

negative at room temperature and changes sign in the vicinity of 170°K, i.e., quite remote from 106°K.

The E and G moduli of polycrystalline Sm are shown in Fig. 7. Their temperature dependence is strikingly similar to that of the elastic moduli and ultrasonic attenuations of Pr (Figs. 1–3). The appearance of a lattice softening in both Pr and Sm is probably due to a common mechanism.

With decreasing temperature, from the ambient, the elastic moduli of Sm (Fig. 7) increase in a normal manner and subsequently form a broad maximum. In this temperature region, K_s (Fig. 8) develops a rather wide hump peaked at 109°K. With further decrease in temperature, K_s exhibits a dip at 70°K. The peak in K_s at 109°K is consistent with the occurrence of anomalies in the vicinity of this temperature in the electrical resistivity,¹⁵ heat capacity,²¹ and other physical properties. The nature of these anomalies was not firmly established.^{19,24} Additional evidence for the similarity in behavior of the elastic moduli in both Pr and Sm is the temperature variation of the α_l and α_t wave attenuations. In Sm (Fig. 9), as in Pr (Fig. 3), α_l displays a

peak, whereas α_t shows a smooth behavior in the temperature region in which the adiabatic compressibilities (Figs. 2 and 8) are anomalous. As was speculated for Pr, these anomalies and the accompanying lattice softening in Sm may be due to an electron-type transition or to temperature-dependent crystallographic change.

The sharp minimum in the elastic moduli of Sm (Fig. 7) at 14°K and the corresponding anomalies observed in the compressibility (Fig. 8) and ultrasonic attenuations (Fig. 9) are characteristic of a magnetic-ordering point. This is in agreement with the behavior of other physical properties of Sm.^{3,15,21}

The temperature dependence of Θ_D of Sm is shown in Fig. 8. The limiting Θ_D , at absolute zero, for the antiferromagnetic phase is 169°K.

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Moment-Conserving Decoupling Procedure for Many-Body Problems

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A new, well-defined procedure for linearizing double-time, statistical Green's functions is proposed. The resultant spectral function automatically conserves the first several frequency moments. This compares very favorably with the usual mean-field decoupling results, which conserve only the first (and, rarely, up to three) frequency moments.

THE Green's function method has been widely used in the study of equilibrium as well as nonequilibrium properties of interacting many-body systems.¹ Since exact solutions to these problems (except for a few one- and two-dimensional cases) can in general not be obtained, approximations have to be introduced. The approximation procedures fall into two distinct categories: (i) The first is the diagrammatic expansion,² which aims at calculating the spectral function to any desired accuracy whenever a perturbation approximation is meaningful; or which are designed to sum a selected subset of the total set of diagrams to many (and possibly infinite) orders when perturbation approxima-

tion itself is not appropriate. (ii) The second category is the Green function or equation of motion decoupling procedure. This consists of self-consistent mean-field approximations, which can often (especially for fermion or boson systems) be interpreted in terms of diagrams but the primary motivation for which is provided by their heuristic simplicity.

The difficulty with the usual decoupling procedures is that they are crude and often they do not lead to a very accurate description of the elementary excitation spectrum of the system. As the structure of the elementary excitation spectrum is embodied in the frequency-wave-vector dependence of the spectral function, the simple decouplings do not lead to accurate representation of the spectral function. Consequently, the frequency moments of the spectral function calculated via the usual mean-field decoupling procedures are not accurately reproduced.

To improve on this situation, we propose a new decoupling scheme which is well defined and which

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¹ D. N. Zubarev, *Usp. Fiz. Nauk* **71**, 71 (1960) [English transl.: *Soviet Phys.—Usp.* **3**, 320 (1960)].

² See, for example, R. D. Mattuck, *A Guide to Feynman Diagrams in the Many-Body Problem* (McGraw-Hill Book Co., New York, 1967).

automatically preserves the first several (or more, if desired) moments of the spectral function. The method is best illustrated by considering simple examples.

Consider first the spin- $\frac{1}{2}$ Ising model with Hamiltonian

$$\mathcal{H} = -\frac{1}{2} \sum_{f_1} \sum_{f_2} I(f_1 f_2) S_{f_1}^z S_{f_2}^z - \mu \sum_f S_f^z. \quad (1)$$

Here $I(ff) = 0$. In the usual notation¹ the equation of motion of the commutator-retarded Green's function of $S_{\sigma}^+(t)$ and $S_{\sigma}^-(t')$ is

$$(E - \mu)G(E) = (\sigma/\pi) + \Gamma(E), \quad (2)$$

$$\Gamma(E) = \sum_f I(fg) \langle\langle S_f^z S_{\sigma}^+; S_{\sigma}^- \rangle\rangle_{(E)}. \quad (3)$$

The usual random-phase-approximation (RPA) decoupling is to ignore the fluctuations of S_f^z around its statistical average σ , i.e.,

$$\Gamma(E) \approx \sigma G(E) \sum_f I(fg) = \sigma J(0)G(E). \quad (4)$$

$G(E)$ is now readily found, and its spectral function $F(\omega)$ is

$$F(\omega) \underset{\text{RPA}}{\approx} 2\sigma \delta(\omega - \omega_0), \quad (5)$$

$$\langle\langle S_{\sigma}^+(t), S_{\sigma}^-(t') \rangle\rangle = \int_{-\infty}^{+\infty} F(\omega) e^{-i\omega(t-t')} d\omega, \quad (6)$$

$$\omega_0 = \mu + \sigma J(0).$$

The $(n+1)$ th frequency moments of the spectral functions, i.e.,

$$\lim_{t \rightarrow t'} \left\langle \left[\left(\frac{d}{dt} \right)^{n-p} S_{\sigma}^+(t), \left(-i \frac{d}{dt'} \right)^p S_{\sigma}^-(t') \right] \right\rangle = \int_{-\infty}^{+\infty} F(\omega) \omega^n d\omega \equiv \tilde{\omega}^{n+1}, \quad (7)$$

are now easily calculated from the equations of motion of S_{σ}^{\pm} and the exact results as well as the RPA prediction using Eq. (5) are

$$\tilde{\omega}^1 = 2\sigma, \quad \tilde{\omega}^2 = 2(a + \mu\sigma), \quad \tilde{\omega}^3 = 2(b + 2\mu a + \mu^2\sigma), \quad (8)$$

$$\tilde{\omega}^4 = 2[c + 3\mu b + 3\mu^2 a + \mu^3\sigma], \quad \tilde{\omega}^{n+1} \underset{\text{RPA}}{=} 2\sigma(\omega_0)^n,$$

$$a = \sum_f I(fg) \langle S_f^z S_{\sigma}^z \rangle,$$

$$b = \sum_{f_1} \sum_{f_2} I(f_1 g) I(f_2 g) \langle S_{f_1}^z S_{f_2}^z S_{\sigma}^z \rangle, \quad (9)$$

$$c = \sum_{f_1} \sum_{f_2} \sum_{f_3} I(f_1 g) I(f_2 g) I(f_3 g) \langle S_{f_1}^z S_{f_2}^z S_{f_3}^z S_{\sigma}^z \rangle.$$

Thus, the RPA gives only the first moment correctly. To achieve a more accurate $F(\omega)$ we propose to proceed as follows: Find the equation of motion of the Green's function on the right-hand side of the original

equation of motion for $G(t-t')$, i.e.,

$$[E - \mu]\Gamma(E) = a/\pi + \Gamma^{(1)}(E), \quad (10)$$

$$\Gamma^{(1)}(E) = \sum_{f_1} \sum_{f_2} I(f_1 g) I(f_2 g) \langle\langle S_{f_1}^z S_{f_2}^z S_{\sigma}^+; S_{\sigma}^- \rangle\rangle_{(E)}. \quad (11)$$

Now require that $\Gamma^{(1)}(E)$ be represented in terms of the two lower-order Green's functions $G(E)$ and $\Gamma(E)$, i.e.,

$$\Gamma^{(1)}(E) = AG(E) + B\Gamma(E). \quad (12)$$

Choose the coefficients A and B so as to preserve the first two frequency moments of the spectral function for $\Gamma^{(1)}(E)$. This gives

$$b = A\sigma + Ba, \quad (\mu b + c) = A(\mu\sigma + a) + B(\mu a + b). \quad (13)$$

These conditions completely specify the unknowns A and B .

$$A = (ac - b^2)/(a^2 - b\sigma), \quad B = (ab - c\sigma)/(a^2 - b\sigma). \quad (14)$$

Insert the decoupling Eq. (12) into Eqs. (2) and (10) and find $G(E)$

$$G(E) = \frac{1}{\pi} \frac{\sigma(E - \mu - B) + a}{(E - \mu)(E - \mu - B) - A}. \quad (15)$$

The spectral function given by Eq. (15) is found to yield the first four moments correctly.

Before proceeding to the study of another physical system (with more interesting time-dependent properties), two things should be emphasized. Firstly, with the above approach we have been able to construct a more accurate Green's function (or equivalently, the spectral function) given the knowledge of the first few frequency moments, which are in themselves time-independent quantities. [Note, that in fact we do find two independent relations between the four unknowns σ , a , b , and c from Eqs. (15) and (2). Therefore, we need to calculate (by conventional methods, such as the high-temperature or the low-temperature series expansions, etc.) only two additional relations for these four quantities.]

For our next example, we choose the case of a system of correlated electrons forming a narrow s band.³ In the notation of Ref. 3, the Green's function equations of motion are

$$EG_{\sigma p}^{\sigma}(E) = \frac{\delta_{\sigma p}}{2\pi} + \sum_f T_{\sigma f} G_{f p}(E) + i\Gamma_{\sigma p}^{\sigma}(E), \quad (16)$$

$$\Gamma_{\sigma p}^{\sigma}(E) [E - I - T_0] - \frac{n_{-\sigma}}{2\pi} \delta_{\sigma, p}$$

$$= \sum_{f \neq \sigma} T_{\sigma f} \langle\langle n_{\sigma-\sigma} C_{f\sigma}; C_{p\sigma}^{\dagger} \rangle\rangle_E$$

$$+ \sum_f T_{\sigma f} \langle\langle C_{\sigma-\sigma}^{\dagger} C_{f-\sigma} C_{\sigma\sigma}; C_{p\sigma}^{\dagger} \rangle\rangle_E$$

$$- \langle\langle C_{f-\sigma}^{\dagger} C_{\sigma-\sigma} C_{\sigma\sigma}; C_{p\sigma}^{\dagger} \rangle\rangle_E. \quad (17)$$

³ J. Hubbard, Proc. Roy. Soc. (London) **A276**, 238 (1963).

Here, for convenience we shall put $T_{g\sigma} = T_0 = 0$. Hubbard³ approximated the terms on the right-hand side of Eq. (17) by $n_{-\sigma} \sum_f T_{gf} G_{fp}^\sigma(E)$. This approximation is reasonable [i.e., much better than the Hartree-Fock approximation, $\Gamma_{gp}^\sigma(E) \sim \sigma G_{gp}^\sigma(E)$], and it conserves the first three frequency moments of the spectral function for the Green's function $G_{gp}^\sigma(E)$. However, because of the inherent two-level nature of the problem, i.e., for arbitrary I , the fourth moment is important for determining the dispersion relation and the spectral weights of the elementary excitations.

Following our procedure, we represent the right-hand side of Eq. (17) as

$$= AG_{gp}^\sigma(E) + CT_{gp}^\sigma(E) + \sum_f [B_{gf} G_{fp}^\sigma(E) + D_{gf} \Gamma_{fp}^\sigma(E)]. \quad (18)$$

Let us determine the first two frequency moments of the spectral functions of the Green's functions, multiply them by the appropriate functions A , B , C , and D as given in Eq. (18) above, and require that these moments be identical with the corresponding moments of the actual sum of the Green's functions, including their appropriate coefficients, occurring on the right-hand side of Eq. (17). This procedure completely determines A , B , C , and D .

$$A = -Cn_{-\sigma} = (1 - n_{-\sigma})^{-1} \times \sum_f T_{gf} [\langle C_{f-\sigma}^\dagger C_{g-\sigma} (1 - n_{g\sigma}) \rangle - \langle C_{g-\sigma}^\dagger C_{f-\sigma} n_{g\sigma} \rangle], \quad (19)$$

$$n_{-\sigma} D_{gf} = n_{-\sigma} T_{gf} - B_{gf} = (1 - n_{-\sigma})^{-1} T_{gf} [\langle n_{g-\sigma} n_{f-\sigma} \rangle - n_{-\sigma}^2 + \langle C_{f\sigma}^\dagger C_{f-\sigma} C_{g-\sigma}^\dagger C_{g\sigma} \rangle + \langle C_{f\sigma}^\dagger C_{f-\sigma}^\dagger C_{g\sigma} C_{g-\sigma} \rangle]. \quad (20)$$

Now replacing the terms on the right-hand side of Eq. (17) by those given in Eq. (18) and using Eqs. (19) and (20) we get

$$2\pi G_k^\sigma(E) = [E - I(1 - n_{-\sigma}) + \Delta_k^\sigma] \times [(E - I + \Delta_k^\sigma)(E - T_k) - In_{-\sigma}(T_k + \Delta_k^\sigma)]^{-1}, \quad (21)$$

where $n_{-\sigma} \Delta_{gf}^\sigma = A \delta_{g,f} - n_{-\sigma} D_{gf}$. The Green's function (21) gives the correct fourth moment for its spectral function. Moreover, it reduces to the correct result in

both the exactly soluble limits, i.e., (i) $T_{gf} = 0$ and (ii) $I = 0$.

A more interesting limiting case is that of infinitely strong intra-atomic correlation, i.e., $I \rightarrow \infty$. To the leading order in the ratio (T/I) we get

$$[2\pi G_k^{(\sigma)}(E)]_{I=\infty} = (1 - n_{-\sigma}) [E - T_k(1 - n_{-\sigma}) + n_{-\sigma} \Delta_k^\sigma]^{-1}. \quad (22)$$

It should be noted that in this limit, for $n_\sigma + n_{-\sigma} \leq 1$, the terms

$$\langle C_{g-\sigma}^\dagger C_{f-\sigma} n_{g\sigma} \rangle, \quad \langle C_{f-\sigma}^\dagger C_{g-\sigma} n_{g\sigma} \rangle, \quad \langle C_{f-\sigma}^\dagger C_{g-\sigma} C_{f\sigma}^\dagger C_{g\sigma} \rangle$$

must become vanishingly small (because they are directly proportional to the statistical weights of situations requiring the arrival of two electrons, or two holes, simultaneously at one spatial location—a happening which is energetically very unfavorable).

The pole of the Green's function, although not complex for the case $I = \infty$, occurs at a different energy from the corresponding noninteracting case, i.e., T_k . The renormalization of the spectrum is only partly as predicted by the Hubbard RPA, i.e., like $(1 - n_{-\sigma})$. Rather, there is an additional energy shift, $-n_{-\sigma} \Delta_k^\sigma$. Note also that the energy shift is partly k -independent, i.e., equal to $-A$, (such shifts are sometimes called the band shifts⁴). This band shift arises because of the electron correlations and is obtained self-consistently in terms of the higher moments of the spectral function. Therefore, it has an entirely different origin than that given by Beeby.⁴ Indeed, in this strong correlation limit, the present result is identical to the infinite I elementary excitation spectrum calculated by Harris and Lange.⁵

In conclusion it may be noted that while we have demonstrated the use of the moment-conserving decoupling procedure by applying it only to the second time derivative of the Green's function of interest, the same method can also be used either at a later stage (when the decoupling must be made in terms of all the preceding Green's functions, thus enabling the conservation of even higher number of frequency moments) or at an earlier stage (in which case it simply reduces to the Hartree-Fock type of approximation).

⁴ J. L. Beeby, Proc. Phys. Soc. (London) **90**, 765 (1967).

⁵ A. B. Harris and R. V. Lange, Phys. Rev. **157**, 295 (1967), Eq. (6.9).