpha\alpha}(\vec{r}t)=\sum_{\vec{k}}e^{i\vec{k}\cdot\vec{r}}\,s^{\alpha\alpha}(\vec{k}t), \tag{72}$$

we observe that in zeroth order $s^{xx}(\vec{r}t)$ does *not* satisfy the spin diffusion equation. It satisfies instead the wave equation. It is well known that for the spin diffusion equation to be applicable, the spin correlation function must be a constant of motion in some physical domain. For the Heisenberg paramagnet the spin correlation function becomes a constant of motion at long wavelengths in the hydrodynamic regime. But for the XY paramagnet, as was pointed out, it is never a constant of motion.

(b) $\langle\dot{S}^x_{-\vec{k}}(0)\dot{S}^x_{\vec{k}}(t)\rangle$: The spin velocity correlation $v^{xx}(\vec{k}t)$ can be obtained using (20) and an identity used earlier (57);

$$[v^{xx}(\vec{k}t)]^{(0)}=\omega_0^2[s^{xx}(\vec{k}t)]^{(0)}. \tag{73}$$

It is commonly assumed[1] for the Heisenberg paramagnet that the decay of $v^{\alpha\alpha}(\vec{k}t)$ is faster than that of $s^{\alpha\alpha}(\vec{k}t)$. For the XY paramagnet in zeroth order $s^{xx}(\vec{k}t)$ and $v^{xx}(\vec{k}t)$ have on the contrary the same "decay" rate.

(c) $\langle\ddot{S}^x_{-\vec{k}}(0)\ddot{S}^x_{\vec{k}}(t)\rangle$: The spin acceleration cor-

relation $\mathfrak{a}^{\alpha\alpha}(\vec{k}t)$ follows similarly;

$$[\mathfrak{a}^{xx}(\vec{k}t)]^{(0)} = \omega_0^4[s^{xx}(\vec{k}t)]^{(0)} \tag{74}$$

XIII. SPECTRAL REPRESENTATION OF BENNETT AND MARTIN

Bennett and Martin[3] have constructed an interesting spectral representation valid in the paramagnet region in the following form: for complex frequencies ω

$$1-\frac{\chi^{\alpha\alpha}(\vec{k}\omega)}{\chi^{\alpha\alpha}(\vec{k}0)} = \left(1+\int_{-\infty}^{\infty} d\omega' \frac{D^{\alpha\alpha}(\vec{k}\omega')}{\omega'^2-\omega^2}\right)^{-1}, \tag{75}$$

where $D^{\alpha\alpha}(\vec{k}\omega)$ is an arbitrary analytic function. Since $D^{\alpha\alpha}(00)$ corresponds to the spin diffusion coefficient, $D^{\alpha\alpha}(\vec{k}\omega)$ is known as the generalized diffusivity. For $\mathrm{Re}\,\omega = \omega'$, one obtains the spectral representation

$$\frac{\mathrm{Im}\chi^{\alpha\alpha}(\vec{k}\omega)}{\chi^{\alpha\alpha}(\vec{k}0)} = \omega D^{\alpha\alpha}(\vec{k}\omega)\left[\omega^2\left(1+\frac{\mathcal{P}}{\pi}\int_{-\infty}^{\infty} d\omega' \frac{D^{\alpha\alpha}(\vec{k}\omega')}{\omega'^2-\omega^2}\right)^2 + [D^{\alpha\alpha}(\vec{k}\omega)]^2\right]^{-1}. \tag{76}$$

Since $D^{\alpha\alpha}(\vec{k}\omega)$ is evidently a better behaved function than $\mathrm{Im}\chi^{\alpha\alpha}(\vec{k}\omega)$, the generalized diffusivity can be in general more easily approximated. From the spectral representation one can also obtain a dispersion relation from which it is possible to describe the boundaries of diffusive and propagating modes.

Now observe that by expanding both sides of (75) in powers of ω, we can relate the generalized diffusivity to the frequency moments $F_{2n}^{\alpha\alpha}(\vec{k})$:

$$F_2^{\alpha\alpha}(\vec{k}) = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega D^{\alpha\alpha}(\vec{k}\omega), \tag{77}$$

$$F_4^{\alpha\alpha}(\vec{k}) = \frac{1}{\pi}\int_{-\infty}^{\infty} d\omega\,\omega^2 D^{\alpha\alpha}(\vec{k}\omega) + \left(\frac{1}{\pi}\int_{-\infty}^{\infty} d\omega D^{\alpha\alpha}(\vec{k}\omega)\right)^2, \tag{78}$$

and so on. Since all the frequency moments exist, the generalized diffusivity must vanish rapidly when $\omega \to \infty$. Bennett and Martin pointed out through the spectral representation (76) that a well-defined propagating mode exists if there is a real solution $\omega = \omega_L(\vec{k})$ for the dispersion relation $A^{\alpha\alpha}(\vec{k}\omega)$:

$$A^{\alpha\alpha}(\vec{k}\omega) = 1+\frac{\mathcal{P}}{\pi}\int_{-\infty}^{\infty} d\omega' \frac{D^{\alpha\alpha}(\vec{k}\omega')}{\omega'^2-\omega^2} \tag{79}$$

such that

$$A^{\alpha\alpha}(\vec{k}\omega_L) = 0. \tag{80}$$

For the XY paramagnet we already have zeroth-order $\mathrm{Im}\chi^{xx}(\vec{k}\omega)$. Hence, we can obtain the zeroth-order generalized diffusivity and, through this, look for the roots of the dispersion relation. Using our zeroth-order result for $\mathrm{Im}\chi^{xx}(\vec{k}\omega)$ we find from (76) that

$$[D^{xx}(\vec{k}\omega)]^{(0)} = \frac{\pi\nu_2^{xx}(\vec{k})}{2\chi^{xx}(\vec{k})}\left[\delta(\omega-\tilde{\omega}_0)+\delta(\omega+\tilde{\omega}_0)\right], \tag{81}$$

where

$$\tilde{\omega}_0 = \omega_0[1-\nu_2^{xx}(\vec{k})/\omega_0^2\chi^{xx}(\vec{k})]^{1/2}. \tag{82}$$

By substituting (81) in (77), (78), and all other higher-expansion terms, one can readily verify all the frequency moments previously obtained. Using (81) in (79), we obtain for the dispersion relation

$$[A^{xx}(\vec{k}\omega)]^{(0)} = 1-\frac{\nu_2^{xx}(\vec{k})/\chi^{xx}(\vec{k})}{\omega^2-\tilde{\omega}_0^2}\ ; \tag{83}$$

thus, $[A^{xx}]^{(0)} = 0$ when $\omega = \pm\omega_0$. There are no other real solutions that satisfy the dispersion relation in zeroth order. This is essentially a restatement of our earlier result that $\mathrm{Im}\chi^{xx}(\vec{k}\omega)$ is singular at $\omega = \pm\omega_0$. In zeroth order this propagating mode is undamped.

Bennett[17] has already anticipated the possible existence of a *high-frequency* propagating mode through the following consideration: Assume that $D^{\alpha\alpha}(\vec{k}\omega)$ vanishes rapidly for ω greater than some cutoff frequency $\omega_c \sim \tau^{-1}$, where $\tau(\vec{k})$ is a characteristic collision time defined as

$$\tau(\vec{k}) = F_2^{\alpha\alpha}(\vec{k})\{F_4^{\alpha\alpha}(\vec{k})-[F_2^{\alpha\alpha}(\vec{k})]^2\}^{-1}. \tag{84}$$

A form for $D^{\alpha\alpha}(\vec{k}\omega)$ which will just satisfy the first two frequency moments (77) and (78) is

$$D^{\alpha\alpha}(\vec{k}\omega) = F_2^{\alpha\alpha}(\vec{k})\tau(\vec{k})\,G^{\alpha\alpha}[\vec{k},\omega\tau(\vec{k})] \tag{85}$$

provided that the well-behaved function $G(k\rho)$ satisfies the requirements that

$$\frac{1}{\pi}\int d\rho\, G^{\alpha\alpha}(\vec{k}\rho) = 1 \tag{86}$$

and

$$\frac{1}{\pi}\int d\rho\,\rho^2 G^{\alpha\alpha}(\vec{k}\rho) = 1. \tag{87}$$

Then the dispersion relation becomes

$$A^{\alpha\alpha}(\vec{k}\omega) = 1+F_2^{\alpha\alpha}(\vec{k})\,\tau^2(\vec{k})\ \mathcal{P}\int_{-\infty}^{\infty} d\rho\,\frac{G^{\alpha\alpha}(\vec{k}\rho)}{\rho^2-\omega^2\tau^2}. \tag{88}$$

Now observe that since, by the assumption on $D^{\alpha\alpha}(\vec{k}\omega)$, $G^{\alpha\alpha}(\vec{k}\rho)$ vanishes rapidly as $\rho \to \infty$, for $\omega\tau \gg 1$ there is a high-frequency solution for the dispersion relation:

$$A^{\alpha\alpha}(\vec{k}\omega) = 1-F_2^{\alpha\alpha}(\vec{k})\tau^2(\vec{k})/\omega^2\tau^2(\vec{k}). \tag{89}$$

The validity of the high-frequency solution thus requires that $\mathfrak{R}^{\alpha\alpha}(\vec{k}) \equiv F_2^{\alpha\alpha}(\vec{k})\tau^2(\vec{k}) \gg 1$. The boundary between the regions where propagating and nonpropagating modes dominate is thus given by the condition $\mathfrak{R}^{\alpha\alpha}(\vec{k}) \approx 1$.

For the XY paramagnet, in zeroth order, we can

readily determine the characteristic time τ and the boundary function $\mathcal{R}^{xx}$:

$$[\tau^{-1}(\vec{k})]^{(0)} = \omega_0[1 - \nu_2^{xx}(\vec{k})/\omega_0^2\chi^{xx}(\vec{k})]^{1/2} \tag{90}$$

and

$$[\mathcal{R}^{xx}(\vec{k})]^{(0)} = [\nu_2^{xx}(\vec{k})/\omega_0^2\chi^{xx}(\vec{k})] \times[1 - \nu_2^{xx}(\vec{k})/\omega_0^2\chi^{xx}(\vec{k})]^{-1}. \tag{91}$$

Thus the high-frequency region refers to the region where either (i) $\omega \gg \omega_0$ or (ii) $\nu_2^{xx}(\vec{k})/\omega_0^2\chi^{xx}(\vec{k}) \to 1$. Observe that the second condition implies $\tau^{xx}(\vec{k}) \to \infty$. That is, the system is firmly in the collisionless regime. Now recall that the second condition is exactly the zeroth-order solution of the static susceptibility (see Sec. IX). Hence, our zeroth order corresponds to a high-frequency approximation.

XIV. EQUIVALENT HAMILTONIAN

While the validity of our zeroth-order approximation cannot be discussed without explicitly considering the first-order term,[4a] it is possible to obtain a limited physical picture of the nature of our approximation. Since (19) depends only on commutation relations, one can find an equivalent Hamiltonian, say $\tilde{\mathcal{H}}_0$, for which zeroth order (19) is exact; that is,

$$[\tilde{\mathcal{H}}_0, S_{\vec{k}}^x] = y_{\vec{k}}^x \tag{92a}$$

and

$$[\tilde{\mathcal{H}}_0, y_{\vec{k}}^x] = \omega_0^2 S_{\vec{k}}^x . \tag{92b}$$

Such a Hamiltonian can be found through the following consideration: In the spirit of molecular-field theory, let $S_r^z = \lambda$, for all r where λ is a constant. Define

$$Q_{\vec{k}}^x = \frac{1}{\sqrt{N}} \sum_r e^{i\vec{k}\cdot\vec{r}} S_r^x \tag{93a}$$

and

$$Q_{\vec{k}}^y = \frac{1}{\sqrt{N}} \sum_r e^{i\vec{k}\cdot\vec{r}} S_r^y . \tag{93b}$$

These operators are assumed to satisfy translational invariance. Then it follows that

$$[Q_{\vec{k}}^x, Q_{\vec{k}'}^y] = i\lambda\delta_{\vec{k}\vec{k}'} . \tag{94}$$

The first two commutators (92a) and (92b) require[18] that

$$[\tilde{\mathcal{H}}_0, Q_{\vec{k}}^x] = i\Omega_{\vec{k}} Q_{\vec{k}}^y \tag{95a}$$

and

$$[\tilde{\mathcal{H}}_0, Q_{\vec{k}}^y] = -i\Omega_{\vec{k}} Q_{\vec{k}}^x , \tag{95b}$$

where $\Omega_{\vec{k}}$ is the energy spectrum. A Hamiltonian which satisfies (95) is

$$\tilde{\mathcal{H}}_0 = -\frac{1}{2\lambda} \sum_{\vec{k}} \Omega_{\vec{k}} (Q_{\vec{k}}^x Q_{-\vec{k}}^x + Q_{\vec{k}}^y Q_{-\vec{k}}^y) . \tag{96}$$

Hence, it follows from (13) that

$$Q_{\vec{k}}^x(t) = Q_{\vec{k}}^x \cos\Omega_{\vec{k}} t - Q_{\vec{k}}^y \sin\Omega_{\vec{k}} t \tag{97a}$$

and

$$Q_{\vec{k}}^y(t) = Q_{\vec{k}}^y \cos\Omega_{\vec{k}} t + Q_{\vec{k}}^x \sin\Omega_{\vec{k}} t . \tag{97b}$$

We observe that (97) is formally identical to (20).

Now if we introduce a set of new operators $Q_{\vec{k}}^\dagger$ and $Q_{\vec{k}}$ defined as

$$Q_{\vec{k}}^\dagger = (1/\sqrt{2\lambda})(Q_{\vec{k}}^x + iQ_{\vec{k}}^y) \tag{98a}$$

and

$$Q_{\vec{k}} = (1/\sqrt{2\lambda})(Q_{\vec{k}}^x - iQ_{\vec{k}}^y), \tag{98b}$$

these operators satisfy the commutation relations of Bose particles,

$$[Q_{\vec{k}}^\dagger, Q_{\vec{k}'}] = \delta_{\vec{k}\vec{k}'} . \tag{99}$$

In terms of the new operators, the equivalent Hamiltonian can be written as

$$\tilde{\mathcal{H}}_0 = \tilde{E}_0 - \sum_{\vec{k}} \Omega_{\vec{k}} n_{\vec{k}}, \tag{100}$$

where $\tilde{E}_0$ and $n_{\vec{k}}$ are, respectively, the "ground"-state energy and the number operator;

$$\tilde{E}_0 = \frac{1}{2} \sum_{\vec{k}} \Omega_{\vec{k}} \tag{101}$$

and

$$n_{\vec{k}} = Q_{\vec{k}}^\dagger Q_{\vec{k}} . \tag{102}$$

Observe that $\tilde{E}_0$ is the ground-state energy if $\Omega_{\vec{k}} < 0$; that is, if the system is an antiferromagnet.

The equivalent Hamiltonian satisfies the familiar commutation relations for harmonic oscillators:

$$[\tilde{\mathcal{H}}_0, Q_{\vec{k}}^\dagger] = \Omega_{\vec{k}} Q_{\vec{k}}^\dagger \tag{103a}$$

and

$$[\tilde{\mathcal{H}}_0, Q_{\vec{k}}] = -\Omega_{\vec{k}} Q_{\vec{k}} . \tag{103b}$$

Hence, it follows that

$$Q_{\vec{k}}^\dagger(t) = Q_{\vec{k}}^\dagger e^{i\Omega_{\vec{k}} t} \tag{104a}$$

and

$$Q_{\vec{k}}(t) = Q_{\vec{k}} e^{-i\Omega_{\vec{k}} t} . \tag{104b}$$

Hence, $Q_{\vec{k}}^\dagger$ and $Q_{\vec{k}}$ are operators which, respectively, create and destroy eigenstates of $\tilde{\mathcal{H}}_0$ with energy $\Omega_{\vec{k}}$. These operators represent normal coordinates. The above result (103) recalls the solution of a dense electron gas problem given by Sawada,[19] in which $\Omega_{\vec{k}}$ represents single-particle and collective (plasma) excitations. For small $\vec{k}$, most of the correlation energy is given by the collective mode, which is essentially independent of

$\vec{k}$ and is undamped. The plasma oscillation is a polarization wave associated with density fluctuations. Thus, it is reasonable to identify ω_0 with $\Omega_{\vec{k}}$. That is, in zeroth order the XY model has a propagating mode, which is physically analogous to the plasma oscillation.[20]

To obtain (103) with the Sawada Hamiltonian, one uses the random-phase approximation (RPA). It is now well established that the RPA is equivalent to a molecular-field approximation.[21] Thus, it is not surprising that our molecular-field approximation $S_r^z = \lambda$ gives rise to an equivalent Hamiltonian which is quite familiar in many-body problems. In Appendix D, our equivalent Hamiltonian is further studied. It is shown there that $\tilde{\mathcal{H}}_0$ is equivalent to taking $q \to \infty$ in $\mathcal{H}_0$ and that, in this limit, high-temperature expansion diagrams are exactly summable.

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APPENDIX A: $\langle S_{\vec{k}}^x y_{\vec{k}}^x \rangle$

From the definition of y_k^x given in Sec. IV, it follows that

$$\langle S_{-\vec{k}}^x y_{\vec{k}}^x \rangle = 2iJ \sum_{(rr')R} e^{i\vec{k}\cdot(\vec{r}-\vec{R})} \langle S_R^x S_r^z S_{r'}^y \rangle . \tag{A1}$$

By expanding the product inside the trace, we see that nonvanishing terms are those with $R = r$ and $R = r'$ only. Hence,

$$\langle S_{-\vec{k}}^x y_{\vec{k}}^x \rangle = J \sum_{(rr')} \langle S_r^y S_{r'}^y \rangle - J \sum_{(rr')} e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} \langle S_r^z S_{r'}^z \rangle . \tag{A2}$$

We have previously shown[4] that the right-hand side of (A2) is precisely $\frac{1}{2}\nu_2^{xx}(\vec{k})$; similarly,

$$\langle y_{-\vec{k}}^x S_{\vec{k}}^x \rangle = -\tfrac{1}{2}\nu_2^{xx}(\vec{k}) . \tag{A3}$$

APPENDIX B: SYMMETRY RELATION FOR $\mathcal{S}^{xx}(\vec{k}\omega)$

Write $\mathcal{S}(\omega)$ (suppressing all the irrelevant symbols) as

$$\mathcal{S}(\omega) = A_+ \delta(\omega - \omega_0) + A_- \delta(\omega + \omega_0) , \tag{B1}$$

where

$$A_\pm = \tfrac{1}{2} Y \pm \tfrac{1}{4} \nu_2/\omega_0 . \tag{B2}$$

Then, if

$$e^{\mp\beta\omega_0} A_\pm = A_\mp , \tag{B3}$$

the symmetry relation (12) is satisfied. Now from (B2), (29), and (49) we can write

$$e^{\beta\omega_0} A_- - e^{-\beta\omega_0} A_+ = \tfrac{1}{2}\nu_2/\omega_0 \tag{B4}$$

and

$$e^{\beta\omega_0} A_- + e^{-\beta\omega_0} A_+ = Y . \tag{B5}$$

By adding and subtracting (B4) and (B5), we obtain the desired relation (B2).

APPENDIX C: FREQUENCY MOMENTS

The zeroth-order frequency moments may be directly calculated using (71). They can also be calculated via (70) using our result (67) as is done here. The frequency moments are

$$F_n^{xx}(\vec{k}) = \int_{-\infty}^{\infty} d\omega\, \omega^n F^{xx}(\vec{k}\omega) , \tag{C1}$$

where in zeroth order

$$[F^{xx}(\vec{k}\omega)]^{(0)} = A\delta(\omega) + \frac{B}{2\pi} \int_{-\infty}^{\infty} dt\, e^{-i\omega t} \cos\omega_0 t , \tag{C2}$$

with

$$A \equiv 1 - B \tag{C3}$$

and

$$B \equiv \nu_2^{xx}(\vec{k})/\omega_0^2 \chi^{xx}(\vec{k}) . \tag{C4}$$

Substituting (C2) in (C1) we get

$$[F_n^{xx}(\vec{k})]^{(0)} = B\left(-i\frac{\partial}{\partial t}\right)^n \cos\omega_0 t \Big|_{t=0} . \tag{C5}$$

All the odd moments evidently vanish. Now since

$$\left(\frac{\partial}{\partial t}\right)^{2n} \cos\omega_0 t = (-\omega_0^2)^n \cos\omega_0 t , \tag{C6}$$

we have the desired result:

$$[F_{2n}^{xx}(\vec{k})]^{(0)} = (\omega_0^2)^{n-1} \nu_2^{xx}(\vec{k})/\chi^{xx}(\vec{k}) . \tag{C7}$$

APPENDIX D: CONSTANT INTERACTION MODEL

If we let $\Omega_{\vec{r}} = J(\vec{r})/\sqrt{q}$ and $\lambda = 1/\sqrt{4q}$ in (96), we recover

$$\tilde{\mathcal{H}}_0 = -\tfrac{1}{2}J - \sum_{rr'}{}' J(\vec{r} - \vec{r}')(S_r^x S_{r'}^x + S_r^y S_{r'}^y) , \tag{D1}$$

where the prime denotes that the sum is over all r and r' but excluding $r = r'$; and $J(\vec{r} - \vec{r}') = J/N$ for *all* values of separation distances. This is a constant-interaction model and one can obtain it from the nearest-neighbor model (1) by letting $q \to \infty$. It is generally known that in the limit $q \to \infty$ the molecular-field treatment of, say, the Heisenberg model becomes exact.[22] For the XY model it is also possible to give an asymptotically exact treatment.

Consider the partition function

$$\tilde{Z} = \mathrm{Tr}\, e^{-\beta\tilde{\mathcal{H}}_0} = e^{\beta J/2} \tilde{Z}' . \tag{D2}$$

Now one can expand $\tilde{Z}'$ in powers of $K \equiv \beta J$;

$$\tilde{Z}' = \sum_{n=0}^{\infty} \left(\frac{K}{N}\right)^n \frac{1}{n!}\, \mathrm{Tr}\, \tilde{P}^n \equiv \sum_n \left(\frac{K}{N}\right)^n \tilde{a}_n , \tag{D3}$$

where $\tilde{P} = N(\tilde{\mathcal{H}}_0 + \frac{1}{2}J)/J$. In the asymptotic limit ($N \to \infty$) we can exactly *sum* the above expansion (D3). Consider the second-order term ($n = 2$). For the nearest-neighbor model P, we obtain

$$\mathrm{Tr}\, P^2 = 2^{N-2} N q\,, \tag{D4}$$

where q is the coordination number. For the constant-interaction model we get instead

$$\mathrm{Tr}\, \tilde{P}^2 = 2^{N-2} N(N-1); \tag{D5}$$

similarly, for $n = 3$,

$$\mathrm{Tr}\, \tilde{P}^3 = 2!\, 2^{N-3} N(N-1)(N-2). \tag{D6}$$

In the fourth order ($n = 4$) we encounter all the nontrivial possibilities. As shown in detail,[23] for the nearest-neighbor model $\mathrm{Tr}\, P^4$ consists of the following:

$$\mathrm{Tr}\, P^4 = 3!\, 2^{N-4} g(4) + \tfrac{1}{2} 3!\, 2^{N-4} g(1,1) + 4 \times 2^{N-3} g(2) + 2^{N-2} g(1), \tag{D7}$$

where $g(m)$ denotes a configurational sum. Here $g(4)$ is a sum on a square, $g(2)$ a sum on a chain of two units, $g(1)$ a sum on a chain of one, and $g(1,1)$ a sum on a separated configuration of two chains each of one unit. In the constant-interaction model, $g(m)$ becomes extremely simple to evaluate. Namely, $g(4) = g(1,1) = N(N-1)(N-2)(N-3)$, $g(2) = N(N-1)(N-2)$, and $g(1) = N(N-1)$. In the limit $N \to \infty$, it is clear that only $g(4)$ and $g(1,1)$ need be retained since these are most divergent.

A similar analysis can be carried out to higher orders. For a given order n, the most *divergent* graphs or configurations are those with n vertices, which can be divided into two classes, linked and unlinked. Of these one needs to consider only the linked graphs since the unlinked can be accounted for by exponentiation (as in the theory of fluids).[24] Thus, exact to the order N^n, we have

$$\tilde{a}_n = \frac{2^{N-n}}{n!} (n-1)!\, N(N-1)(N-2)\cdots(N-n) = 2^{N-n}(n-1)! \binom{N}{n}. \tag{D8}$$

Substituting (D8) into (D3) and by exponentiation we finally obtain

$$\tilde{Z} = 2^N \exp\left[\frac{K}{2} + \sum_n \left(\frac{K}{2N}\right)^n (n-1)! \binom{N}{n}\right]. \tag{D9}$$

Now if we use the Stirling approximation, the argument of the exponent (D9) can be easily summed and we obtain

$$\tilde{Z} \approx 2^N (1 - \tfrac{1}{2} K) + O(N^{-1} 2^N). \tag{D10}$$

In the constant-interaction model the fluctuation above T_c can be written in the following special form:

$$\tilde{Y} \equiv \sum_{r=1}^{N} \langle S_0^x S_r^x \rangle = \frac{\partial}{\partial K} \ln \tilde{Z}. \tag{D11}$$

Hence, it follows directly that

$$\tilde{Y} \sim (T - T_c)^{-1}, \tag{D12}$$

where $T_c = J/2k_B$. This is just a molecular-field result.

In light of our earlier remark in Sec. XIV, this result is hardly surprising. What is, however, interesting is that for the constant-interaction model it is only necessary to consider, in each order, the most divergent graph, which is a ring graph (and is thus summable). This is very similar to the perturbative solution of Gell-Mann and Brueckner for a high-density electron gas.[25]

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[1] See, for example, W. Marshall and R. D. Lowde, Rep. Prog. Phys. **31**, 705 (1968). We shall closely follow the notations used in this work.

[2] Examples of recent works are S. W. Lovesey and M. A. Meserve, Phys. Rev. Lett. **28**, 614 (1972); G. F. Reiter, Phys. Rev. B **5**, 222 (1972); J. Van Leeuwen and J. D. Gunton, Phys. Rev. B **6**, 231 (1972); M. F. Collins, Phys. Rev. B **4**, 1588 (1971); M. DeLeener and P. Resibois, Phys. Rev. **178**, 819 (1969); G. A. T. Allan and D. D. Betts, Can. J. Phys. **46**, 799 (1968); M. F. Collins and W. Marshall, Proc. Phys. Soc. Lond. **92**, 390 (1967).

[3] H. S. Bennett and P. C. Martin, Phys. Rev. **138**, A608 (1965).

[4] (a) M. H. Lee, Phys. Rev. B 8, 1203 (1973). (b) In Appendix A of Ref. 4(a), the "smallness" of the perturbation is discussed in some detail, where a similar question arises in considering quantum mechanical effects on the critical behavior.

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

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

[7] D. D. Betts, C. J. Elliott, and M. H. Lee, Can. J. Phys. **48**, 1566 (1970); R. V. Ditzian and D. D. Betts, Can. J. Phys. **50**, 129 (1972).

[8] Dynamically, $S_{\vec{k}}^z(t)$ in the XY model has essentially the same behavior as $S_{\vec{k}}^z(t)$ in the Heisenberg model.

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

[10] D. Pines and P. Nozières, *Theory of Quantum Liquids* (Benjamin, New York, 1966).

[11] It will be seen that once the first-order terms are included in (16), the sharply peaked functions become broadened and can have a width (see Ref. 5).

[12] The Lorentzian shape follows from the assumption that the spatial correlation functions fall off according to the Ornstein-Zernicke relation and the time fluctuations of the correlations decay exponentially. See M. T. Hutchings, M. P. Schulhof, and H. J. Guggenheim [Phys. Rev. B **5**, 154 (1972)] for an interesting recent experimental interpretation.

[13] There is an interesting inequality for the isothermal and isolated susceptibilities. See R. M. Wilcox, Phys. Rev. **174**, 624 (1968); H. Falk, Phys. Rev. **165**, 602 (1968); G. A. T. Allan and D. D. Betts, J. Appl. Phys. **39**, 1351 (1968).

[14] This is a customary procedure. But since these moments cannot be easily calculated except for $n = 1$ and possibly $n = 2$, the susceptibility or relaxation function is somewhat arbitrarily approximated by the first two moments (see Ref. 1).

[15] H. Falk and L. W. Bruch, Phys. Rev. **180**, 442 (1969).

[16] See, for example, M. F. Collins and W. Marshall (in Ref. 2).

[17]H. S. Bennett, Phys. Rev. **174,** 629 (1968); Phys. Rev. **176,** 650 (1968).
[18]The commutators (92a) and (92b) must first be symmetrized. This may be accomplished by letting $y^x \to \omega_0 y^x$ or by interpreting y^x in the molecular-field approximation with $\lambda = (4q)^{-1/2}$ (see Appendix D).
[19]K. Sawada, Phys. Rev. **106,** 372 (1957).
[20]Recently, S. R. Mattingly and D. D. Betts [Can. J. Phys. **50,** 2415 (1972)] showed, based on series expansions of the XY model, that there exists an undamped mode at $\omega \approx qJ$.
[21]R. Brout, *Phase Transitions* (Benjamin, New York, 1965).
[22]J. S. Smart, *Effective Field Theories Of Magnetism* (Saunders, Philadelphia, Pa., 1966).
[23]M. H. Lee, J. Math. Phys. **12,** 61 (1971).
[24]J. Van Leeuwen, J. Groneveld, and J. de Boer, Physica (Utr.) **25,** 792 (1959).
[25]M. Gell-Mann and K. Brueckner, Phys. Rev. **106,** 364 (1957). See also, R. Brout, *Many Electron Problems* (Interscience, New York, 1963).