Critical dynamics of isotropic phonon model

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The critical-dynamics equations in the strong-fluctuation region are obtained for a model with a nonconserving n-component order parameter φ_i and with interaction $(\varphi_i\varphi_i)^2$ in three-dimensional space. The equations are derived by expanding the Ward identities for the temperature Green functions and vertices in terms of the total interaction vertex. In the case when the fluctuations of φ_i are optical phonons, the retarded paired correlation function of the order parameter squared is calculated. Also calculated are the order-parameter retarded-Green-function corrections necessitated by multifrequency scattering processes, in the region where these corrections are small. In various limiting cases, expressions are obtained that describe the shapes of the spectra of the scattering of light and of neutrons by soft optical photons, as well as the frequency and temperature dependences of the sound damping near second-order phase transitions.

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The correlation-coalescence rule established by Polyakov[1] and Kadanoff[2] and the dynamic scaling hypothesis[3] are at present the basic phenomenological premises concerning the spatial and frequency dispersion of the correlation functions of fluctuating quantities near a second-order phase transition. They permit the exponents of the power-law momentum asymptotics of the correlation functions and of the asymptotics of their characteristic frequencies $\omega_i(k)$ in the fluctuation regions $kr_c \gg i$ to be connected with the critical indices that describe the temperature dependences of the susceptibilities and of the kinetic coefficients at $k=0$. At the same time, the dynamic-scaling hypothesis leaves open the question of the nature of the singularities that cause the frequency dispersion of the susceptibilities. For linear dynamic susceptibilities considered within the dynamic-scaling framework it can be assumed as a rule that their characteristic frequencies $\omega_i(k)$ determine the positions of the poles that describe the excitation of one quasiparticle by an external field. Allowance for the effect of multiparticle excitations is possible only in the microscopic theory. Generally speaking, this influence can be noticeable for linear susceptibilities only at frequencies $\omega \ll \mathrm{Re}\,\omega_i(k)$ or $\omega \gg \mathrm{Re}\,\omega_i(k)$. A more important role is played by the microscopic theory in the study of the character of the dispersion of higher-order correlation functions over fluctuating fields whose singularities are due precisely to the multiparticle excitations, and are not simple poles.

An essential feature of multiparticle processes is that the momenta of the individual excited quasiparticles can generally speaking be arbitrarily large. This makes it necessary in the microscopic dynamic theory to take exact account of the spatial dispersion of the vertices and of the correlation functions of the fluctuating fields. In the present-day variants of the theory of interacting modes,[4–6] however, this dispersion can be described only phenomenologically.

In the present paper we obtain critical-dynamics equations for a model with nonconserved n-component order parameter φ_i and with $(\varphi_i\varphi_i)^2$ interaction in three-dimensional space, by expanding Ward's identity for the temperature Green functions and the vertices in terms of the total interaction vertex. The solutions of these equations have at $\omega=0$ and $kr_c \gg 1$ momentum asymptotics that agree with the correlation-coalescence rule,[1] and go over at $\omega=0$ and $k=0$ into the corresponding results for the homogeneous static quantities.[7] These equations were used to obtain the paired retarded correltion function $C_R(k,\omega)$ of the square of the order parameter and to calculate, in the lowest order in the invariant charge, the corrections to the retarded correlator of φ_i, the Green's functions $G_R(k,\omega)$, for the case when the order parameter is an optical phonon. The expressions obtained for these functions permit a qualitative, and in individual cases also a quantitative description of the shapes of the scattering spectra of light and of neutrons from soft optical phonons, as well as the frequency and temperature dependences of the sound damping near structural second-order phase transitions.

§ 1. WARD'S IDENTITY AND CRITICAL-DYNAMICS EQUATIONS

The functions $G_R(k,\omega)$ and $C_R(k,\omega)$ are analytic continuations of the temperature correlators $G(K)$ and $C(k)$ to the real axis from discrete imaginary frequencies $i\omega_m$ in the upper complex ω plane. These correlators are defined by the relations

$$\delta_{ij}G(K)=\frac{1}{\beta}\int_0^\beta d\sigma\int d^3x e^{i(KX)}\langle T_\sigma\{\varphi_i(X)\varphi_j(0)\}\rangle,$$

$$C(K)=\frac{1}{4\beta V}\int_0^\beta d\sigma\int d^3x e^{i(KX)}t_{ij}\langle T_\sigma\{\varphi_i(X)\varphi_j(X)\varphi_k(0)\varphi_l(0)\}\rangle t_{kl} -\frac{1}{4}\delta_{K,0}[t_{ij}\langle\varphi_i(0)\varphi_j(0)\rangle]^2, \qquad (1)$$

where $X=\{x,\sigma\}$, $K=\{k,\omega_m\}$, $(KX)=kx-\omega_m\sigma$, and β is the reciprocal temperature. The matrices t_{ij} were introduced for convenience in the calculations that follow; in the final expressions we shall put $t_{ij}=\delta_{ij}$.

We introduce also the vertex

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$$T_{ij}(P,K)=G^{-1}(P+K)G^{-1}(P)D_{ij}(P,K),$$

where

$$D_{ij}(P,K)=\frac{1}{2\beta^2 V}\int d^4X\int d^4Y \exp i[(PX)+(KY)]$$
$$\times\langle T_\sigma\{\varphi_i(X)\varphi_j(0)\varphi_k(Y)\varphi_l(Y)\}\rangle t_{kl}$$
$$-{}^1/_2\delta_{K,0}G_{ij}(P)\langle\varphi_k(0)\varphi_l(0)\rangle t_{kl}.$$

It follows from the definition of this vertex that at $t_{ij}=\delta_{ij}$

$$T_{ij}(P,0)=\frac{\partial G^{-1}(P)}{\partial\tau}\delta_{ij}\equiv T(P)\delta_{ij}, \tag{2}$$

where τ is the coefficient of the term $\varphi_i\varphi_i$ in the Hamiltonian.

The diagram expansion of T_{ij} (P,K) is a sum of diagrams with two tails and one corner, the latter corresponding to a bare vertex t_{ij}, while the expansion of $C(K)$ contains diagrams with two such corners. The inner lines can be regarded as corresponding to the complete Green functions $G(P)$, leaving out the diagrams with self-energy insets. Just as in the static case,[7] differentiation of $G(P)$ with respect to τ in each diagram, with allowance for the equality $\partial G(P)/\partial\tau=-G^2(P)T(P)$ yields Ward's identities—the diagram expansions of $\partial C(K)/\partial\tau$ and $\partial T_{ij}(P,K)/\partial\tau$. (An identical procedure yields an expression for the derivative, with respect to τ, of the total interaction vertex $\Gamma_{ijkl}(K_1,K_2,K_3,K_4)$.

The expansions obtained in this manner for the derivatives contain, besides $G(P)$ and $T(P)$, also the bare vertices t_{ij} and

$$\Gamma^{(0)}_{ijkl}={}^1/_3u(\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}).$$

They can be expressed in terms of the total vertices by iterating the corresponding perturbation-theory series, assuming the total vertex Γ_{ikl} to be small. It is convenient here to regard the bare vertices as dependent on the external momenta:

$$t_{ij}=t_{ij}(P,K),\quad \Gamma^{(0)}_{ijkl}=\Gamma^{(0)}_{ijkl}(K_1,K_2,K_3,K_4).$$

Once they are excluded, the Ward identities for T_{ij} and Γ_{ijkl} together with Eq. (2) form a closed system of equations, whose right-hand sides are represented by expansions over Γ_{ijkl}. In the lowest order of this expansion, they take the form

$$\frac{\partial}{\partial\tau}\Gamma_{ijkl}(K_1,K_2,K_3,K_4)$$
$$=6\sum_{Q_4}\int\frac{d^3q}{(2\pi)^3}\Gamma_{ijmn}(K_1,K_2,Q,-Q-K_1-K_2)$$
$$\times\Gamma_{mnkl}(-Q,Q+K_1+K_2,K_3,K_4)G(Q+K_1+K_2)G^2(Q)T(Q)$$
$$+(j\leftrightarrow k,2\leftrightarrow 3)+(i\leftrightarrow k,1\leftrightarrow 3), \tag{3}$$

$$\frac{\partial}{\partial\tau}T_{ij}(P,K)=6\sum_{Q_4}\int\frac{d^3q}{(2\pi)^3}\Gamma_{ijlm}(-P,K+P,Q,-Q-K)$$
$$\times T_{lm}(Q,K)G(Q-K)G^2(Q)T(Q). \tag{4}$$

If the reciprocal radius of the correlations

$$\varkappa=[\partial\ln G^{-1}(P)/\partial p^2]^{-1/2}_{P=0}$$

is of the order of u, the solutions (2)–(4) should go over into the corresponding bare quantities, so that we obtain the following boundary conditions at $\varkappa_0\sim u$:

$$\Gamma_{ijkl}(K_1,K_2,K_3,K_4)|_{\varkappa=\varkappa_0}={}^1/_3u(\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}),$$
$$T_{ij}(P,K)|_{\varkappa=\varkappa_0}=t_{ij},\qquad G(P)|_{\varkappa=\varkappa_0}=G_0(P)|_{\tau=\varkappa_0^2}.$$

The equation for $C(K)$ takes in the lowest order in Γ_{ijkl} the form

$$\frac{\partial}{\partial\tau}C(K)$$
$$=-\sum_{Q_4}\int\frac{d^3q}{(2\pi)^3}T_{lm}(Q,K)T_{lm}(-Q,-K)G(K-Q)G^2(Q)T(Q) \tag{5}$$

with the boundary condition

$$C(K)|_{\varkappa=\varkappa_0}=\frac{1}{2}t_{lm}t_{lm}\pi(K),$$
$$\pi(K)=\sum_{Q_4}\int\frac{d^3q}{(2\pi)^3}G_0(K-Q)G_0(Q)|_{\tau=\varkappa_0^2}.$$

The integration region in (3)–(5) is bounded by the cutoff momentum $\Lambda\sim u$.

The fluctuations of the order parameter in the vicinity of the phase tansition are quasiclassical, so that $G(q,0)\gg G(q,\omega_m)$ at all $\omega_m\neq 0$ and $q<\Lambda$. The presence of $G^2(Q)$ in the right-hand sides of (3)–(5) allows us to assume that the leading contribution to the sums over the frequencies $Q_4=\omega_m$ is made by the integrals with $Q_4=0$, in which $G^2(q,0)$ restricts the integration to values $q\lesssim\varkappa$.

Therefore, assuming the vertices Γ_{ijkl} and T_{ij} to be slowly varying functions of the four-dimensional momentum, we can, in the right-hand sides of (3)–(5), as $\varkappa\to 0$, replace the vertices that depend on the external momenta by their values at $Q=0$. The procedure used in Ref. 7 in the static case to renormalize the Ward identities reduces in fact to the same approximation. Therefore Eqs. (3)–(5) simplified in this manner will coincide at zero external momenta, in the lowest order in Γ, with the corresponding static equations.[7]

Following the indicated procedure in (3)–(5) and assuming also that $K_1=-K_2=P$ and $K_3=0$ in (3), we obtain the following closed system of equations:

$$\frac{\partial}{\partial\tau}\Gamma_{ijkl}(P)=-3\Gamma_{ijmn}(P)\Gamma_{mnkl}(0)\frac{\partial\Pi(0)}{\partial\tau}$$
$$-3[\Gamma_{imkn}(P)\Gamma_{mjnl}(P)+\Gamma_{imln}(P)\Gamma_{mjnk}(P)]\frac{\partial\Pi(P)}{\partial\tau}, \tag{6}$$

$$\frac{\partial}{\partial\tau}T(P)=-\frac{3}{n}\Gamma_{llmm}(P)T_0\frac{\partial\Pi(0)}{\partial\tau}, \tag{7}$$

$$\frac{\partial}{\partial\tau}T_{ij}(0,K)=-3\Gamma_{jmil}(K)T_{lm}(0,K)\frac{\partial\Pi(K)}{\partial\tau}, \tag{8}$$

$$\frac{\partial}{\partial\tau}C(K)=\frac{1}{2}T_{lm}(0,K)T_{lm}(0,-K)\frac{\partial\Pi(K)}{\partial\tau}, \tag{9}$$

$$\frac{\partial}{\partial\tau}G^{-1}(P)=T(P), \tag{10}$$

where

$$\Gamma_{ijkl}(P)=\Gamma_{ijkl}(P,-P,0,0),\qquad T_0=T(0),$$
$$\Pi(P)=\sum_{Q_4}\int\frac{d^3q}{(2\pi)^3}G(K-Q)G(Q). \tag{11}$$

Although it is impossible to justify rigorously the procedure used to derive Eqs. (3)–(5) and the qualitative arguments used to obtain (6)–(10), we can nevertheless regard the agreement between the asymptotic solutions of Eqs. (6)–(10) and the results of the phenomenological treatment[1] and of the microscopic calculations (see below) as an indication that the employed approximations are acceptable.

§ 2. VERTICES AND TEMPERATURE CORRELATION FUNCTIONS

It is easy to obtain from (6) and (7) at $P=0$

$$\Gamma_{ijkl}(0)={}^1/_3\Gamma_0(\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}),$$
$$\Gamma_0^{-1}=(n+8)[\Pi(0)-\pi(0)]+u^{-1},$$
$$T_0=(\Gamma_0/u)^{\xi_1},\qquad \xi_1=(n+2)/(n+8).$$

Inasmuch as $\varkappa\to 0$ we have

$$\Pi(0)\sim\varkappa^{-1+2\eta},\qquad T_0\sim\varkappa^{2-\eta-1/\nu},$$

we get

$$\xi_1=\frac{2-\eta-1/\nu}{1-2\eta}\approx 2-\frac{1}{\nu}, \tag{12}$$

where η is the Fisher exponent and ν is the correlation-radius exponent.

The solution of (6) can be represented in the form

$$3\Gamma_{ijkl}(P)$$
$$=[(n+2)/n]\Gamma_1(P)\delta_{ij}\delta_{kl}+\Gamma_2(P)[\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}-(2/n)\delta_{ij}\delta_{kl}],$$

where the $\Gamma_i(P)$ satisfy the equations

$$\dot\Gamma_1(P)=\frac{n+2}{n+8}\Gamma_1(P)$$
$$-\frac{2}{n}\dot\Pi(P)[(n+2)\Gamma_1^2(P)+2(n-1)\Gamma_2^2(P)],$$
$$\dot\Gamma_2(P)=\frac{2}{n+8}\Gamma_2(P) \tag{13}$$
$$-\frac{1}{n}\dot\Pi(P)\Gamma_2(P)[4(n+2)\Gamma_1(P)+(n-2)(n+4)\Gamma_2(P)],$$
$$\Gamma_i(P)|_{\varkappa=\varkappa_0},$$

in which the dot denotes differentiation with respect to $\ln\Gamma_0$.

We introduce new varibles $F_i(P)$ defined by

$$\Gamma_i(P)=\Gamma(P)F_i(P),$$

where

$$\Gamma^{-1}(P)=(n+8)[\Pi(P)-\pi(P)]+u^{-1}. \tag{14}$$

For $F_i(P)$ we obtain from (13)

$$F_i(P)=\left[\frac{\Gamma_0}{\Gamma(P)}\right]^{\xi_i}+\frac{1}{n(n+8)}\int_u^{\Gamma_0}\frac{d\Gamma_0'}{\Gamma'(P)}\frac{\partial\Gamma'(P)}{\partial\Gamma_0'}A_i(P),$$
$$A_1(P)=n(F_1^2+2F_2^2-3F_1)+2(F_1^2-F_2^2),\quad \xi_1=(n+2)/(n+8),$$
$$A_2(P)=4(n+2)F_1+(n-2)(n+4)F_2-n(n+6),\ \xi_2=2/(n+8). \tag{15}$$

In the lowest order in the invariant charge $g=\Gamma_0\Pi(0)\approx(n+8)^{-1}$ (Ref. 7) we have $F_i(P)\approx[\Gamma_0/\Gamma(P)]^{\xi_i}$, since the second term in the right-hand side of (15) is proportional to $(n+8)^{-2}$. Indeed, the quantities $A_i(P)$ can be represented as sums of terms proportional to

$$F_i(P)-1\approx\xi_i\ln[\Gamma_0/\Gamma(P)]\sim(n+8)^{-1},$$

and whose integrals are finite at all values of P and $\varkappa$. Thus,

$$\Gamma_i(P)\approx\Gamma(P)[\Gamma_0/\Gamma(P)]^{\xi_i}. \tag{16}$$

At $n=1$ the expression for the scalar vertex of the interaction is given by Eq. (16) with $\xi_1=1/3$.

Putting $T_{ij}(0,K)=\delta_{ij}R(K)$, we obtain from (8)

$$R(K)$$
$$=\exp\left\{-\frac{n+2}{n}\int_u^{\Gamma_0}d\Gamma_0'\frac{\partial\Pi(K)}{\partial\Gamma_0'}[\Gamma_1'(K)+(n-1)\Gamma_2'(K)]\right\}.$$

Replacing $\Gamma_i(K)$ by $\Gamma(K)$ we obtain an expression for $R(K)$ accurate to terms of order ξ_i:

$$R(K)=[\Gamma(K)/u]^{\xi_1}. \tag{17}$$

From (9) and (17) we have

$$C(K)=\frac{n}{2}\left\{\pi(K)+\frac{1}{(n+8)u}\frac{\nu}{\alpha}\left[\left(\frac{u}{\Gamma(K)}\right)^{\alpha/\nu}-1\right]\right\},$$
$$\alpha/\nu=(1-2\xi_1)(1-2\eta)\approx(1-2\xi_1)=(4-n)/(n+8). \tag{18}$$

It follows from (7) and (16) that

$$T(P)=T_0+\int_{T_0}^1 dT_0'\left\{1-\left[\frac{\Gamma'(P)}{\Gamma_0'}\right]^{1-\xi_1}\right\}. \tag{19}$$

Using (10) and (19) we can represent $G(P)$ in the form

$$G^{-1}(P)=\tilde G^{-1}(P)+\Sigma(P),$$

where

$$\tilde G^{-1}(P)=r+G_0^{-1}(P)-G_0^{-1}(0),\qquad r\equiv G^{-1}(0)\approx\varkappa^2, \tag{20}$$

$$\Sigma(P)=\int_r^{r_0}dr'\left[1-\frac{T'(P)}{T'}\right]$$
$$\approx\int_{T_0}dT_0'\left(\frac{r'}{T_0'}-\frac{r}{T_0}\right)\left\{\left[\frac{\Gamma'(P)}{\Gamma_0'}\right]^{1-\xi_1}-1\right\} \tag{21}$$

It will be shown below that in the region $\max(\varkappa,p)\gg\varkappa_0 e^{-1/\eta}$ we have $G(p,0)\approx\tilde G(p,0)$. At $P_4\equiv\omega_m=0$ we have $\tilde G^{-1}(p,0)=\varkappa^2+p^2$, so that

$$\Pi(p,0)\approx\frac{1}{4\pi p}\operatorname{arctg}\frac{p}{2\varkappa}.$$

Substituting this expession in (14) and (16)–(19) we obtain at $\varkappa\ll p\ll\varkappa_0$ and $\alpha>0$

$$\Gamma_1(p,0)\sim p^{1-\xi_1}\varkappa^{\xi_1}\sim p^{1/\nu-1}T_0,$$
$$T(p,0)\sim p^{1-\xi_1}\varkappa^{2\xi_1-1}\sim p^{1/\nu-1}C(0),$$
$$R(p,0)\sim p^{\xi_1}\approx p^{2-1/\nu}.$$

The exponents in these asymptotic equations agree, apart from the index η, with those obtained in Ref. 1.

§ 3. THE RETARDED CORRELATION FUNCTIONS G_R AND C_R

An equation for $G_R(p,\omega)$ can be obtained by analytically continuing expressions (11), (20), and (21) from the discrete imaginary frequencies $i\omega_m$ in the upper half-plane ($\omega_m = 2\pi m/\beta\hbar \geqslant 0$). To this end we represent $\Pi(P)$ in the form

$$\Pi(P)=\frac{1}{(2\pi)^3}\int d^3p_1\int d^3p_2\delta(p_1+p_2-p)A(p_1,p_2,\omega_m), \quad (22)$$

$$A(p_1,p_2,\omega_m)=\sum_{\omega_n}G(p_1,\omega_n)G(p_2,\omega_m-\omega_n). \quad (23)$$

At $\omega_m\geqslant 0$, in the quasiclassical approximation, the summation over the frequencies ω_n in (23) can be restricted to the interval $0\leqslant\omega_n\leqslant\omega_m$, inasmuch as there are no terms with $G(p,0)$ outside this interval. We can then expess A in terms of $G_R(p,\omega)$ as follows:

$$A(p_1,p_2,\omega_m)=\frac{\beta\hbar}{2\pi i}\oint\frac{d\omega'}{\exp(\beta\hbar\omega')-1}G_R(p_1,\omega')G_R(p_2,i\omega_m-\omega'). \quad (24)$$

The integration contour in (24) contains the segment $[0,i\omega_m]$ on the imaginary axis. Moving it off to infinity, the integral in (14) can be transformed into a sum of integrals over contours that contain the singularities of the functions G_R (the contribution from the poles $[\exp(\beta\hbar\omega')-1]^{-1}$ can be neglected in the quasiclassical approximation). We shall assume that the singularities of $G_R(p,\omega)$ in the lower half-plane include simple poles that tend to the point $\omega=0$ as $\varkappa\to 0$ and $p\to 0$. The integrals over the contours around these poles make then the main contribution to A, a contribution that diverges as $\varkappa\to 0$ and $p_i\to 0$ as a result of the clamping of these contours between the poles G_R and $[\exp(\beta\hbar\omega')-1]^{-1}$ at $\omega'=i\omega_m$ and $\omega'=0$. Thus

$$A(p_1,p_2,\omega_m)\approx-\frac{\beta\hbar}{2\pi i}\left(\oint_{C_1}+\oint_{C_2}\right),$$

where the contour C_1 contains the poles $G_R(p_1,\omega')$ and C_2 the poles $G_R(p_2,i\omega m-\omega')$. Substituting $\omega''=i\omega_m-\omega'$ in the integral with respect to C_2, we obtain

$$A(p_1,p_2,\omega_m)=-\frac{\beta\hbar}{2\pi i}\left\{\oint_{C_1}\frac{d\omega'}{\exp(\beta\hbar\omega')-1}G_R(p_1,\omega')G_R(p_2,i\omega_m-\omega')-\oint_{C_2'}\frac{d\omega''}{\exp(-\beta\hbar\omega'')-1}G_R(p_1,i\omega_m-\omega'')G_R(p_2,\omega'')\right\}. \quad (25)$$

The analytic continuation of (25) reduces to the substitution $i\omega_m\to\omega$, so that for the continuation of (22), assuming that $|\beta\hbar\omega'|\ll 1$ on C_1 and $|\beta\hbar\omega''|\ll 1$ on C'_2 we obtain

$$\Pi_R(p,\omega)=-\frac{1}{\pi i}\int\frac{d^3p_1}{(2\pi)^3}\oint_{C_1}\frac{d\omega'}{\omega'}G_R(p_1,\omega')G_R(p-p_1,\omega-\omega'). \quad (26)$$

For $G_R(p,\omega)$ we have from (14), (20), and (21)

$$G_R^{-1}(p,\omega)=\tilde{G}_R^{-1}(p,\omega)+\Sigma_R(p,\omega), \quad (27)$$

$$\Sigma_R(p,\omega)=\int_{T_0}^{1}dT_0'\left(\frac{r'}{T_0'}-\frac{r}{T_0}\right)\left\{\left[\frac{\Gamma_R'(p,\omega)}{\Gamma_0'}\right]^{1-\xi_1}-1\right\} \quad (28)$$

$$\Gamma_R^{-1}(p,\omega)=(n+8)\left[\Pi_R(p,\omega)-\pi_R(p,\omega)\right]+u^{-1}. \quad (29)$$

By the term with exponent $1-\xi_1$ in (28) is meant that analytic branch of this function which is real at real Γ_R with a cut along the line that starts out from zero and lies outside the region of the values of Γ_R at $\operatorname{Im}\omega>0$.

A characteristic feature of Eqs. (26)–(29) that determine $G_R(p,\omega)$ is that all the functions G_R contained in them have frequencies $|\omega'|\lesssim\max(|\omega_i(p)|,|\omega|)$, where $\omega_i(p)$ are the frequencies of the poles of G_R. Assuming that the fluctuations of φ_i are slowest motions in the system, i.e., that $|\omega_i(p)|t_e\ll 1$ (t_e is the longest characteristic time of the noncritical fluctuations,[1]) and considering only the frequency region with $\omega t_e\ll 1$, we can regard the frequency ω in (26)–(29) as satisfying this condition and represent G_{0R}^{-1} (and with it also $\tilde{G}_R^{-1}$) by an expansion in powers of ω:

$$G_{0R}^{-1}(p,\omega)=\tau+p^2-2i\omega L-M\omega^2. \quad (30)$$

Inclusion in (30) of the term quadratic in ω allows us to consider the case when the fluctuations of the order parameter are propagating excitations, for example soft optical phonons near a second-order structural phase transition. In the effective field region $\tau>\varkappa_0^2$ the soft phonons are well-defined elementary excitations at $L^2\ll M\varkappa_0^2$. It will be shown below that in the region of strong fluctuations ($\varkappa\ll\varkappa_0$) there exists a section in which

$$G_R^{-1}(p,\omega)\approx\tilde{G}_R^{-1}(p,\omega)=\varkappa^2+p^2-2i\omega L-\omega^2M \quad (31)$$

and the condition $L^2\ll M\varkappa^2$ can be satisfied (at sufficiently small L), so that the phonons remain weakly damped. Only this section will be considered in the present paper.

Regarding Σ_R as a small correction to $\tilde{G}_R^{-1}$ in (27), we substitute (31) in (26). The result of the integration is of the form

$$\Pi_R(p,\omega)=\frac{1}{4\pi ip}\ln\frac{(S+2\varkappa)(R+2L-iM\omega)+ip(R+2L)}{(S+2\varkappa)(R+2L-iM\omega)-ip(R+2L)}$$

$$R=[4L^2+M(p^2-4iL\omega-M\omega^2)]^{1/2},$$

$$S=(4\varkappa^2+p^2-4iL\omega-M\omega^2)^{1/2} \quad (32)$$

The square roots and the logarithms in (32) denote the branches of those functions which are analytic in the plane, with a cut along the negative real axis, and take on real values on the positive real axis, with $R>0$ and $S>0$ on this axis. It can be shown that at $\mathrm{Im}\,\omega>0$ the quantity Π_R of (32) satisfies the inequalities

$$(\mathrm{Re}\,\omega)\frac{\partial}{\partial\varkappa}\mathrm{Im}\,\Pi_R(p,\omega)<0,\quad \mathrm{Re}\,\omega\neq 0,$$

$$\frac{\partial}{\partial\varkappa}\Pi_R(p,\omega)<0,\quad \mathrm{Re}\,\omega=0,$$

by virtue of which Γ_R has no values on the real negative axis at $\mathrm{Im}\,\omega>0$. An expression for Σ_R that is analytic in the upper ω half-plane can therefore be obtained by substituting (32) in (29) and (28) and choosing the power-law branch in (28) with a cut along this semiaxis.

At

$$\max(2L\omega, M\omega^2, p^2)\ll\varkappa^2\ll\varkappa_0^2\min(2L/M^{1/2}p, 1)$$

it follows from (28), (29), and (32) that

$$\Sigma_R(p,\omega)={}^1/_2\xi_1(A^{1-1/\nu}-1)+{}^3/_4\eta A^{1-1/\nu}(\Delta+{}^1/_3A^2p^2)\ln(\varkappa_0/\varkappa),$$

$$A=\frac{R+2L}{R+2L-i\omega H},\quad \Delta=p^2-4iL\omega-M\omega^2,$$

$$\eta=\frac{1}{12}\xi_1(1-\xi_1)=\frac{1}{2}\frac{n+2}{(n+8)^2}. \qquad (33)$$

At

$$\varkappa^2\ll\max(2L\omega, M\omega^2, p^2)\ll\varkappa_0^2\min(2L/M^{1/2}p, 1)$$

and $\alpha>0$ we have

$$\Sigma_R(p,\omega)={}^1/_2\xi_1(A^{1-1/\nu}-1)-{}^3/_8\eta A^{1-1/\nu}(\Delta+{}^1/_3A^2p^2)\ln(\Delta/\varkappa_0^2)$$

$$-\xi_1(\nu/\alpha)\varkappa^{(1-\alpha)/\nu}[8\pi\Pi_R^{(0)}(p,\omega)]^{1-1/\nu},$$

$$\Pi_R^{(0)}(p,\omega)=\Pi_R(p,\omega)|_{\varkappa=0}. \qquad (34)$$

The cuts of the powers and of the logarithm in (33) and (34) are taken along the negative real axis.

At $\omega=0$ Eq. (34) takes the form

$$\Sigma_R(p,0)=-\eta p^2\ln\frac{p}{\varkappa_0}-\xi_1\frac{\nu}{\alpha}\varkappa^{(1-\alpha)/\nu}\left(\frac{p}{\pi}\right)^{1/\nu-1}. \qquad (35)$$

The first term in the right-hand side of (35) can be regarded as the first term of the expansion of $p^2(p/\varkappa_0)^{-\eta}$, by identifying the parameter η introduced in (33) with the Fisher index. Its value coincides with the result of the ε-expansion.[4] The second term in (35) is equal, accurate to the factor $\pi^{1-1/\nu}$, to the expression obtained in Ref. 8.

In the case of relaxation dynamics [$M=0$ in (30)] it follows from (30) that

$$G_R(p,\omega)=\varkappa^2+p^2[1+\eta\ln(\varkappa_0/\varkappa)]-2i\omega L[1+{}^3/_2\eta\ln(\varkappa_0/\varkappa)].$$

The influence of the multiparticle processes at small ω and p reduces thus to a renormalization of the coefficient of p^2 and of the damping constant L. The expression for the renormalized constant

$$\tilde L=L\left[1+{}^3/_2\eta\ln\left(\frac{\varkappa_0}{\varkappa}\right)\right],$$

can be regarded, in accord with the results obtained in the method of the dynamic renormalization group,[4] as an expansion of the power-law relation

$$\tilde L=L(\varkappa_0/\varkappa)^{3/2\eta}.$$

We have then for the relaxation dynamic index z

$$z=2-\eta-d\ln\tilde L/d\ln\varkappa=2+{}^1/_2\eta,$$

which is close to the result of the ε-expansion for the model without conservation laws[4]:

$$z=2+c\eta,\quad c=6\ln{}^4/_3-1\approx 0.73.$$

It follows from (33) and (34) that smallness of Σ_R compared with $\tilde G_R^{-1}$ is ensured in the corresponding regions by the inequality

$$\max(2L\omega, M\omega^2, p^2, \varkappa^2)\gg\varkappa_0^2e^{-2/\eta}. \qquad (36)$$

When the condition (36) is satisfied the analytic continuation (18) of $C(K)$ is given by

$$C_R(k,\omega)$$

$$=\frac{n}{2}\left\{\pi_R(k,\omega)+\frac{1}{(n+8)u}\frac{\nu}{\alpha}\left[\left(\frac{u}{\Gamma_R(k,\omega)}\right)^{\alpha/\nu}-1\right]\right\},$$

where Γ_R is determined by (29) with Π_R from (32), and the cut of the function raised to the power α/ν is taken along the negative real axis. If the expression in the left-hand side of (36) is much smaller than $\varkappa_0^2$ and $\alpha>0$, we have

$$C_R(k,\omega)$$

$$\approx\frac{n}{2}\frac{\nu}{\alpha}[(n+8)u]^{\alpha/\nu-1}|\Pi_R(k,\omega)|^{\alpha/\nu}\exp\left(i\frac{\alpha}{\nu}\mathrm{arctg}\frac{\Pi_R''}{\Pi_R'}\right),$$

$$\Pi_R=\Pi_R'+i\Pi_R''. \qquad (37)$$

We note that the condition (36) allows us to neglect the exponent in the power-law functions. To find G_R and C_R outside the region where this neglect is impossible, we must take into account the terms of the next order in Γ_{ijkl} in Eqs. (3)–(5), terms that introduce corrections proportional to g^2 into Γ_R (29) and ξ_1 (12). The contribution of these corrections to η is only of the order of g^3, but their contribution to the exponents α and ν, which is proportional to ξ_1, is of the order of g^2 and must be taken into account in order to satisfy the scaling relations between the critical exponents.

§ 4. SCATTERING SPECTRA AND DAMPING OF SOUND

The results can be used to interpret dynamic critical phenomena in the vicinity of second-order structural phase transitions, such as the anomalous damping of sound and critical scattering of light and of neutrons. The spectral intensity of the scattering of light and neutrons by soft optical phonons is determined by the imaginary parts of the functions G_R and C_R. It is convenient to express the function G_R in terms of parameters that characterize the line shape of the soft mode:

$$M^{-1}G_R^{-1}(p,\omega)=\Omega^2+v^2p^2-2i\omega\Gamma-\omega^2+v^2\Sigma_R(p,\omega),$$
$$v^2=M^{-1},\quad \Omega=v\varkappa,\quad \Gamma=v^2L.$$

It follows from (33) that at $\Omega \gg \max(2\Gamma, vp)$ there exists in the first-order spectrum, besides the soft mode, a quadrupole-scattering peak with intensity

$$I_1(p,\omega) \propto \omega^{-1}\operatorname{Im} G_R(p,\omega) \approx -{}^1/_2\xi_1\Omega_0{}^2\Omega^{-4}\omega^{-1}\operatorname{Im} A^{1-1/\nu}.$$

Its width is of the order of max $(2\Gamma, vp)$ and the intensity at the maximum is

$$I_1(p,0)=6\eta\frac{\Omega_0^2}{\Omega^2}\left\{\left[1+\left(\frac{vp}{2\Gamma}\right)^2\right]^{1/2}+1\right\}^{-1} I_{SM},$$

where $I_{SM}=(2\Omega^2\Gamma)^{-1}$ is the intensity at the soft-mode maximum.

For the spectral intensity of the second-order scattering

$$I_2(k,\omega)\propto\omega^{-1}C_R(k,\omega)$$

we obtain $\alpha>0$ from (37) the following approximate expressions:

I. $\Gamma \ll vk \ll \Omega$:

a) $|\omega|<vk$,

$$I_2(k,\omega)\propto\left(\frac{v^2k^2-\omega^2}{\Omega^2v^2k^2}\right)^{\alpha/2\nu}\omega^{-1}\operatorname{arctg}\frac{\omega}{(v^2k^2-\omega^2)^{1/2}};$$

b) $|\omega|>2\Omega$,

$$I_2(k,\omega)\propto|\omega|^{-1-\alpha/\nu}\operatorname{arctg}(\omega^2/4\Omega^2-1)^{1/2}.$$

II. $(\omega, vk)\gg\max(\Gamma,\Omega^2\Gamma^{-1})$:

$$I_2(k,\omega)\propto(vk)^{-\alpha/\nu}|\omega|^{-1}\left|\ln\frac{(\omega+vk)^2+4\Gamma^2}{(\omega-vk)^2+4\Gamma^2}\right|^{\alpha/\nu},$$

$$\Gamma=\Gamma\left(\frac{\Omega+\Gamma}{2\Gamma}\right)^2.$$

III. $vk\ll\Gamma\ll\Omega$:

a) $|\omega|\ll\Omega$,

$$I_2(k,\omega)\propto\Omega^{-\alpha/\nu}(\omega^2+8\Gamma^2)^{-1};$$

b) $|\omega|>2\Omega$, the same as in Ib.

IV. $vk\ll\Omega\ll\Gamma$:

a) $|\omega|\ll\Omega$,

$$I_2(k,\omega)\propto\Omega^{-\alpha/\nu}t_r/x^{1+\alpha/\nu}(x+1);$$
$$x=2^{-1/2}[(1+\omega^2t_r^2)^{1/2}+1]^{1/2},\quad t_r=\Gamma\Omega^{-2};$$

b) $|\omega|\gg\Gamma$,

$$I_2(k,\omega)\propto|\omega|^{-1-\alpha/\nu}\operatorname{arctg}\left[\left(1+\frac{\omega^2}{16\Gamma^2}\right)^{1/2}+\frac{|\omega|}{4\Gamma}\right]^3.$$

V. $\Omega\ll vk\ll\Gamma$:

a) $|\omega|\ll vk$,

$$I_2(k,\omega)\propto(vk)^{-\alpha/\nu}|\omega|^{-1}\frac{u}{1+u^2}\left(\operatorname{arctg}\frac{|\omega|t_h}{2y^3}\right)^{-1+\alpha/\nu}$$
$$y=2^{-1/2}[(1+\omega^2t_h^2)^{1/2}-1]^{1/2},\quad t_h=4\Gamma/v^2k^2;$$

b) $|\omega|\gg\Gamma$, the same as in IV b.

In cases I and II the shape of the spectra can be intepreted in terms of phonon processes. In a process without a change in the number of phonons, the conservation laws are of the form

$$\omega=\Omega(p_2)-\Omega(p_1),\quad \Omega(p_i)=(\Omega^2+v^2p_i^2)^{1/2},\quad \mathbf{p}_2=\mathbf{p}_1+\mathbf{k}, \tag{38}$$

while in a process with excitation (or absorption) of a pair of critical phonons

$$|\omega|=\Omega(p_1)+\Omega(p_2),\quad \mathbf{p}_1+\mathbf{p}_2=\mathbf{k}. \tag{39}$$

The process (38) has threshold $\omega_{\max}=vk$, which is reached at

$$p_i\gg\max(k,\varkappa),\quad (\mathbf{p}_i\mathbf{k})\approx p_ik, \tag{40}$$

while the process (38) has a threshold $\omega_{\min}=(4\Omega^2+v^2k^2)^{1/2}$ at

$$\mathbf{p}_1\approx\mathbf{p}_2\approx{}^1/_2\mathbf{k}. \tag{41}$$

In case I the spectral intensity displays the existence of these thresholds, since the photons near these thresholds are well defined excitations ($\Omega(p_i)\gg\Gamma, \omega\gg\Gamma$). In case II the dispersion of the group velocity $u(p)=v^2p/\Omega(p)$ of the phonons excited near the merging thresholds $\omega_{\min}\approx\omega_{\max}=vk$ becomes small enough for them to form phonon packets that are not smeared out during the free path time Γ^{-1}. Indeed, for the smearing time of a packet with momentum $q\sim p_i$ we have from (40)

$$t(q)=\left[\frac{du(q)}{dq^{-1}}\right]^{-1}\approx\frac{vq}{\Omega^2}\gtrsim\frac{vk}{\Omega^2}\gg\Gamma^{-1}. \tag{42}$$

The group velocity of such packets, $\mathbf{u}(q)\approx v\mathbf{k}/k$, coincides with the phase velocity $\omega\mathbf{k}/k^2$ of the external excitations. The packets satisfy thus the phase-resonance condition that causes an rapid growth of the damping at $\omega\approx vk$. The presence of a peak in the spectral intensity can be interpreted as the result of excitation in the gas of phonon wave packets analogous to second sound in a gas of acoustic phonons.

In the interpretation of the singularities of the spectra in cases III–V it must be recognized that relations (38) and (39) are satisfied accurate to the reciprocal free path time of the phonons Γ. In case III this causes smearing of the lower threshold by an amount of the order of Γ, where as at high frequencies $|\omega|>2\Omega$ this smearing, just as in Ib, can be neglected. When condition IV is satisfied the phonons excited in the process (39) at $|\omega|\ll\Omega$ turn out to be overdamped, $\Omega(p_i)\lesssim\Gamma$. Scattering by them leads to the appearance of a central peak of width proportional to the reciprocal relaxation time $\Omega^2\Gamma^{-1}$. In the processes (38) there can be excited weakly damped phonons with arbitrarily large momenta, and this leads to the presence of a tail in the spectral intensity at frequencies higher than the reciprocal free path time of

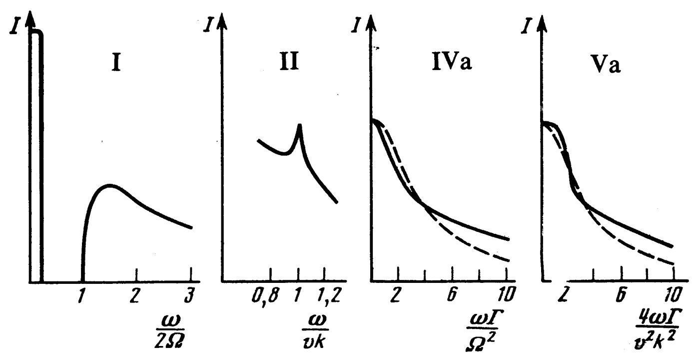

FIG. 1. Spectral intensity of second-order scattering. The Roman numbers denote the corresponding equations in the text. The plot II pertains to $2\Gamma/vk=10^{-3}$. The dashed curves in cases IVa and Va show the Lorentzians with the equivalent half-widths, $3.5\Omega^2\Gamma^{-1}$ and $0.8v^2k^2\Gamma^{-1}$, respectively.

these phonons, $\omega > \Gamma$. In V, just as in II, the condition (42) may be satisfied for the excited phonons, but by virtue of $vk \ll \Gamma$ excitations of second-sound type are relaxing. Their relaxation can be regarded as heat transfer in the gas of phonon packets, with a characteristic time $t_h = 4\Gamma/v^2k^2$ that determines the width of the central peak. The integral intensity of the central peak in cases III and IV is proportional to the heat capacity: $I \propto \Omega^{\alpha/\nu} \propto \tau^{-\alpha}$, and in case V we have $I \propto (vk)^{-\alpha/\nu}$. The spectral intensities for some of the considered cases (at $n = 1$) are shown in Fig. 1.

The expressions presented above for the spectral intensity, with the exception of cases II, IVb, and Vb, can be represented in the scaling form:

$$I_2(k, \omega) = \varkappa^{-\alpha/\nu} t f(\omega t, \varkappa/k), \quad t \sim \varkappa^{-z}$$

The dynamic index z (Ref. 3), however, has different values. Thus, $z = 2$ in IVa and Va, $z = 1$ in I and IIb, and $z = 0$ in IIIa.

In the region where the influence of the elastic degrees of freedom on the order-parameter fluctuations can be neglected,[9] the function $I_2(k,\omega)$ determines also the damping decrement of the longitudinal sound at $T > T_c$. Indeed, in this region the self-energy part of the temperature propagator of the acoustic phonons, by virtue of the presence of striction interaction of the type $u_{ii}\varphi_j\varphi_j$ constitutes a sum of diagrams having two corners and proportional to the temperature correlator $C(K)$. As a result, the correction to the dynamic bulk elastic modulus $B(k,\omega)$ turns out to be proportional to $C_R(k,\omega)$, so that we have for the bulk-viscosity coefficent $\eta_L(k,\omega)$

$$\eta_L(k, \omega) = -\omega^{-1} \operatorname{Im} B(k, \omega) \propto I_2(k, \omega),$$

and for the longitudinal-coefficient damping coefficient $\alpha_L(\omega)$ we obtain

$$\alpha_L(\omega) \propto \omega^2 \eta_L\left(\frac{\omega}{c_L}, \omega\right) \propto \omega^2 I_2(\omega/c_L, \omega),$$

where c_L is the speed of the longitudinal sound. At $c_L < v$ and $\alpha > 0$ we have from I–V the following:

1. $\Gamma \ll \Omega$:
   a) $\omega \ll \Gamma c_L/v, \quad \alpha_L(\omega) \propto \omega^2 \Omega^{-\alpha/\nu} \Gamma^{-1}$;
   b) $\Gamma c_L/v \ll \omega \ll \Omega c_L/v, \quad \alpha_L(\omega) \propto \omega \Omega^{-\alpha/\nu}$.
2. $\Omega \ll \Gamma c_L/v$:
   a) $\omega \ll \Omega^2 \Gamma^{-1}, \quad \alpha_L(\omega) \propto \omega^2 \Omega^{-2-\alpha/\nu} \Gamma$;
   b) $\Omega^2 \Gamma^{-1} \ll \omega \ll \Omega c_L/v, \quad \alpha_L(\omega) \propto \omega^{1-\alpha/2\nu}$;
   c) $\Omega c_L/v \ll \omega \ll \Gamma c_L/v, \quad \alpha_L(\omega) \propto \omega^{1-\alpha/2\nu} \quad (c_L/v \ll 1)$.

The presently available theoretical results on sound damping near structural phase transitions correspond to region 2a (Ref. 10). The value of the critical exponent $\rho = zv + \alpha \approx 2\nu + \alpha$ obtained in Ref. 10 for the contribution made to $\alpha_L(\omega)$ from the longitudinal viscosity coefficient $\eta_L(0,\omega)$ agrees, accurate to η, with the result 2a. A frequency dispersion of $\alpha(\omega)$ analogous to 2a, b, c, was observed near a structural phase transition in $KMnF_3$.[11]

Expessions I–V for the sectral intensity $I_2(k,\omega)$ permit at least a qualitative description of a number of singularities observed in the second-order scattering spectra in the vicinity of structural phase transitions. Thus, in displacive phase transitions with weakly damped soft mode the characteristic feature of the scattering spectra at $T > T_c$ is, according to Ib and IIIb, the presence of a maximum of two-phonon scattering at a frequency on the order of 2Ω. Such peaks, having an asymmetric shape that agrees qualitatively with Ib, were actually observed in $Hg_2(Cl_x Br_{1-x})_2$. Another feature of the second-order spectrum is the presence of a rather broad and slowly growing $(I \propto \tau^{-\alpha})$ central peak. It appears that the anomalous temperature dependence of such a peak will take place in a sufficiently large temperature range only for crystals with relaxation dynamics ($\Omega \ll \Gamma$ already in the effective-field region) (see IVa). By way of example we cite the experimental observation[13] of quasielastic scattering in an order–disorder transition in NH_4Cl, with a temperature dependence that agrees with IVa.

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[1)]Besides the order-parameter fluctuations there are also other slow (hydrodynamic) motions (sound, heat conduction) with characteristic frequencies much lower than t_e^{-1}. We disregard here their interaction with the order parameter.

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