Generalized Cauchy relation and elastic constants for liquid metals

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A generalized Cauchy relation that connects the pressure in the system with the high-frequency elastic moduli is obtained for liquid metals. It is shown that the presence of an electron subsystem in the metal leads to violation of the Cauchy relation. This violation is characteristic of systems with central paired interaction. Explicit expressions are obtained for the corrections to the high-frequency elastic moduli and to the Cauchy relation on account of multiparticle interaction between the ions.

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1. INTRODUCTION

In connection with advances in neutron experimental techniques, the question of the role of multiparticle interactions in liquids is now being intensively studied.[1-4] An estimate of the influence of the multiparticle forces on the properties of simple liquids such as argon is made difficult by the lack of reliable data on the potentials of the multiparticle interactions and multiparticle distribution functions. The situation is more favorable for liquid metals, where the potentials of the interparticle interactions can be calculated "from first principles" and multiparticle effects can be correspondingly separated. A multiparticle theory of metals in the crystalline phase was developed by Brovman and Kagan (see the review[5]) and has found numerous experimental confirmations.[5,6] For liquid metals it is customary to confine oneself in the theory to the pair-interaction approximation,[7] and no direct experiments aimed at observing multiparticle effects are known. It is known, however, that multiparticle effects, first, can substantially renormalize the paired interaction,[8] and second, irreducible three-, four-, ... particle interactions can turn out to be of the same order as the paired.[5] It has therefore become necessary to take simultaneous account of paired and multiparticle interactions. One can indicate in this connection metal properties that, on the one hand, are sensitive to multiparticle forces, and on the other can be calculated (to a certain approximation) knowing only the paired static structure factor, which has been well investigated in experiment. We have in mind the elastic constants of liquid metals. It is known that under fast external action a liquid reveals elastic properties, that can be characterized by appropriate elastic constants.[9,10] A connection between the high-frequency elastic constants and moduli, on the one hand, and the structure of a liquid and the interparticle potential, on the other, has been established in Refs. 10–12 under the assumption that the interparticle interaction is paired and central. It was found that this calls for satisfaction of the so-called generalized Cauchy relation, which connects the pressure P in the system with the elastic moduli

$$K-{}^5/_3G=2(P-nk_BT), \tag{1}$$

where K and G are the high-frequency hydrostatic compression and shear moduli, respectively, T is the temperature, n is the particle-number-density, and k_B is the Boltzmann constant. The principal assumptions that lead to (1) are incorrect for metals, so that the Cauchy relation in the form (1) need not be satisfied. In the present paper we obtain a generalization of relation (1) to include the case of liquid metals. An essential feature of the generalization is that account is taken of three- and four-particle interactions in addition to two-particle, and it is shown that Eq. (1) is violated by multiparticle interactions. The new Cauchy relation contains only a two-particle structure factor and does not depend on the multiparticle distribution functions; this facilitates its experimental verification.

2. FREE ENERGY AND EQUATION OF STATE OF LIQUID METALS

We use the results of Refs. 5 and 7, according to which the thermodynamic potential Ω of a metal, as an aggregate of interacting ions and electrons, is replaced in the adiabatic approximation by the thermodynamic potential of a single-component system of ions with effective interaction determines by the polarization properties of the electrons:

$$\Omega=-k_BT\ln \mathrm{Sp}\exp\left[\frac{\mu_iN_i-H_i-\Omega_e}{k_BT}\right]. \tag{2}$$

Here H_i, N_i, and μ_i are respectively the Hamiltonian, the number of ions, and their chemical potential, Ω_e was obtained by averaging over the electron variables, and the trace means the operation of averaging over the ion variables. Under the assumption that the coupling between the electron and ion subsystems is effected by a weak pseudopotential (PP), Ω_e can be represented as a series in powers of PP:

$$\Omega_e=\sum_{n=0}^{\infty}\Omega_e^{(n)}, \tag{3}$$

where $\Omega_e^{(n)}$ corresponds to the n-th order in the PP. $\Omega_e^{(0)}$ corresponds in this case to the contribution made to Ω by the homogeneous electron gas (against the background of the compensating charge), and $\Omega_e^{(1)}$ is determined by the non-Coulomb part of the PP. The terms with $n\geqslant2$ contribute to the effective Hamiltonian of the ions. Using quantum field theory methods,[13] we can obtain for them the following expressions[5,7]:

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$$\Omega_e^{(2)}=-\frac{N_i^2}{2V}\sum_{\mathbf{K}\neq 0}\frac{\pi(\mathbf{k})}{\varepsilon(\mathbf{k})}|\rho_i(\mathbf{k})w_0(\mathbf{k})|^2, \tag{4}$$

$$\Omega_e^{(n)}=\frac{V}{nv_0^n}\sum_{\mathbf{k}_1,\ldots,\mathbf{k}_n\neq 0}\tilde{\Lambda}_n(\mathbf{k}_1,\ldots,\mathbf{k}_n)\rho_i(\mathbf{k}_1)\ldots\rho_i(\mathbf{k}_n)\Delta(\mathbf{k}_1+\ldots+\mathbf{k}_n),\quad n\geqslant 3. \tag{5}$$

Here

$$\rho_i(\mathbf{k})=\frac{1}{N_i}\sum_{j=1}^{N_i}e^{-i\mathbf{k}\mathbf{R}_j},\quad w_0(\mathbf{k})=\int w_0(\mathbf{r})e^{-i\mathbf{k}\mathbf{r}}\,d\mathbf{r}, \tag{6}$$

$w_0(\mathbf{r})$ is the PP of the electron-ion interaction (assumed to be local), $\pi(\mathbf{k})$ and $\varepsilon(\mathbf{k})$ are the static polarization opperator and the dielectric constant of the electron gas,

$$\tilde{\Lambda}_n(\mathbf{k}_1,\ldots,\mathbf{k}_n)=\Lambda_n(\mathbf{k}_1,\ldots,\mathbf{k}_n)\frac{w_0(\mathbf{k}_1)}{\varepsilon(\mathbf{k}_1)}\cdots\frac{w_0(\mathbf{k}_n)}{\varepsilon(\mathbf{k}_n)}, \tag{7}$$

where Λ_n are the multipoles introduced in Ref. 5 and are in fact the n-th order polarization functions of the electron gas, R_j are the coordinates of the ions, $v_0=V/N_i$ is the specific volume of the ion, and $\Delta(\mathbf{k})$ is the Kronecker symbol. (In the multipoles used by us, in contrast to Ref. 5, the factor $1/n$ is separated explicitly.)

In what follows it is convenient to change over from the Ω-potential to the Helmholtz free energy F. It is known that for this purpose it is necessary to write[14]

$$F=\Omega-\mu_e\frac{\partial\Omega}{\partial\mu_e}-\mu_i\frac{\partial\Omega}{\partial\mu_i},$$

where μ_e is the chemical potential (CP) of the electrons. We thus obtain

$$F=\Omega_e^{(0)}+\Omega_e^{(1)}+\sum_{n\geq 2}U_n^{(0)}-k_BT\ln\operatorname{Sp}\exp\left[-\frac{H^*}{k_BT}\right], \tag{8}$$

Here $U_n^{(0)}$ is a structureless term of n-th order in the PP and H^* is the effective Hamiltonian of the ions,

$$H^*=H_i+\sum_n\sum_{m=2}^{n}U_n^{(m)},$$

where $U_n^{(m)}$ is the potential energy of the indirect ion-ion interaction of n-th order in the PP, and describes the irreducible m-particle interaction.

Simultaneously with the change from Ω to F it is necessary to carry out in all terms of (8) a renormalization of the CP. We use for this purpose the expansion (2) and write

$$\langle N_e\rangle=-\sum_{n=0}^{\infty}\left\langle\frac{\partial\Omega_e^{(n)}}{\partial\mu_e}\right\rangle,$$

where the angle brackets denote the statistical-averaging operation. On the other hand, μ_e is determined from the relation

$$\langle N_e\rangle=-\left\langle\frac{\partial\Omega_e^{(0)}}{\partial\mu_e}\right\rangle_{\mu_e=\mu_e^{(0)}},$$

where $\mu_e^{(0)}$ is the CP of the electrons in the absence of ions, given T, V, and N_e. From the last two equations we obtain the renormalized CP. In second order in the PP, which we shall need hereafter, we obtain the CP shift

$$\Delta\mu_e^{(2)}=-\frac{1}{2Vv_0\pi(0)}\sum_{\mathbf{k}\neq 0}\frac{\partial\pi(\mathbf{k})}{\partial\mu_e^{(0)}}\left|\frac{w_0(\mathbf{k})}{\varepsilon(\mathbf{k})}\right|^2S(\mathbf{k}), \tag{9}$$

where $S(\mathbf{k})$ is the static structure factor of the ions.

We obtain now the equation of state of a liquid metal, accurate to terms quadratic in PP. To this end, we differentiate the free energy (8) with respect to volume. The derivative of the first term yields the electronic contribution to the pressure, which can be expressed in terms of the polarization operator (see Ref. 5). The derivative of the second term is obtained directly. When finding the derivatives of the last two terms it is necessary to take into account also the implicit volume dependence, which can be obtained with the aid of a similarity transformation.[5,9] We obtain thus

$$P=\frac{k_BT}{v_0}+\frac{n_e^2}{2\pi(0)}+\frac{bz}{v_0^2}+\frac{1}{2(2\pi)^3v_0}\int d\mathbf{k}\,S(\mathbf{k})\left[\varphi(\mathbf{k})+k_x\frac{\partial\varphi}{\partial k_x}+n_e\frac{\partial\varphi}{\partial n_e}\right]-\frac{1}{2}\int_0^{n_e}n_e^2\frac{\partial}{\partial n_e}\left[\frac{1}{\pi(0)}\right]dn_e, \tag{10}$$

where n_e is the electron density and z is the valence of the metal. Here $\varphi(\mathbf{k})$ is the Fourier transform of the paired ion-ion potential in the approximation quadratic in the PP:

$$\varphi(\mathbf{k})=\frac{4\pi z^2e^2}{\mathbf{k}^2}-\frac{\pi(\mathbf{k})|w_0(\mathbf{k})|^2}{\varepsilon(\mathbf{k})}. \tag{11}$$

Not counting the kinetic contribution (k_BT/v_0), expression (10) is equivalent to the equation of state of the metal in the crystalline phase,[5] the only difference being that summation over the reciprocal-lattice vectors is replaced by integration with respect to $\mathbf{k}$, with a statistical weight $S(\mathbf{k})$ that takes into account the presence of short-range order in the system.

We shall use Eq. (10) later to obtain the Cauchy relation.

3. MICROSCOPIC DETERMINATION OF THE STRESS TENSOR

It can be shown[12] that the high-frequency elastic moduli and constants of liquids are expressed in terms of equal-time correlation functions of the Fourier transforms of the components of the microscopic stress tensor $\sigma^{\alpha\beta}(\mathbf{q})$. In standard notation[15]

$$c_{11}=\frac{1}{Vk_BT}\lim_{\mathbf{q}\to 0}\langle\sigma^{zz}(-\mathbf{q})\sigma^{zz}(\mathbf{q})\rangle, \tag{12}$$

$$c_{12}=\frac{1}{Vk_BT}\lim_{\mathbf{q}\to 0}\langle\sigma^{zz}(-\mathbf{q})\sigma^{xx}(\mathbf{q})\rangle, \tag{13}$$

$$c_{44}=\frac{1}{Vk_BT}\lim_{\mathbf{q}\to 0}\langle\sigma^{zx}(-\mathbf{q})\sigma^{zx}(\mathbf{q})\rangle. \tag{14}$$

For isotropic media, such as liquids, only two of the constants corresponding to the two possible types of deformation, compression (tension) and shear, are independent. To find the components $\sigma^{\alpha\beta}(\mathbf{q})$ we write down the microscopic expression for the momentum flux density vector in the Fourier representation

$$j^\alpha(\mathbf{q})=\sum_{i=1}^{N_i}mv_i^\alpha e^{-i\mathbf{q}\mathbf{R}_i}$$

(m is the particle mass, v_i^α is the α-th component of the velocity of the i-th particle) and obtain the time dependence of $j^\alpha(\mathbf{q})$:

$$\frac{\partial j^\alpha(\mathbf{q})}{\partial t}=\sum_{l=1}^{N_t}\left(-\frac{\partial U}{\partial R_l^\alpha}-imq^\beta v_l^\alpha v_l^\beta\right)e^{-i\mathbf{q}\mathbf{R}_l}. \tag{15}$$

Here $U=U(\mathbf{R}_1,\ldots,\mathbf{R}_{Nt})$ is the potential energy of the system. Representing Eq. (15) in the form

$$\partial j^\alpha(\mathbf{q})/\partial t=iq^\beta\sigma^{\alpha\beta}(\mathbf{q}), \tag{16}$$

we obtain the microscopic definition of the stress tensor. For systems with paired central interaction, the problem of finding $\sigma^{\alpha\beta}$ (in the coordinate representation) was solved in Ref. 16. For liquid metals, we take into account besides the paired interactions also the multiparticle interactions and carry out the analysis in the Fourier representation, inasmuch as in this representation[5] one can obtain the explicit form of $U(\mathbf{R}_1,\ldots,\mathbf{R}_{Nt})$. According to (4) and (5), the potential energy (with the constant term excluded) is represented by a sum of irreducible paired, triple, etc. interactions:

$$U(\mathbf{R}_1,\ldots,\mathbf{R}_{N_i})=\sum_{n=2}^{N_i}U_n(\mathbf{R}_1,\ldots,\mathbf{R}_{N_i}), \tag{17}$$

where U_m describes the energy of the n-particle ion-ion interactions. Confining ourselves hereafter, in the calculation of the elastic constants, to the approximation quadratic in PP, we can easily establish that, with the required accuracy, it suffices to retain in (17) the terms U_2, U_3, and U_4. With the aid of (4) and (5) we obtain

$$\begin{aligned}U_2=\frac{1}{2}\sum_{l_1l_2}{}'\frac{1}{V}\sum_{\mathbf{k}_1}\Big[\varphi(\mathbf{k}_1)&+\frac{2}{V}\sum_{\mathbf{k}_2}\tilde{\Lambda}_3(\mathbf{k}_1,\mathbf{k}_2,-\mathbf{k}_1-\mathbf{k}_2)\\&-\frac{2}{v_0}\tilde{\Lambda}_3(\mathbf{k}_1,-\mathbf{k}_1,0)-\frac{6}{v_0V}\sum_{\mathbf{k}_2}\tilde{\Lambda}_4(\mathbf{k}_1\ \mathbf{k}_2,-\mathbf{k}_1-\mathbf{k}_2,0)\\&+\frac{3}{v_0^2}\tilde{\Lambda}_4(\mathbf{k}_1,-\mathbf{k}_1,0,0)\Big]\exp[-i\mathbf{k}_1(\mathbf{R}_{l_1}-\mathbf{R}_{l_2})]\equiv\frac{1}{2}\sum_{l_1l_2}{}'\Phi_2(\mathbf{R}_{l_1}-\mathbf{R}_{l_2}),\end{aligned} \tag{18}$$

$$\begin{aligned}U_3=\frac{1}{3}\sum_{l_1l_2l_3}{}'\frac{1}{V^2}\sum_{\mathbf{k}_1\mathbf{k}_2}\Big\{&\tilde{\Lambda}_3(\mathbf{k}_1,\mathbf{k}_2,-\mathbf{k}_1-\mathbf{k}_2)-\frac{3}{v_0}\tilde{\Lambda}_4(\mathbf{k}_1,\mathbf{k}_2,-\mathbf{k}_1-\mathbf{k}_2,0)\\&+\frac{9}{4V}\sum_{\mathbf{k}_3}[\tilde{\Lambda}_4(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,-\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3)+\tilde{\Lambda}_4(\mathbf{k}_1,\mathbf{k}_2-\mathbf{k}_3,\mathbf{k}_3,-\mathbf{k}_1-\mathbf{k}_2)]\Big\}\\&\times\exp[-i\mathbf{k}_1(\mathbf{R}_{l_1}-\mathbf{R}_{l_3})-i\mathbf{k}_2(\mathbf{R}_{l_2}-\mathbf{R}_{l_3})]\equiv\frac{1}{3!}\sum_{l_1l_2l_3}{}'\Phi_3(\mathbf{R}_{l_1},\mathbf{R}_{l_2},\mathbf{R}_{l_3}),\end{aligned} \tag{19}$$

$$\begin{aligned}U_4=\frac{1}{4}\sum_{l_1\ldots l_4}{}'\frac{1}{V^3}\sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}&\tilde{\Lambda}_4(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,-\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3)\\\times\exp[-i\mathbf{k}_1(\mathbf{R}_{l_1}-\mathbf{R}_{l_4})-i\mathbf{k}_2(\mathbf{R}_{l_2}-\mathbf{R}_{l_4})&-i\mathbf{k}_3(\mathbf{R}_{l_3}-\mathbf{R}_{l_4})]\equiv\frac{1}{4!}\sum_{l_1\ldots l_4}{}'\Phi_4(\mathbf{R}_{l_1},\ldots,\mathbf{R}_{l_4}).\end{aligned} \tag{20}$$

The succeeding transformations consist of successively substituting expressions (18)–(20) in (15) and separating $\sigma^{\alpha\beta}(\mathbf{q})$ in accord with (16). Carrying out this substitution and recognizing that we are interested in the limit of small $\mathbf{q}$, we obtain after changing from summation to integration the contributions made to $\sigma^{\alpha\beta}(\mathbf{q})$ by the n-particle interactions in the form

$$\begin{aligned}\sigma_n^{\alpha\beta}(\mathbf{q})=\frac{1-n}{2n}\frac{1}{(2\pi)^{3(n-1)}}\int d\mathbf{k}_1\ldots\int d\mathbf{k}_{n-1}\Big\{&\frac{\partial}{\partial k_1^\beta}[k_1^\alpha\Phi_n(\mathbf{k}_1,\ldots,\mathbf{k}_{n-1})]\\&+\frac{\partial}{\partial k_1^\alpha}[k_1^\beta\Phi_n(\mathbf{k}_1,\ldots,\mathbf{k}_{n-1})]\Big\}\sum_{l_1\ldots l_n}{}'\exp[-i\mathbf{k}_1(\mathbf{R}_{l_1}-\mathbf{R}_{l_n})-\ldots\\&-i\mathbf{k}_{n-1}(\mathbf{R}_{l_{n-1}}-\mathbf{R}_{l_n})-i\mathbf{q}\mathbf{R}_{l_n}],\quad n\geqslant2,\end{aligned} \tag{21}$$

where $\Phi_n(\mathbf{k}_1,\ldots,\mathbf{k}_{n-1})$ is the Fourier transform of the potential of the n-particle interaction.

4. ELASTIC MODULI AND GENERALIZED CAUCHY RELATION

The elastic constants for liquids are defined as the coupling coefficients between the rate of change of the microscopic stress tensor and the microscopic strain-rate tensor $\Lambda^{\gamma\delta}(\mathbf{q})$ (Ref. 12):

$$\dot{\sigma}^{\alpha\beta}(\mathbf{q})=c^{\alpha\beta\gamma\delta}(\mathbf{q})\Lambda^{\gamma\delta}(\mathbf{q}). \tag{22}$$

The macroscopic constants are obtained from $c^{\alpha\beta\gamma\delta}(\mathbf{q})$ by taking the limit as $\mathbf{q}\to0$. Multiplying (22) by $\Lambda^{\lambda\mu}(-\mathbf{q})$ and averaging over phase space, we obtain

$$\langle\Lambda^{\lambda\mu}(-\mathbf{q})\dot{\sigma}^{\alpha\beta}(\mathbf{q})\rangle=c^{\alpha\beta\gamma\delta}(\mathbf{q})\langle\Lambda^{\lambda\mu}(-\mathbf{q})\Lambda^{\gamma\delta}(\mathbf{q})\rangle. \tag{23}$$

The correlator in the right-hand side of (23) is calculated directly, and the left-hand side can be determined by substituting in it (21). To average over the ion coordinates, we introduce the multiparticle distribution functions.[10] With their aid, the left-hand side of (23) is expressed in terms of the Fourier transform of the two-, three-, and four-particle distribution functions. Separating the irreducible parts of the latter, we easily verify that after taking the limit as $\mathbf{q}\to0$ there remain, in the approximation quadratic in the PP, only the contributions from the irreducible second-order distribution function. Adding the kinetic contribution to the stress tensor [the second term of (15)], we obtain ultimately for the elastic constants

$$c_{11}=\frac{3k_BT}{v_0}+\frac{\varphi(0)}{v_0^2}+\frac{1}{(2\pi)^3v_0}\int d\mathbf{k}\,S(\mathbf{k})\left[\varphi(\mathbf{k})+2k_x\frac{\partial\varphi}{\partial k_x}+\frac{1}{2}k_x^2\frac{\partial^2\varphi}{\partial k_x^2}\right]+\Delta c, \tag{24}$$

$$\begin{aligned}c_{12}=\frac{k_BT}{v_0}+\frac{\varphi(0)}{v_0^2}+\frac{1}{(2\pi)^3v_0}\int d\mathbf{k}\,S(\mathbf{k})\Big[&\varphi(\mathbf{k})\\&+\frac{3}{2}k_x\frac{\partial\varphi}{\partial k_x}+\frac{1}{2}k_xk_y\frac{\partial^2\varphi}{\partial k_x\partial k_y}\Big]+\Delta c,\end{aligned} \tag{25}$$

$$c_{44}=\frac{k_BT}{v_0}+\frac{1}{2(2\pi)^3v_0}\int d\mathbf{k}\,S(\mathbf{k})k_x^2\frac{\partial^2\varphi}{\partial k_y^2}, \tag{26}$$

where Δc is the correction to the elastic constants to account for the multiparticle forces:

$$\begin{aligned}\Delta c=\frac{1}{(2\pi)^3v_0}\int d\mathbf{k}\,S(\mathbf{k})\Big[&4\tilde{\Lambda}_3(\mathbf{k},-\mathbf{k},0)\\&+2k_x\frac{\partial\tilde{\Lambda}_3(\mathbf{k},-\mathbf{k},0)}{\partial k_x}+\frac{3}{v_0}\tilde{\Lambda}_4(\mathbf{k},-\mathbf{k},0,0)\Big].\end{aligned} \tag{27}$$

It is easy to verify that the following relation holds

$$c_{44}={}^1/_2(c_{11}-c_{12}), \tag{28}$$

as should be the case for isotropic media.

If Eqs. (24)–(26) are compared with the corresponding expressions for metals in the crystalline phase, then it turns out that, just as in the case (10), for solid metals the integration with respect to $\mathbf{k}$ with the weight function $S(\mathbf{k})$ is replaced by summation over the reciprocal-lattice vectors. The relation (28), however, does not hold for crystals.

Equations (24)–(26) make it possible to obtain the contribution of multiparticle interactions to the high-frequency elastic moduli. The moduli K and G are connected with the elastic constants by the relations

$$K={}^1/_3(c_{11}+2c_{12}),\quad G={}^1/_2(c_{11}-c_{12})\equiv c_{44}. \tag{29}$$

Substituting (24)–(26) in (29) and comparing with (10) we obtain the generalized Cauchy relation

$$\begin{aligned} K-\frac{5}{3}G=2\Big\{&P-\frac{k_BT}{v_0}+\frac{1}{2}\int\limits_0^{n_e} n_e^2\frac{\partial}{\partial n_e}\left[\frac{1}{\pi(0)}\right]dn_e\Big\}\\ &-\frac{n_e}{(2\pi)^3v_0}\int d\mathbf{k}\,S(\mathbf{k})\Big\{\frac{\partial}{\partial n_e}\left[\frac{\pi(\mathbf{k})}{\varepsilon(\mathbf{k})}\right]|w_0(\mathbf{k})|^2\\ +k_x\frac{\partial}{\partial k_x}&\left(\frac{\partial}{\partial n_e}\left[\frac{\pi(\mathbf{k})}{\varepsilon(\mathbf{k})}\right]|w_0(\mathbf{k})|^2\right)+\frac{1}{2}|w_0(\mathbf{k})|^2 n_e\frac{\partial^2}{\partial n_e^2}\left[\frac{\pi(\mathbf{k})}{\varepsilon(\mathbf{k})}\right]\Big\}. \end{aligned} \tag{30}$$

To obtain (30) we used identities for multipoles Λ_n for the case when some of the arguments vanish, and took into account also the renormalization (9) of the CP.

5. DISCUSSION OF RESULTS

Comparison of (30) and (1) shows that there are two causes of the violation of the Cauchy relation (1) in liquid metals: the first is connected with the presence in the metal of an electron subsystem (the integral with respect to density in (30), and the second is connected with the dependence of the effective ion-ion interaction on the density.

The analysis of expressions (24)–(26) for the elastic constants (and for the corresponding moduli) is similar to the analysis in the case of solid metals,[5] and we shall not repeat it here. We note only circumstances that are typical of liquid metals.

The estimate of the contribution of the metal particle interactions to the Cauchy relation depends on the possibility of independently determining the left- and right-side of (30). The existing electron-gas models allow a sufficiently accurate calculation of the integrals in (30), and the static structure factor $S(\mathbf{k})$ can be taken from data on neutron scattering by liquid metals. The elastic moduli, in principle, can also be obtained from neutron experiments, in which the dynamic structure factor of the metal $S(\mathbf{k}, \omega)$ is determined, since it is known that K and G are defined in terms of the long-wave limits of the frequency moments $S(\mathbf{k}, \omega)$.[17] The numerical calculations are made difficult, however, by the fact that the results of experiments aimed at determining $S(\mathbf{k}, \omega)$ are usually represented not in tabulated but in graphic form, and the accuracy of the latter is low. Another possibility of estimating K and G is to use the results of computer experiments–the molecular dynamics (MD) method. Many calculations of the properties of liquids have by now been calculated by the MD method. They show that in liquids there can propagate short-wave perturbations (including shear waves), i.e., collective excitations similar to phonons in crystals.[18,19] However, all the calculations for liquid metals were carried out in the paired-interaction approximation. It appears that MD experiments with allowance for multiparticle interactions would be advisable. We note that for nonconducting liquids such as argon, such calculations are available, although the three-particle potential for argon is known only in asymptotic form (at large distances), whereas for metals it can be calculated with high accuracy.

As already indicated, the elastic moduli are determined in terms of the second and fourth frequency moments $S(\mathbf{k}, \omega)$. The renormalization of K and G on account of multiparticle interactions means renormalization of the corresponding moments $S(\mathbf{k}, \omega)$. At the present time one of the principal methods of studying the microdynamics of liquids is the reconstruction of the dynamic structure factor from its moments. A renormalization of the moments $S(\mathbf{k}, \omega)$ means that in principle it is possible to find the contribution of multiparticle interactions to all types of collective motions in liquids, and also to the kinetic coefficients (viscosity, self-diffusion), which are defined in terms of $S(\mathbf{k}, \omega)$. This question will be considered in a separate paper.

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