[2]W. L. McMillan, Phys. Rev. 167, 331 (1968).
[3]M. Strongin, O. F. Kammerer, J. E. Crow, R. D. Parks, D. H. Douglass, Jr., and M. A. Jensen, Phys. Rev. Letters 21, 1320 (1968); J. M. Dickey and A. Paskin, *ibid.* 21, 1441 (1968).
[4]J. W. Garland, K. H. Bennemann, and F. M. Mueller, Phys. Rev. Letters 21, 1315 (1968).
[5]V. Buckel and R. Hilsch, Z. Physik 132, 420 (1952); 138, 109 (1954).
[6]M. Strongin and O. F. Kammerer, J. Appl. Phys. 39, 2509 (1968).
[7]D. G. Naugle, R. E. Glover, III, and W. Moormann, International Conference on Science of Superconductivity, Stanford University, August, 1969 (unpublished).
[8]Koji Kajimura and Nobuo Mikoshiba, J. Low-Temp. Phys. 4, 331 (1971).
[9]W. E. Masker and R. D. Parks, Phys. Rev. B 1, 2164 (1970).
[10]L. G. Aslamazov and A. I. Larkin, Fiz. Tverd. Tela 10, 1104 (1968)[Soviet Phys. Solid State 10, 875 (1968)].
[11]Richard S. Thompson, Phys. Rev. B 1, 327 (1970).
[12]J. E. Crow, R. S. Thompson, M. A. Klenin, and A. K. Bhatnagar, Phys. Rev. Letters 24, 371 (1970).
[13]R. D. Parks, preprint of talk delivered at the Twelfth International Conference of Low Temperature Physics.
[14]M. Strongin, J. M. Dickey, and J. E. Crow, Solid State Commun. 8, 1647 (1970).

PHYSICAL REVIEW B VOLUME 3, NUMBER 7 1 APRIL 1971

Effects of Phonons and Impurities on Single-Particle-Mode Neutron Scattering in Chromium

J. B. Sokoloff
Physics Department, Northeastern University, Boston, Massachusetts 02115

Contrary to a comment made in a recent paper on inelastic neutron scattering in antiferromagnetic chromium, it is argued here that at low temperatures the electron-phonon interaction does not cause significant broadening of the single-particle-mode peak in the inelastic-neutron-scattering cross section at the gap energy. The addition of vanadium impurities is then suggested as a means of lowering the gap energy in order to make it easier to perform the experiment to observe this peak in the scattering and thus measure the gap energy by neutron diffraction. Estimates are given of the scattering cross section.

In a previous publication[1] (to be referred to as I), it was argued that there should be a peak [actually a singularity of the form $(\omega-\Delta)^{-1/2}$, where Δ is the gap energy] in the inelastic-neutron-scattering cross section for antiferromagnetic chromium metal at neutron energy transfers equal to the gap between the magnetically split hands. In a recent publication, Liu has argued that such a peak will be rendered unobservable when the effects of the electron-phonon interaction are included.[2] It will be shown in this note that although the arguments of Ref. 2 may be possibly valid at room temperature, they are certainly not correct at temperatures far below room temperature, at which not too many phonons exist to scatter electrons. At such low temperatures (e.g., liquid-nitrogen temperature), the results of I are not invalidated by the electron-phonon interaction. A method of lowering the gap energy to make it more easily observable by neutron diffraction will also be discussed.

Reference 2 treats the phonons as impurities, but phonons are different from impurities. For example, whereas there are impurities at all temperatures, there are no phonons at zero temperature. Our treatment of the electron-phonon interaction will follow Abrikosov, Gorkov, and Dzyaloshinski.[3] We find the self-energy of the one-electron Green's function from Eq. (21.26) in Ref. 3,

$$\Sigma(\vec{p},\epsilon)=\frac{g^2}{(2\pi)^4\pi}\int d^3p_1\int_{-\infty}^{\infty}d\omega\int_{-\infty}^{\infty}d\epsilon_1\frac{\mathrm{Im}G(\vec{p}_1,\epsilon_1)\,\mathrm{Im}D(\vec{p}-\vec{p}_1,\omega)}{\omega+\epsilon_1-\epsilon-i\delta}\left[\tanh\left(\frac{\epsilon_1}{2KT}\right)+\coth\left(\frac{\omega}{2KT}\right)\right], \quad (1)$$

where ϵ, ϵ_1, and ω are electron and phonon energies, $\vec{p}$ and $\vec{p}-\vec{p}_1$ are electron and phonon momenta, and G and D are electron and phonon Green's functions, respectively. Since G is a 2×2 matrix for the spin-density wave state, Σ is a 2×2 matrix.

In order to consider the rounding out of the peak at the gap energy in the density of states, following Zittartz,[4] we find the off-diagonal component of Eq. (1). Using Zittartz's one-electron Green's function,[4] we find

$$\Sigma_{\text{off-diag}}(\vec{p},\epsilon)=-\frac{g^2}{(2\pi)^4}\int d^3p_1\int_{-\infty}^{\infty}d\omega\sum_{\alpha=1,2}\frac{\mathrm{Im}D(\vec{p}-\vec{p}_1,\omega)}{\omega+\omega_\alpha(\vec{p}_1)-\epsilon-i\delta}(-1)^\alpha$$

$$\times\left[\tanh\left(\frac{\omega_\alpha(\vec{p}_1)}{2KT}\right)+\coth\left(\frac{\omega}{2KT}\right)\right]\frac{\Delta}{\omega_1(\vec{p}_1)-\omega_2(\vec{p}_1)}\,, \tag{2}$$

where Δ is the gap energy and

$$\omega_\alpha(\vec{p}_1)=\left(\frac{1}{m_a}-\frac{1}{m_b}\right)\xi_1+(-1)^\alpha\left[\xi_1^2\left(\frac{1}{m_a}+\frac{1}{m_b}\right)^2+\Delta^2\right]^{1/2}, \tag{3}$$

where

$$\xi_1=\tfrac{1}{2}(p_1^2-p_0^2)\,,$$

and where m_a and m_b are the effective masses of the bands that interact to produce the spin-density wave. Taking KT equal to zero in Eq. (2) (this is a good approximation if $KT\ll K\theta_D,\Delta$), using Eq. (21.21) in Ref. 3 for $D(\vec{p}-\vec{p}_1,\omega)$, and taking the phonon lifetime equal to zero, we obtain

$$\Sigma_{\text{off-diag}}(\vec{p},\epsilon)=\frac{g^2\pi}{(2\pi)^4}\int d^3p_1\frac{\Delta}{\omega_1(\vec{p}_1)-\omega_2(\vec{p}_1)}\frac{\omega_0^2(\vec{k})}{2\omega(\vec{k})}\left(\frac{1}{\omega(\vec{k})+\omega_2(\vec{p}_1)-\epsilon-i\delta}-\frac{1}{-\omega(\vec{k})+\omega_1(\vec{p}_1)-\epsilon-i\delta}\right), \tag{4}$$

where $\omega_0(\vec{k})$ and $\omega(\vec{k})$ are the bare and renormalized phonon energies, respectively, and $\vec{k}=\vec{p}-\vec{p}_1$. The imaginary part of $\Sigma_{\text{off-diag}}$ is proportional to the difference of two δ functions whose arguments are the energy denominators in Eq. (4). Since neither denominator vanishes if $\epsilon=\Delta$, the imaginary part is zero.

Now we will find the real part of Eq. (4). Following Refs. 3 and 4, we make the following change of variables:

$$\int d^3p_1=\frac{2\pi}{|\vec{p}_1|}\int_0^{k_D}k\,dk\int_{\xi_1(|\vec{p}_1|-k)}^{\xi_1(|\vec{p}_1|+k)}d\xi_1\,. \tag{5}$$

Here we have assumed a Debye cutoff for the phonon wave vector. To simplify the integrals, we replace Eq. (3) by

$$\omega_\alpha(\vec{p}_1)=(-1)^\alpha(\tfrac{1}{2}\Delta-b\xi)\,, \tag{6}$$

where b is a number of order $1/m_a$ or $1/m_b$, and we restrict ξ_1 to have values between $-\epsilon_0/b$ and 0, where $\epsilon_0\gg\Delta$. Then, using Eqs. (5) and (6) and taking $\omega_0(\vec{k})\sim\omega(\vec{k})=vk=\omega$, Eq. (4) becomes

$$\Sigma_{\text{off-diag}}(\vec{p},\epsilon)=-\frac{g^2}{(2\pi)^2}\frac{1}{4pb\,v^2}\int_0^{\omega_D}\omega^2\,d\omega\ln\left|\frac{1}{\omega+\frac{1}{2}\Delta-\epsilon}\right|. \tag{7}$$

In obtaining this result, we assumed $\epsilon_0\gg\Delta\gg\omega_D$ as well as making the assumption (Ref. 3) that the important ω in the integral of Eq. (3) is $\omega\sim\omega_D$. With these assumptions, it was possible to take

$$\Delta/[\omega_1(\vec{p}_1)-\omega_2(\vec{p}_1)]=-1\,,$$

because when p_1 differs from p_0 sufficiently for this not to be true, the integrand in Eq. (4) is of order ω_D/Δ, which we neglect. Performing the integral in Eq. (7), we find

$$\Sigma_{\text{off-diag}}(\vec{p},\epsilon)\approx-\frac{\eta}{8}\frac{k_p^2}{p_0^2}\frac{\omega_D}{3}\ln\frac{\epsilon_0}{\omega_D}+O\left(\frac{\epsilon-\Delta}{\Delta}\right), \tag{8}$$

where η is a constant of order unity given by

$$\eta=g^2p_0m/2\pi^2$$

from under Eq. (21.16) in Ref. 3.

We note that Eq. (8) does not have the sharp energy dependence of the correction to the self-energy operator given in Eq. (32) of Ref. 4. The phonon correction obtained here never becomes large enough to cause the rounding of the peak in the density of states at the gap energy. The correction given by Eq. (8) will renormalize Δ, but will not have a significant effect on the shape of the density of states. Since the peak in the density of states is not rounded out, there is no reason to believe that the neutron-scattering cross section will be rounded out. As is indicated by Ref. 2, the neutron-scattering cross section is not broadened if the density of states is not. In pure chromium for which Δ is about[5] 150 meV and ω_D is about 25 meV, it is reasonable to take $\Delta\gg\omega_D$. Thus, it should be possible to observe a peak at

150 meV in the neutron-scattering cross section of pure chromium at low temperatures, as predicted by I.

Unfortunately, it is at the present time difficult to perform inelastic neutron scattering with an energy transfer of 150 meV. One possible way of getting around this difficulty is to reduce the Néel temperatures, and hence the gap, by adding vanadium impurities to chromium.[6] Although the impurities will lower the gap energy, they will also broaden out the peak in the way predicted by Zittartz.[4]

The inelastic-neutron-scattering cross section for the peak at the gap energy may be estimated using the results of I. We may define a density of interband transitions by

$$\rho(\epsilon) = \frac{1}{N} \sum_{\vec{k}} \delta(\epsilon - D(\vec{k})), \tag{9a}$$

where

$$D(\vec{k}) = \tfrac{1}{2}[\epsilon_a(\vec{k}) - \epsilon_b(\vec{k})], \tag{9b}$$

where ϵ_a and ϵ_b are the energies of the two paramagnetic state bands mixed to form the spin-density wave state, and $\vec{Q}$ is the wave vector of the spin-density wave. Assuming $\rho(\epsilon)$ to be constant between $\epsilon = 0$ and w (the effective bandwidth), and using Eqs. (23), (28b), (53), and (62) of the first paper in Ref. 1, we may estimate the cross section of this peak relative to the total intensity on the spin-wave peak at 50 meV. Taking $w = 1$ eV and assuming a "window" (width of the peak at the gap energy over which we count neutrons) equal to about 20% of the gap energy, we find that the total area under the spin-wave peak at 50 meV is about 12 times greater than the intensity of the single-particle-mode peak at 150 meV. If the gap is reduced to about one-third of this value (which can be attained by adding about 2% vanadium[6]) and if we keep the ratio of the "window" to the gap energy at 20%, the cross section of the single-mode peak will be about cut in half. Since the window is now $\frac{1}{3}$ as large, the sharpness of the peak has not really been reduced. By lowering the gap energy, we gain the advantage of being able to measure the peak more easily because of the greater neutron flux available at low neutron energies. The presence of vanadium impurities, however, will broaden out the peak. We can get an idea of the extent of this broadening by noting that Zittartz[4] has shown that the energy at which the density of states becomes zero is lowered in the presence of impurities from Δ to an energy ω_g given by

$$\omega_g/\Delta = (1 - \alpha^{2/3})^{3/2}, \tag{10}$$

where $\alpha = \Gamma/\Delta$, where Γ is the one-electron level width in the paramagnetic state due to impurity scattering ($\Gamma = \hbar/T$, where T is the electron lifetime). To get the paramagnetic-state residual resistivity, we extrapolate the straight line for higher concentrations in Fig. 4 of Ref. 6 to the concentration 2%, which is the vanadium concentration necessary to lower the gap by a factor of $\frac{1}{3}$. Substituting this resistivity in the Drude formula, we obtain Γ and hence α. Substituting in Eq. (10), we find that $\omega_g/\Delta = 0.6$. The real broadening of the peak is probably not as great as this since the effective width (e.g., width at which the density of states falls to half its maximum value) is probably less. The peak in the neutron scattering should be broadened by about the same amount, as indicated in Ref. 2. Thus when we add vanadium impurities to lower the gap energy, we pay for it in increased broadening of the peak. It should be possible, however, to choose an optimum vanadium concentration with the right experimental setup to do this experiment.

The broadening out of the single-particle-mode peak on the inelastic-neutron-scattering cross section for antiferromagnetic chromium due to the electron-phonon interaction has been shown to have no qualitative effect on the cross section at temperatures far below the Debye temperature. Also an experimental method has been suggested for lowering the gap energy in order to make it more easily observable by neutron diffraction. The fact that our model of the electronic structure of chromium is highly simplified will result in some errors in our estimates, but probably not extremely important errors. The energy-band calculation of Asano and Yamashita shows that the gap is nearly the same for almost all directions of $\vec{k}$ in the Brillouin zone for those Fermi-surface sections wiped out by the gap.[7]

[1] J. B. Sokoloff, Phys. Rev. 185, 770 (1969); 185, 783 (1969).

[2] S. H. Liu, Phys. Rev. B 2, 2664 (1970).

[3] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics*, translated by R. A. Silverman (Prentice-Hall, Englewood Cliffs, N. J., 1963), pp. 176–186.

[4] J. Zittartz, Phys. Rev. 164, 575 (1967).

[5] A. S. Barker, Jr., B. I. Halperin, and T. M. Rice, Phys. Rev. Letters 20, 384 (1968).

[6] A. L. Trego and A. R. Mackintosh, Phys. Rev. 166, 495 (1966).

[7] S. Asano and J. Yamashita, J. Phys. Soc. Japan 23, 714 (1967).