Spin Density Waves in an Electron Gas

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It is shown rigorously that the paramagnetic state of an electron gas is never the Hartree-Fock ground state, even in the high-density—or weak-interaction—limit. The paramagnetic state is always unstable with respect to formation of a static spin density wave. The instability occurs for spin-density waves having a wave vector $Q \approx 2k_F$, the diameter of the Fermi sphere. It follows that the (Hartree-Fock) spin susceptibility of the paramagnetic state is not a monotonic decreasing function with increasing Q, but rather a function with a singularity near $Q=2k_F$. Rather convincing experimental evidence that the antiferromagnetic ground state of chromium is a large-amplitude spin density wave state is summarized. A number of consequences of such states are discussed, including the problem of detecting them by neutron diffraction.

I. INTRODUCTION

AN idealized electron gas—namely, N electrons confined to a box of volume V and having a uniform, rigid background of positive charge to guarantee electrical neutrality—has been the subject of much theoretical study during the past thirty years. The elementary theory is the Hartree-Fock (HF) approximation, which defines the best N-electron wave functions that can be written as a single Slater determinant of one-electron wave functions. HF states have almost always been employed as the N-electron basis functions for further refinements of the theory. In any event, the nature of the HF ground state is of some interest.

Traditionally, the belief has been that an electron gas can have either a paramagnetic or ferromagnetic HF ground state, depending on the electron density, $n=N/V$. The paramagnetic state is a Slater determinant of plane waves, having occupied all one-electron states with wave vector $\mathbf{k}$ lying within a Fermi sphere of radius k_F, for both spin states. The HF energy per electron of the paramagnetic state is

$$(W/N)_p = (3\hbar^2 k_F^2/10m) - (3e^2 k_F/4\pi), \quad (1)$$

the sum of the kinetic energy and the exchange energy. The relation between n and k_F is

$$n = k_F^3/3\pi^2. \quad (2)$$

The ferromagnetic state for an electron gas of identical density is a Slater determinant having all electron states within a sphere of radius $2^{1/3}k_F$ occupied, but only for spin up, say. The HF energy per electron of the ferromagnetic state is

$$(W/N)_f = 2^{2/3}(3\hbar^2 k_F^2/10m) - 2^{1/3}(3e^2 k_F/4\pi). \quad (3)$$

A comparison of Eqs. (1) and (3) indicates that the ferromagnetic state has lower energy than the paramagnetic state when

$$k_F < 5me^2/(2^{1/3}+1)2\pi\hbar^2 \approx 0.66\times 10^8 \text{ cm}^{-1}. \quad (4)$$

Consequently, a high-density electron gas would be paramagnetic and a low-density one would be ferromagnetic. This criterion was first derived by Bloch.[1] The ferromagnetic state considered above is completely polarized. Partially polarized states must also be compared, but one can easily show that they always have higher energy than the smaller of (1) and (3). If the electron density is extremely low, Wigner[2] has shown that a HF state with electrons localized near lattice positions would have lower energy than (3). The system, then, could no longer be described as an electron gas.

In Sec. III it will be shown, contrary to general belief, that the paramagnetic state is never the HF ground state. Specifically, the paramagnetic state is always unstable with respect to formation of a static spin-density wave (SDW). In fact, the instability is sufficiently great that a general proof valid even in the high-density—or weak-interaction—limit can be constructed. A low-density electron gas will still be ferromagnetic (in the HF approximation), but the critical density will be smaller than that corresponding to (4). It seems safe to presume that the HF ground state is indeed a SDW state (except for the low-density ferromagnetic range) although, strictly speaking, all that has been proved is that is has lower energy than the historical HF "ground state."

The SDW instability of an electron gas in the HF approximation has been pointed out earlier[3] by the writer, although the demonstration given there was, for the sake of simplicity, limited to a one-dimensional gas. The original surmise had arisen from a study of a three-dimensional electron gas, similar to that presented here in Sec. III. Several authors[4,5] have suggested that such HF instabilities cannot occur in the three-dimensional case, either generally or for weak interactions. However, their arguments have neglected the wave-vector dependence of exchange interactions characteristic of Coulomb forces. It is true that SDW instabilities are less general in three dimensions that in one, e.g., they are never ground states for δ-function interactions in three dimensions.[6] So considerable care is required to

[1] F. Bloch, Z. Physik **57**, 545 (1929).

[2] E. P. Wigner, Trans. Faraday Soc. **34**, 678 (1938).

[3] A. W. Overhauser, Phys. Rev. Letters **4**, 462 (1960).

[4] W. Kohn and S. J. Nettel, Phys. Rev. Letters **5**, 8 (1960).

[5] A. Yoshimori, Phys. Rev. **124**, 326 (1961).

[6] This question has been investigated partially by Yoshimori (see reference 5) who studied the instability resulting from δ-func-

establish the nature of the ground state in any particular case. It is necessary to emphasize that a consideration of only small deviations from the paramagnetic state is not sufficient for establishing the stability of that state. For example, the critical electron density corresponding to (4) is 35% larger than the critical density that would have been obtained if only small ferromagnetic deviations from the paramagnetic state were tested.

Of course, the ultimate question of physical interest is the nature of the true ground state of an electron gas. Until methods are developed which do not depend on a prejudgment of the final outcome, recourse to experimental behavior can serve as a guide, even though real metals do not conform to the idealized model. Correlation corrections will tend to suppress SDW's just as they tend to suppress ferromagnetism. Therefore it is not surprising that almost all metals appear to have paramagnetic ground states. But there are some exceptions. Considerable experimental evidence indicates that the antiferromagnetic ground state of chromium is just a large amplitude SDW state. This is discussed in Sec. VIII. The recently discovered anomalies in the magnetic susceptibilities of vanadium[7] and molybdenum[8] may also arise from a SDW transition. The susceptibility maximum observed near 100°K in palladium[9] is another candidate. A SDW of small amplitude would have very minor physical manifestation, so the (remote) possibility of a more frequent occurrence cannot be easily ruled out on the basis of existing experimental evidence.

In the following section the nature of a SDW in the HF approximation will be elaborated. It will be assumed that the reader is familiar with HF theory. The usual derivation of the HF equations does not require that the one-electron functions be separable into products of pure space and pure spin functions, although such a factorization has almost always been imposed. This unnecessary constraint must be dropped in order to allow a treatment of spiral SDW's.

II. NATURE OF A SPIN DENSITY WAVE

Exchange interactions arising from repulsive forces always favor the parallel alignment of spins. Partial or complete ferromagnetic polarization of an electron gas increases the magnitude of the exchange energy. However the cost, in terms of increased kinetic energy, is very high. Ferromagnetic polarization introduces a long-range parallelism of spins as well as a short range, but it is the latter that is more important with respect to the exchange energy. It is not unreasonable, then, to consider states of an electron gas which have a net fractional spin polarization $\mathbf{P}(\mathbf{r})$ at every point, but with the direction of $\mathbf{P}$ varying continuously with position. A spiral SDW is the simplest example:

$$\mathbf{P}=P(\mathbf{x}\cos Qz+\mathbf{y}\sin Qz). \tag{5}$$

The axis $\mathbf{Q}$ of the SDW, taken here to be the $\mathbf{z}$ direction, need not be perpendicular to the plane of polarization defined by the unit vectors $\mathbf{x}$ and $\mathbf{y}$. No generality is lost, however, by considering this special case. It should be noted that (5) describes a static polarization, the phase and amplitude of the wave being independent of time.

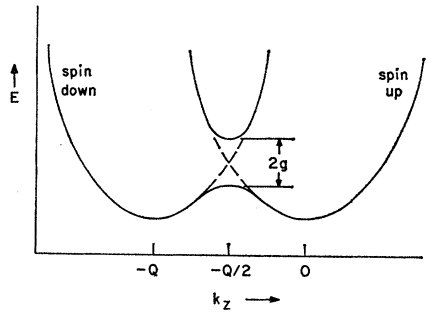

FIG. 1. Single-particle energy level spectrum for a spiral spin density wave. The spin-down branch has been displaced Q to the left of the spin-up branch in order that the unperturbed states coupled by the SDW exchange potential have the same abscissa. Only lower branch states will be occupied in a SDW ground state.

As will be shown below, a spin polarization of the form (5) leads to an off-diagonal contribution A'' to the one electron exchange potential $A\equiv A'+A''$,

$$A=A'-g\boldsymbol{\sigma}\cdot(\mathbf{x}\cos Qz+\mathbf{y}\sin Qz), \tag{6}$$

where $\boldsymbol{\sigma}$ is the Pauli spin operator. A' is the diagonal part (in the pure plane-wave representation) of the one-electron exchange energy. The amplitude g of the off-diagonal contribution will, in general, be dependent on the wave vector of the electron considered. If the spin operators are substituted explicitly,

$$A''=-g\begin{pmatrix}0 & e^{-iQz}\\ e^{iQz} & 0\end{pmatrix}, \tag{7}$$

The operator A'' connects plane-wave states in pairs: $\mathbf{k},\ \alpha \rightleftarrows (\mathbf{k}+\mathbf{Q}),\ \beta$, where α and β are the spin-up and spin-down spin functions. Consequently, the HF equation,

$$[(p^2/2m)+A]\psi=E\psi, \tag{8}$$

can be solved formally. The eigenvalues are those of a two-dimensional secular equation:

$$E_{\mathbf{k}}=\tfrac{1}{2}(\epsilon_{\mathbf{k}}+\epsilon_{\mathbf{k}+\mathbf{Q}})\pm[\tfrac{1}{4}(\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}+\mathbf{Q}})^2+g^2]^{1/2}. \tag{9}$$

The one-electron energy $\epsilon_{\mathbf{k}}$ is the free electron energy plus the diagonal part A' of the one-electron exchange energy; see (15a,b). The two branches of the eigenvalue

tion interactions, but without allowance for the repopulation of k space or large SDW deformations. The present writer has extended this study by evaluating the HF energy for both large and small SDW's, with k space always repopulated in such a way that the Fermi surface is a surface of constant HF (one-electron) energy. A similar study has been carried out independently by Conyers Herring (private communication). SDW ground states do not occur for δ-function interactions, whatever their strength.

[7] J. Burger and M. A. Taylor, Phys. Rev. Letters **6**, 185 (1961).

[8] H. Kojima, R. S. Tebble and D. E. G. Williams, Proc. Roy. Soc. (London) **A260**, 237 (1961).

[9] F. E. Hoare and J. C. Matthews, Proc. Roy. Soc. (London) **A212**, 137 (1952).

spectrum are shown in Fig. 1. The exact wave functions for the lower branch are

$$\varphi_{\mathbf{k}}=\{\alpha\cos\theta\exp(i\mathbf{k}\cdot\mathbf{r}) +\beta\sin\theta\exp[i(\mathbf{k}+\mathbf{Q})\cdot\mathbf{r}]\}/V^{1/2}, \quad (10)$$

where

$$\cos\theta(\mathbf{k})\equiv g/[g^2+(\epsilon_{\mathbf{k}}-E_{\mathbf{k}})^2]^{1/2}. \quad (11)$$

The algebraic signs have been defined so that $0\leq\theta\leq\frac{1}{2}\pi$. The wave functions for the upper branch can be obtained from (10) by replacing θ with $\theta+\frac{1}{2}\pi$. However, states of the upper branch will not be occupied in the ground state. They are, of course, orthogonal to the lower branch. They become occupied at finite temperatures, and cause a decrease in the SDW amplitude.

The square modulus of (10) is a constant, $1/V$, because the two terms have orthogonal spin functions. Therefore a charge density wave does not accompany a SDW. That is why a Coulomb potential term need not appear in the HF equation (8).

The exchange operator A that arises in the HF scheme is defined by the following operator equation, valid for any two-component wave function $\psi(\mathbf{r})$.

$$A\psi(\mathbf{r}_1)=-\sum_{\mathbf{k}}\left[\int(e^2/r_{12})\varphi_{\mathbf{k}}^{\dagger}(\mathbf{r}_2)\psi(\mathbf{r}_2)d^3r_2\right]\varphi_{\mathbf{k}}(\mathbf{r}_1). \quad (12)$$

For the present problem the $\varphi_{\mathbf{k}}$ are the occupied states (10). The matrix elements of A between the pure plane wave states, $\mathbf{k}'$, α and $(\mathbf{k}'+\mathbf{Q})$, β, can be evaluated explicitly. By definition they are,

$$-g(\mathbf{k}')\equiv V^{-1}\int\alpha^{\dagger}\exp[-i\mathbf{k}'\cdot\mathbf{r}]A \times\beta\exp[i(\mathbf{k}'+\mathbf{Q})\cdot\mathbf{r}]d^3r. \quad (13)$$

The indicated coordinate integrations of (12) and (13) can be carried out, and there remains only the integrations in $\mathbf{k}$ space for the occupied states $\varphi_{\mathbf{k}}$:

$$g(\mathbf{k}')=\int\frac{4\pi e^2}{|\mathbf{k}'-\mathbf{k}|^2}\sin\theta\cos\theta\frac{d^3k}{8\pi^3}. \quad (14)$$

This is an integral equation for $g(\mathbf{k})$ since $\theta(\mathbf{k})$ is a function of $g(\mathbf{k})$, as given by (11). Actually, the dependence is quite intricate since θ also depends through $\epsilon_{\mathbf{k}}$ on the diagonal elements A' of the exchange operator (12). For a spin-up plane wave,

$$\epsilon_{\mathbf{k}'}=\frac{\hbar^2|\mathbf{k}'|^2}{2m}-\int\frac{4\pi e^2}{|\mathbf{k}'-\mathbf{k}|^2}\cos^2\theta\frac{d^3k}{8\pi^3}, \quad (15a)$$

and for a spin-down plane wave,

$$\epsilon_{\mathbf{k}'+\mathbf{Q}}=\frac{\hbar^2|\mathbf{k}'+\mathbf{Q}|^2}{2m}-\int\frac{4\pi e^2}{|\mathbf{k}'-\mathbf{k}|^2}\sin^2\theta\frac{d^3k}{8\pi^3}. \quad (15b)$$

An exact solution of the HF equations reduces therefore to a solution of the coupled integral equations (14) and (15), together with the algebraic relations (9) and (11). Needless to say, explicit nontrivial solutions cannot be written down easily, although it follows from the demonstration of this paper that such solutions always exist.

The expectation value W of the Hamiltonian for a single Slater determinant of the functions (10) can be evaluated in a straightforward manner:

$$\frac{W}{V}=\frac{\hbar^2}{2m}\int(k^2\cos^2\theta+|\mathbf{k}+\mathbf{Q}|^2\sin^2\theta)\frac{d^3k}{8\pi^3} -\frac{1}{2}\int\int\frac{4\pi e^2}{|\mathbf{k}'-\mathbf{k}|^2}\cos^2(\theta'-\theta)\frac{d^3k}{8\pi^3}\frac{d^3k'}{8\pi^3}. \quad (16)$$

The first term is the kinetic energy and the second is the exchange energy. The only difference between the exchange integral for two pure plane-wave states and two states such as (10) is the additional factor $\cos^2(\theta'-\theta)$ for the latter. (Of course, the pure plane-wave case has a similar factor, which is either 1 or 0, depending on whether the pair has parallel or antiparallel spin.) If $\theta'=\theta$, the two spins will be parallel at every point, even though their direction of polarization varies from point to point. This direction lies on the surface of a cone having semivertical angle 2θ. The azimuthal angle of the polarization is Qz. The latter component is responsible for the net local spin polarization of the entire electron gas, as given by (5). The fractional amplitude P is readily found to be

$$P=\int\sin2\theta(d^3k/8\pi^3n). \quad (17)$$

The energy (16) is a functional of the parameter $\theta(\mathbf{k})$, and the problem at hand is to find that $\theta(\mathbf{k})$ which minimizes W. The integral equation (14) defines the solution of this variational problem. The region in k space which is taken to be occupied can also be varied, provided its total volume is $8\pi^3n$. Of course, each choice requires a separate variational calculation.

The paramagnetic state of an electron gas is a trivial solution of (14) although, as will be shown in Sec. III, it is a saddle point of W rather than an absolute minimum. The occupied region of k space for the paramagnetic state (according to the convention of Fig. 1) is two spheres of radius k_F, one centered at $k_z=0$ and the other at $k_z=-2k_F$. (They touch at the point $k_z=-k_F$, $k_x=k_y=0$.) The solution is $\theta=0$ for states in the sphere centered at $k_z=0$, and $\theta=\frac{1}{2}\pi$ for states in the other sphere, as illustrated by the dashed curve of Fig. 2. A nonzero, conical spin polarization arises whenever θ takes on values between 0 and $\frac{1}{2}\pi$. The qualitative behavior of $\theta(\mathbf{k})$ for a SDW state is indicated by the continuous curve in Fig. 2.

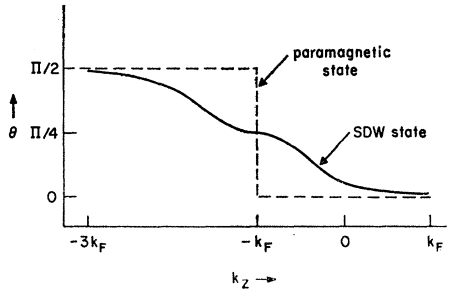

FIG. 2. Variation of the parameter θ with k_z for the low energy branch of Fig. 1. The SDW wave vector Q is taken equal to the diameter $2k_F$ of the Fermi sphere.

The integral equation can be solved easily if the wave-vector dependence of the exchange integral is neglected. This is not only an instructive exercise but the result will be used in the general proof of the following section. Let $4\pi e^2/|\mathbf{k}'-\mathbf{k}|^2$ be replaced by the constant γ. The $\mathbf{k}'$ dependence vanishes from the right-hand side of (14), so g is then a constant, independent of $\mathbf{k}$. Using (9) and (11) one finds that (14) can be written,

$$g=\gamma\int\frac{g}{2[\mu^2(k_z+\frac{1}{2}Q)^2+g^2]^{1/2}}\frac{d^3k}{8\pi^3}, \tag{18}$$

where

$$\mu\equiv(-\partial\epsilon_{\mathbf{k}}/\partial k_z)_{k_z=-\frac{1}{2}Q}. \tag{19}$$

The volume of integration must now be selected. For reasons that will become clear later, it will be taken to be a circular cylinder of radius R and length L, centered in the space of Fig. 1 at $k_z=-\frac{1}{2}Q$, and with the clyinder axis parallel to the z axis. The integration in (18) can now be carried out and the resulting equation solved explicitly for g.

$$g=\mu L/2\sinh\beta, \tag{20}$$

where

$$\beta=8\pi^2\mu/\gamma R^2. \tag{21}$$

The only other solution of (18) is the trivial one, $g=0$.

The quantity of major interest is the energy difference between the solution (20) and the trivial one. This can be evaluated directly from (16), after replacing the exchange integral by γ, as before.

$$\Delta W/V=-(\mu L^2R^2/32\pi^2)(\coth\beta-1). \tag{22}$$

This result is negative definite, so that the SDW solution always has lower energy than the trivial solution. It must be appreciated, of course, that (22) is the SDW energy relative to that of a pure plane wave state for which the occupied region in k space is a cylinder, and not the pair of touching spheres that would minimize the kinetic energy. The foregoing calculation can be employed to show that SDW states exist whenever the occupied region of k space (as defined by Fig. 1) has a finite area of intersection with the plane $k_z=-\frac{1}{2}Q$. This conclusion means that exact solutions of the HF equations having SDW character always exist, but it does not imply that the HF ground state has that character. For it is possible that the energy of repopulation associated with the achievement of a finite area of intersection is larger than the subsequent energy decrease resulting from the SDW deformation. Such is the case for short-range interactions in the weak-coupling limit.[10] But it is not the case for Coulomb interactions. No matter how weak the coupling nor how high the density, the paramagnetic state of an electron gas is unstable in the HF approximation.

III. GENERAL PROOF OF THE SDW INSTABILITY

The method employed will be dependent on the well-known variational theorem. It will be shown that an N-electron determinantal wave function having SDW character and lower energy than the paramagnetic state can always be constructed. The wave function will by no means be close to the optimum one energetically, but it will provide a brief, yet rigorous demonstration of the existence of the instability.

Let the Fermi surface be truncated, as shown in Fig. 3, so that the circular interface Σ has radius R, assumed small compared to k_F. The wave vector $\mathbf{Q}$ of the SDW that will arise will be slightly smaller than $2k_F$:

$$Q=2k_F-(R^2/k_F), \tag{23}$$

to the lowest power in R. The radius of each sphere must also be increased slightly to make up for the volume, $\pi R^4/2k_F$, of the two truncated spherical segments. This repopulation requires a kinetic energy increase ΔT given, to the lowest power of R, by

$$\Delta T/V=(\hbar^2/96\pi^2mk_F)R^6. \tag{24}$$

The R^6 dependence arises because the number of displaced electrons is proportional to R^4, and their energy increase to R^2.

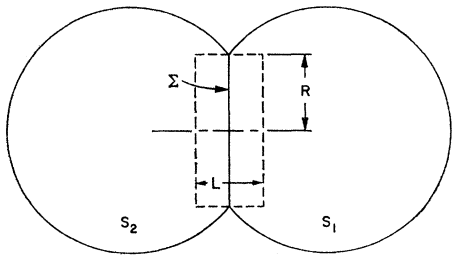

FIG. 3. Truncated spheres, S_1 and S_2, for spin-up and spin-down electrons, respectively. S_2 is displaced Q to the left of S_1, as in Fig. 1, so that the truncated faces Σ coincide. Electron states allowed to participate in a SDW deformation, during proof of the instability theorem, lie within the circular cylinder of length L and radius R.

[10] This can be shown, for example, by the argument of Kohn and Nettel (see reference 4), which is not valid, it must be pointed out, for Coulomb interactions. This result may be surmised easily from the R dependence of Eqs. (21), (22), and (24).

The foregoing repopulation also causes an increase in the exchange energy of the electron gas. The exchange potential A' of an electron, arising from its interaction with all the others, is

$$A'(k)=-\frac{e^2k_F}{\pi}\left[1+\frac{k_F^2-k^2}{2k_Fk}\ln\left|\frac{k_F+k}{k_F-k}\right|\right], \quad (25)$$

which can be derived by evaluating the integral in (15), employing the paramagnetic state solution for θ. The maximum exchange energy increase for a single electron involved in the repopulation is, for small R,

$$(\Delta A')_{\max}=(e^2R^2/\pi k_F)\ln(2k_F/R). \quad (26)$$

A simple integration determines ΔJ, the total exchange energy increase resulting from the repopulation:

$$\frac{\Delta J}{V}=\left[\frac{-7}{12}+\ln\frac{2k_F}{R}\right]\frac{e^2R^6}{96\pi^3k_F^2}, \quad (27)$$

which is about a factor of 6 smaller than the product of (26) and the number of displaced electrons per unit volume.

Consider now those states lying within a circular cylinder of radius R and length L, as shown in Fig. 3. The cylinder lies entirely within the truncated spheres S and S'. Those states outside the cylinder will be kept undeformed, whereas those inside will be allowed to generate a SDW, as described in the preceding section. States having the same k_z will be taken to have equal deformations, θ. Therefore, when the interaction between two groups of states located at k_z and k_z' is computed, it will be useful to know the average value M of the exchange integral:

$$M\equiv\langle 4\pi e^2/|\mathbf{k}'-\mathbf{k}|^2\rangle_{\text{av}}. \quad (28)$$

The average is over all $\mathbf{k}'$ and $\mathbf{k}$ lying, respectively, on two circular planes inside the cylinder, separated by $\zeta=k_z'-k_z$. Only elementary integrations enter the computation of this average. The result is

$$M=(4\pi e^2/R^2)f(u), \quad (29)$$

where $u=\zeta^2/R^2$ and

$$f(u)=2\ln[(u+(u^2+4u)^{1/2})/2u]+\tfrac{1}{2}[(u^2+4u)^{1/2}-u]-1. \quad (30)$$

This is a monotonic decreasing function with increasing u, varying as $\ln(1/u)$ for small u and as $1/u$ for large u. The average (29) will now be written as the sum of two contributions,

$$M=\gamma+D, \quad (31)$$

where

$$\gamma=(4\pi e^2/R^2)f(L^2/R^2). \quad (32)$$

The constant γ is the smallest average interaction between two circular planes of the cylinder, corresponding to the average for the two faces at opposite ends. Consequently, the remainder D is positive for all other pairs.

The one-electron wave functions for the states inside the cylinder will be taken to be those defined by the solution (20) of the preceding section, with γ given by (32). The parameter β becomes essentially independent of R if we fix the shape of the cylinder as follows:

$$L=\lambda R, \quad (33)$$

where λ is a constant. Then,

$$\beta=2\pi\mu/e^2f(\lambda^2). \quad (34)$$

It follows from (22) that the SDW lowers the energy by a term proportional to R^4, whereas the repopulation energy, (24)+(27), increases it by a term essentially proportional to R^6. Since the value of R is at our disposal, the net energy change can always be made negative.

The foregoing argument indicates the basic strategy of the proof, but two difficult points remain. The energy (22) includes, to be sure, the entire kinetic-energy increase arising from the deformation, but only the exchange-energy decrease arising from the constant term γ of (31). Naturally, the total energy (16) includes as well the exchange-energy difference ΔJ_D arising from the remainder D in (31), summed over all pairs of states within the cylinder. Furthermore, the entire exchange interaction between states inside the cylinder and those outside has yet to be considered. The latter contribution is the more troublesome one.

The contribution ΔJ_D is readily shown to be negative by considering an infinite sequence of steps by which the trivial solution in the cylinder is changed to the nontrivial one. One begins, say, by changing the θ values for $k_z>-\frac{1}{2}Q$ from $\theta=0$ to their final ones for each infinitesimal interval $(\Delta k_z)_i$ in sequence, beginning at the interface Σ. Each resulting energy increment is a change in an energy W_i which involves a sum of interactions of the interval i with intervals $i+p$ and $i-p$, equally spaced on opposite sides of the interval i:

$$W_i=-\tfrac{1}{2}\textstyle\sum_p[\cos^2(\theta_i-0)+\cos^2(\theta_i-\theta_{i-p})]D_p. \quad (35)$$

The interval $i+p$ (to the right of i) still has its $\theta=0$. The important point to note is that the function in square brackets has its minimum magnitude as a function of θ_i at $\theta_i=0$ and $\theta_i=\theta_{i-p}\leq\frac{1}{2}\pi$. Therefore, since $\theta(k_z)$ is a monotonic decreasing function of k_z, the change in θ_i from 0 to its final value—intermediate between 0 and θ_{i-p}—must increase the magnitude of the exchange interaction. D_p, in (35), is the interaction between the interval i and $i\pm p$ and is positive, being just the product of $D(\zeta)$ by the numbers of states for the two intervals of each pair. If the interval $i+p$ lies outside of the cylinder, the first term of (35) must be omitted, leaving the increase of the second term completely—instead of only partially—uncancelled. A similar sequence of steps must be carried out for

$k_z < -\frac{1}{2}Q$, and by a corresponding argument each step increases the magnitude of the exchange interaction. Therefore,

$$\Delta J_D < 0. \tag{36}$$

Consequently, the remainder D of the exchange interaction (31), summed throughout the cylinder, necessarily enhances the instability under consideration.

Finally, the exchange interaction between states inside the cylinder and those outside must be accounted for. This should be done at the outset by including an exchange potential $\bar{A}'(\mathbf{k})$ in the single-particle energy $\epsilon_{\mathbf{k}}$. The parameter that enters the theory in this regard is μ, defined in (19):

$$\mu = (\hbar^2 Q/2m) + (-\partial \bar{A}'/\partial k_z)_{k_z=-\frac{1}{2}Q}. \tag{37}$$

$\bar{A}'$ differs from A', given by (25), in that the contribution of the half-cylinder inside the truncated sphere must not be included in the integration of (15). When this contribution is subtracted from (25), the well-known singular slope of the potential at the Fermi surface is removed for electron states on the interface Σ. This subtraction is accomplished most directly by employing (29) and (30) in the integrations, which then yield a value for μ appropriately averaged over the circular cross section of the cylinder:

$$\mu = \hbar^2 Q/2m + (e^2/\pi) \ln(4k_F/L). \tag{38}$$

Actually, the magnitude of the slope at the interface Σ is a trifle smaller than (38). However, employment of the value (38) will prevent the exchange potential from being underestimated anywhere in the cylinder. Direct verification of this result is straight forward, but tedious. It can be seen intuitively rather easily, since $\frac{1}{2}L$ times the second term of (38) is equal to the difference in A' for states at the interface Σ and states $\frac{1}{2}L$ nearer the center of the sphere. (The contribution of the half-cylinder to this energy difference is zero, by symmetry. And the curvature of $\bar{A}'$ is such that the average energy difference $\bar{A}'(k_z) - \bar{A}'(-\frac{1}{2}Q)$ is smaller in magnitude than $|k_z + \frac{1}{2}Q|$ times the second term of (38), for all states inside the cylinder.)

Substitution of (38) into (34) together with the use of (33) determines the parameter β,

$$\beta = (\pi\hbar^2 Q/me^2 f) + (2/f) \ln(4k_F/\lambda R). \tag{39}$$

The deformation energy (22) with μ and β given by (38) and (39) now includes adequately the exchange interactions under consideration. Since β depends slightly on R, (22) no longer varies precisely as R^4. The proof of the instability requires only that ΔW be proportional to a smaller power than R^6 for small R. When $R \to 0$, β becomes large, and

$$(\coth\beta - 1) \to 2e^{-2\beta}. \tag{40}$$

The deformation energy ΔW then varies essentially as follows:

$$-\Delta W \propto R^{4+(4/f)}, \tag{41}$$

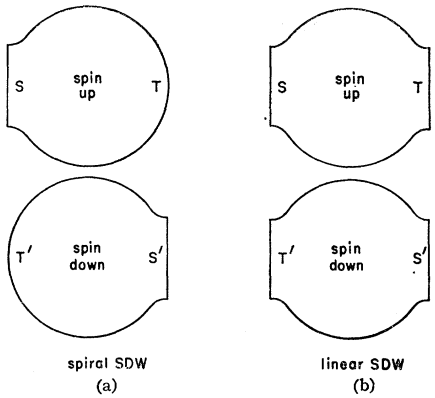

FIG. 4. Occupied regions of k space (a) for a right-handed spiral SDW, and (b) for a linear SDW. A right-handed spiral exchange potential perturbs strongly the electron states near S and S', whereas a left-handed spiral perturbs the states near T and T'.

in the small R limit. Since $f(\lambda^2)$ can be chosen arbitrarily large by selecting $\lambda = L/R$ sufficiently small, the exponent appearing in (41) is easily made smaller than six. For example, a cylindrical shape corresponding to $\lambda = 0.2$, for which $f = 2.6$, is adequate.

The validity of the foregoing demonstration does not depend on the magnitude of e^2 or k_F. Consequently, the SDW instability exists in the HF approximation even in the weak-coupling or high-density limit.[11] To be sure, the magnitude of the instability and the optimum value of R become very small in this limit. The HF ground state would then not correspond to a single SDW, but would probably contain a large number, $\sim(k_F/R)^2$, of SDW's, having $\mathbf{Q}$'s appropriately oriented throughout the available solid angle. The total instability would thereby be increased by a similar numerical factor.

The magnitude of the instability derived above is, of course, only a lower limit. Allowing the exchange potential to perturb states outside the cylinder will lower the energy of the SDW state even more, and will increase the amplitude of the exchange potential, thereby causing still larger deformations, etc. A further enhancement will arise when k space is repopulated so that the Fermi surface is a surface of constant energy $E_{\mathbf{k}}$. Numerical calculations that include such features are planned, and should provide a smaller upper bound than heretofore for the energy of the HF ground state.

IV. LINEAR SPIN DENSITY WAVES

The occupied region of k space for a right-handed spiral SDW, corresponding to (5), is illustrated in Fig. 4(a), where the spin-up and spin-down distributions are indicated separately. The states that are most strongly perturbed by the SDW exchange potential (7) are those located near S and S' of Fig. 4, for spin-up and spin-down electrons, respectively. The energy gap

[11] The instability of an electron gas has also been studied recently by F. Iwamoto and K. Sawada, Phys. Rev. **126**, 887 (1962). They succeeded in finding only a low-density instability.

occurs at the plane $k_z=-\frac{1}{2}Q$ for spin-up electrons and at the plane $k_z=\frac{1}{2}Q$ for spin-down electrons. If the self-consistent amplitude g of the SDW exchange potential is comparable to the Fermi energy, all of the occupied states will be strongly perturbed, and the fractional spin polarization P will be large. In this circumstance one would not anticipate further instabilities from additional SDW formation since most of the available exchange energy decrease has been achieved. A second SDW would necessarily "interfere" with the first one.

However, if the amplitude of the first SDW is small compared to the Fermi energy, the states near T and T' of Fig. 4 will hardly be perturbed at all, and can participate fully in a left-handed spiral SDW instability, say:

$$\mathbf{P}=P(\mathbf{x}\cos Qz-\mathbf{y}\sin Qz). \tag{42}$$

Consequently, the energy decrease resulting from SDW formation will be almost doubled. There will be some interference, since the contribution of states near T and T' to the right-handed spiral will be reduced, and the contribution of states near S and S' to the left-handed spiral will be similarly moderated. The occupied region of k space for two colinear spirals is illustrated in Fig. 4(b). The total polarization is the sum of (5) and (42).

$$\mathbf{P}_{\rm tot}=P_0\boldsymbol{\varepsilon}\cos Qz, \tag{43}$$

where $P_0=2P$. A polarization wave of this form will be referred to as a linear SDW. It should be remembered that the theory of a SDW is insensitive to the direction of spin polarization, so that the unit vector $\boldsymbol{\varepsilon}$ of (43) can have any orientation with respect to $\mathbf{Q}$. (For the particular example employed above, it would have been the $\mathbf{x}$ direction.) Of course, in a real metal dipolar interaction, spin-orbit coupling, and other possible mechanisms could operate to select say a transverse or longitudinal polarization preferentially.

The orientation of $\mathbf{Q}$ is arbitrary for an idealized, isotropic electron gas. Very likely, in a real metal one or more symmetry directions would be selected. From (21) and (22) it can be seen that a high density of states at the Fermi surface is the most important factor influencing the magnitude of a SDW instability. Therefore, one would anticipate that the $\mathbf{Q}$ directions would intersect the Fermi surface where the local density of states is a maximum. For example, if a portion of the Fermi surface makes a close approach to a Brillouin zone boundary, the local density of states will be large. A SDW instability with $\mathbf{Q}$ parallel to, but somewhat smaller, say, than the reciprocal lattice vector associated with the zone boundary might be anticipated. The Fermi surface would then be truncated by a SDW energy gap lying inside of the zone boundary. Topologically, the Fermi surface would be equivalent to one slightly larger in enclosed volume and intersecting instead the zone boundary.

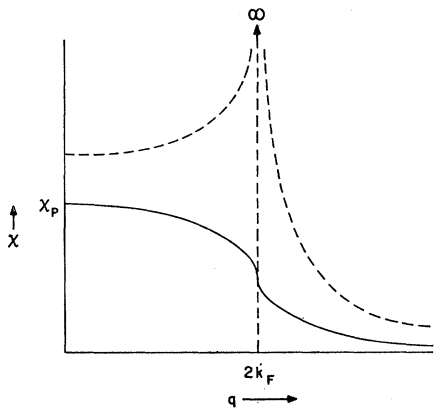

FIG. 5. Schematic illustration of the wave-vector-dependent spin susceptibility. The solid curve is that of a noninteracting electron gas, with intercept χ_P, at $q=0$, being the well-known static Pauli susceptibility. The dashed curve is that of an electron gas, with Coulomb interactions, in the Hartree-Fock approximation.

The multiple SDW instability that permits a linear SDW (which can usually be regarded as two colinear spirals) may also allow the simultaneous existence of several linear SDW's. The amplitude of each could not be too large, of course, For example, the ground state of a cubic metal could contain three linear SDW's with $\mathbf{Q}$'s parallel to each of the three cubic axes, or possibly four linear SDW's with $\mathbf{Q}$'s parallel to each of the four [111] axes, etc. It must be emphasized that the direction of the polarization vector $\boldsymbol{\varepsilon}$ of each linear SDW can be different. This is possible because each SDW arises essentially from a different group of electron states in k space. For example, each linear SDW could be longitudinally polarized. To illustrate the point, the total spin polarization density for the case of a three linear SDW ground state could be

$$\mathbf{P}=P_0(\mathbf{x}\cos Qx+\mathbf{y}\cos Qy+\mathbf{z}\cos Qz). \tag{44}$$

A cyclic permutation of the polarization vectors in (44) would correspond to three linear SDW's, each having transverse polarization. The antiferromagnetic ground state of chromium is similar to that given by (44), as will be discussed in Sec. VIII.

V. SPIN SUSCEPTIBILITY OF THE PARAMAGNETIC STATE

The wave-vector-dependent spin susceptibility of a noninteracting electron gas is

$$\chi(q)=\chi_P\left[\frac{1}{2}+\frac{4k_F^2-q^2}{8k_Fq}\ln\left|\frac{2k_F+q}{2k_F-q}\right|\right], \tag{45}$$

where $\chi_P\equiv\chi(0)$ is the well-known Pauli susceptibility. Equation (45) is a monotonic decreasing function with increasing q, as shown schematically by the solid curve in Fig. 5. The spin susceptibility of an interacting electron gas has been studied by Wolff,[12] who found that

[12] P. A. Wolff, Phys. Rev. 120, 814 (1960).

the HF spin susceptibility remained a monotonic decreasing function of q in an approximate treatment employing δ-function interactions. However, the SDW instability derived in Sec. III shows that the HF spin susceptibility of the paramagnetic state cannot be a monotonic function for the case of Coulomb interactions. The existence of the instability requires that $\chi(q)$ have a singularity near $q=2k_F$, as shown schematically by the dashed curve of Fig. 5. Whether or not there is a susceptibility minimum between the intercept,

$$\chi(0)=\chi_P[1-(me^2/\pi\hbar^2k_F)]^{-1}, \tag{46}$$

and the singularity near $2k_F$ very likely depends on the electron density.

The spin susceptibility (for $q\neq 0$) is ordinarily evaluated by perturbation theory[12a] without allowing for the repopulation of k space that will occur as a consequence of the self-consistent potential. This omission is justified because the repopulated volume is proportional to the square of the potential and cannot contribute a first order term to the spin polarization. It will have been noted, however, that the proof of the instability given in Sec. III employed a repopulation of k space. The question arises, then, whether the instability would have occurred without including repopulation. The answer is yes. The repopulated volume occuring in the proof is proportional to R^4, and from (20) and (33) the exchange potential is proportional essentially to R. Therefore, if the repopulated volume were depleted, at most an additional energy term of order R^5 would be needed. But by an appropriate choice of λ, Eq. (33), the SDW deformation energy can be made to vary with a power of R less than five, as shown in (41). Consequently, the instability would still have occurred, despite a neglect of repopulation, but it would have been less severe.

It would seem to be purely academic to discuss the spin susceptibility of an unstable state. The motivation is, of course, the fact that the HF instability discussed here is probably not indicative of the character of the true ground state for most metals. That would require the true susceptibility peak, as in Fig. 5, to have at most a finite height for typical metals. The important point remains, though, that a susceptibility maximum near $q=2k_F$ is a likely consequence of Coulomb interactions, and has not been pointed out previously. The occurrence of such a maximum has interesting implications with regard to the magnetic properties of metals and alloys, as is discussed briefly below.

The present paper is concerned primarily with the possible existence of the SDW ground states. These may indeed be rare; but the existence of SDW excited states is more general. One may select an arbitrary wave vector $\mathbf{q}$, and then repopulate k space so that the Fermi surface has a finite area in common with the planes, $\mathbf{k}=\pm\frac{1}{2}\mathbf{q}$. It follows that the repopulated plane wave state is unstable with respect to SDW deformations, for any repulsive interaction, however weak. (The proof is essentially equivalent to the one-dimensional case.[3]) Therefore, exact SDW solutions of the HF equations always exist. And they encompass a continuous range of SDW polarization amplitudes, $0\leq P<1$, for all wave vectors $q>0$. The HF equations of a SDW excited state should of course include appropriately the effective potential of any interactions that stabilize the excitation, when such are present.

SDW excited states have been employed previously[13] by the writer to explain the apparent antiferromagnetic properties of paramagnetic alloys. The HF theory of a SDW was formulated there within the framework of perturbation theory, which does not adequately approximate the exact HF formulation given here in Sec. II. However, the associated treatment of the interaction of localized spins with SDW excited states, and the long-range antiferromagnetic order that can occur at low temperature remains essentially unaffected. A possible misgiving with regard to such an antiferromagnetic mechanism might arise from the incorrect view that $\chi(q)$ is a monotonic decreasing function of q. The excitation energy of a SDW state, with a given fractional polarization P, is inversely proportional to $\chi(q)$. The lowest energy excitation (for a fixed P) would then correspond to $q=0$, and would favor ferromagnetism rather than antiferromagnetism. This argument is incomplete, as pointed out below, since energy contributions from SDW excitations having wave vectors differing from $\mathbf{q}$ by a reciprocal lattice vector must also be included. In any case, the observation that $\chi(q)$ need not have its maximum at $q=0$ obviates even the plausibility of such a misgiving.

The effective exchange interaction between a localized spin $\mathbf{S}_j$ and, say, a linear SDW such as (43) would be

$$H_j=-G(q)\mathbf{S}_j\cdot\boldsymbol{\varepsilon}P_0\cos(\mathbf{q}\cdot\mathbf{R}_j), \tag{47}$$

where $\mathbf{R}_j$ is the position of the localized spin $\mathbf{S}_j$, and $G(q)$ is an appropriate exchange interaction constant between the spin and a SDW of wave vector $\mathbf{q}$. $G(q)$ will depend on q, since the exchange interaction should have a "form factor," associated of course with the finite size of the localized orbital. It is the interaction energy (47), depending linearly on P_0, which can overcome the SDW excitation energy:

$$W(q)=n^2\mu^2P_0^2/4\chi(q), \tag{48}$$

[12a] The reader should appreciate that the Hartree-Fock perturbation theory (with exchange) is required. This formalism has been given by H. W. Peng, Proc. Roy. Soc. (London) **A178**, 499 (1941), and has been used explicitly by C. Herring, Phys. Rev. **85**, 1003 (1952); **87**, 60 (1952) in a collective electron treatment of a ferromagnetic Bloch wall.

[13] A. W. Overhauser, J. Phys. Chem. Solids **13**, 71 (1960). The reader should note that an alternative explanation that ignores the possibility of long-range order, proposed by W. Marshall, Phys. Rev. **118**, 1519 (1961), when evaluated quantitatively, does not in fact account for the experimental heat capacity of Cu-Mn alloys at the observed Mn concentrations.

where μ is the Bohr magneton, $W(q)$ is the excitation energy per unit volume of a linear SDW with maximum fractional polarization P_0, $\chi(q)$ is the spin susceptibility per unit volume. At 0°K all spins $\mathbf{S}_j$ will be oriented by the interaction (47), causing a net energy decrease per cc arising from the sum of (47) and (48):

$$\Delta W = -(2SN_p/\pi n\mu)^2 G^2(q)\chi(q), \tag{49}$$

where N_p is the concentration of localized spins. Ignore, now, for the sake of simplicity all other SDW excitations. The wave vector of the long-range order would then be expected to be that value of q which maximizes $G^2\chi$. If this occurs for $q\neq 0$, antiferromagnetic order is possible. If the maximum occurs at $q=0$, a ferromagnetic or, possibly, a superparamagnetic[14] state may result. The striking difference between the properties of dilute Cu-Mn alloys[15] and dilute Cu-Co alloys[16] may possibly be explained on this basis—the result of significantly different form factors $G(q)$ for the two species of paramagnetic solute.

A considerable amount of additional effort is needed to explore details of SDW mechanisms in magnetic ordering. The foregoing remarks are intended only to illustrate the elementary physical basis of the method. The point of view is that the natural coordinates for elaborating the theory are the spin directions $\mathbf{S}_j$ and the amplitudes $P_\mathbf{q}$ of the SDW excitations for all $\mathbf{q}$. To order P^2 the latter coordinates can be eliminated, their physical effect replaced by equivalent interactions between all pairs of spins.[17] But the temptation to truncate such indirect interactions for pragmatic reasons —considering say only pairs that are relatively near—is always present and can lead to spurious conclusions. Indeed, for an ordered ground state described by a wave vector $\mathbf{Q}$ (including the ferromagnetic case, $Q=0$), the amplitudes $P_\mathbf{q}$ are identically zero for all $\mathbf{q}$ excepting $\mathbf{Q}$ itself and those which differ from $\mathbf{Q}$ by a reciprocal lattice vector (times 2π). This result can be recovered in the indirect interaction model only if the interactions are summed exactly for all pairs, regardless of range. In the SDW description just one—or at most a few—SDW's play a role in an ordered ground state, or in ordered thermally excited states treated by a molecular field or random phase approximation.

Errors that are more difficult to avoid when the indirect interaction model is employed occur in cases when a single SDW is highly excited—e.g., the helical spin structures occurring in the rare earth metals. Terms of higher order than P^2 and the repopulation of k space, for example, become important and will play perhaps a crucial role in such phenomena as order-order transitions, the temperature variation of the helical pitch, resistivity anomalies, etc. Such nonlinear phenomena arise naturally in the theory of an individual SDW. Consequently, this approach is the appropriate and generally valid one.

VI. DETECTION OF SDW'S BY NEUTRON DIFFRACTION

Direct observation of the Fourier components of magnetization density by neutron diffraction is the standard technique for determining antiferromagnetic order. Detection of SDW ground states in metals, when present, may nevertheless be quite difficult. Very likely the fractional polarization of a SDW is of the order of one percent, so that scattering amplitudes would be a hundred times smaller than typical. A further difficulty is that the wave vector $\mathbf{Q}$ of a SDW is determined by the diameter of the Fermi surface, not by the lattice parameter. Consequently, the neutron-scattering vector $\mathbf{K}$ will generally be unpredictable and will correspond to an unknown point in reciprocal space, both in magnitude and direction.

Consider first the case of a spiral SDW in an ideal electron gas, with the circle of polarization perpendicular to $\mathbf{Q}$, as in (5). The allowed scattering vectors are,

$$\mathbf{K}=\pm\mathbf{Q}. \tag{50}$$

It has been pointed out that if the incident neutrons are unpolarized, each of the two scattered beams will be completely polarized,[18] provided the diffraction sample contains only right-handed (or left-handed) spirals. Since there is no magnetostatic energy tending to cause domain formation in an antiferromagnet, and since SDW's are a conduction electron phenomenon with consequent long range coherence, it is likely that subdivision into domains will not occur in good specimens. This possibility requires that particular caution must be used in searching for SDW reflections. For suppose there is a single SDW in, for example, an otherwise cubic crystal. All equivalent directions in reciprocal space must be scanned since $\mathbf{Q}$ would be parallel to just one of them.

Consider next a linear SDW in an ideal electron gas, such as (43). The allowed reflections will be the two given by (50), but only if the polarization vector $\boldsymbol{\varepsilon}$ has a component perpendicular to $\mathbf{K}$. For if $\boldsymbol{\varepsilon}$ and $\mathbf{K}$ are parallel, the magnetic induction B will be identically zero, and there will be no magnetic interaction with neutrons. A longitudinally polarized linear SDW in an ideal electron gas is invisible to neutrons.

In real metals the wave functions of conduction electrons have, of course, a periodic modulation within

[14] C. P. Bean and J. D. Livingston, J. Appl. Phys. **30**, 120S (1959).

[15] J. E. Zimmerman and F. E. Hoare, J. Phys. Chem. Solids **17**, 52 (1960); L. T. Crane and J. E. Zimmerman, *ibid.* **21**, 310 (1961).

[16] L. T. Crane and J. E. Zimmerman, Phys. Rev. **123**, 113 (1961).

[17] M. A. Ruderman and C. Kittel, Phys. Rev. **96**, 99 (1954); K. Yosida, *ibid.* **106**, 893 (1957). These calculations cannot be considered quantitative until they are carried out with a self-consistent field method including exchange interactions, and until appropriate form factors $G(q)$ are also incorporated.

[18] A. W. Overhauser, Bull. Am. Phys. Soc. **7**, 241 (1962).

each unit cell of the crystal, e.g.,

$$\psi_{\mathbf{k}}=u_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}_\alpha}. \tag{51}$$

If we neglect the $\mathbf{k}$ dependence of the Bloch periodic part, $u_{\mathbf{k}}(\mathbf{r})$, the one-electron functions for a SDW deformation will be,

$$\varphi_{\mathbf{k}}=u(\mathbf{r})\{\alpha\cos\theta\exp(i\mathbf{k}\cdot\mathbf{r}) +\beta\sin\theta\exp[i(\mathbf{k}+\mathbf{Q})\cdot\mathbf{r}]\}, \tag{52}$$

which is a slight generalization of the wave function (10). The conjecture that has been made here is that the spin polarization within a unit cell follows the phase of the SDW, as in the empty lattice case, but that the amplitude is modulated by the additional multiplicative factor $|u(\mathbf{r})|^2$. For a linear SDW the magnetization density $\mathbf{M}(\mathbf{r})$ would be,

$$\mathbf{M}(\mathbf{r})=n\mu|u(\mathbf{r})|^2\varepsilon P_0\cos(\mathbf{Q}\cdot\mathbf{r}), \tag{53}$$

with $u(\mathbf{r})$ normalized in a unit volume. The conduction electron density of a unit cell can be Fourier analyzed in the usual way:

$$|u(\mathbf{r})|^2=\sum_{\mathbf{G}} f_{\mathbf{G}}\exp(2\pi i\mathbf{G}\cdot\mathbf{r}), \tag{54}$$

where $\{\mathbf{G}\}$ are the reciprocal lattice vectors and $\{f_{\mathbf{G}}\}$ are the Fourier coefficients, or form factors. It follows from (53) and (54) that the Fourier components of the magnetization density, and therefore the allowed scattering vectors, are

$$\mathbf{K}=2\pi\mathbf{G}\pm\mathbf{Q}. \tag{55}$$

In other words, there will be two magnetic reflections associated with each reciprocal lattice vector $\mathbf{G}$, and we shall refer to them as the satellites of $\mathbf{G}$. The satellites of a particular $\mathbf{G}$ might lie closer to another $\mathbf{G}$ since $\mathbf{Q}$ can be large, but it should be easy to make the proper identification. Such assignments would be clear from relative intensity measurements, since from (53) and (54), the relative intensity is determined by $f_{\mathbf{G}}^2$, the form factor of $\mathbf{G}$ rather than the form factor of the scattering vector $\mathbf{K}$.

The form factor of valence electrons ordinarily decreases rapidly in magnitude with increasing wave vector. Consequently, the only intense reflections from a conduction electron SDW will be the satellites of the origin ($G=0$). The other satellites should be present in principle, but one would expect them to be extremely weak. A longitudinally polarized linear SDW in a conduction band should not be completely invisible. The satellites of the origin would have zero intensity for the same reason given previously. But the weak satellites of the other reciprocal points, for which $\boldsymbol{\varepsilon}$ is not parallel to $\mathbf{K}$, would theoretically be present.

The foregoing model was based on a "flexible spin" hypothesis, in which it was assumed that the spin polarization density conforms smoothly to the phase of the SDW within each unit cell. This model is probably an adequate one for SDW's arising entirely from conduction electrons. We must now consider the other extreme; a rigid spin hypothesis—in which it is assumed that the cellular part of the wave function is so completely centralized by the ion core potential that the direction and amplitude of the spin polarization density within a unit cell is determined by the phase of the SDW at the center of the cell. Undoubtedly the "truth" will always be somewhere between the two extremes. But the latter extreme may be an appropriate model for a d-band SDW, or for a SDW in which oriented localized moments (as in the rare-earth metals) are the major contribution to the magnetization density.

Let $u(\mathbf{s})$ be redefined so that it is nonzero only in the unit cell centered at the origin of coordinate space. In the rigid-spin model, the magnetization density of a linear SDW will be given by

$$\mathbf{M}(\mathbf{r})=\mu\varepsilon P_0\sum_{\mathbf{L}}|u(\mathbf{r}-\mathbf{L})|^2\cos(\mathbf{Q}\cdot\mathbf{L}), \tag{56}$$

where $\{\mathbf{L}\}$ are the lattice sites. If $f_{\mathbf{K}}$ is the Fourier transform of $|u(\mathbf{s})|^2$, then the Fourier coefficient $\mathbf{M}_{\mathbf{K}}$ of $\mathbf{M}(\mathbf{r})$ is,

$$\mathbf{M}_{\mathbf{K}}=\mu\varepsilon P_0 f_{\mathbf{K}}\sum_{\mathbf{L}}\exp(2\pi i\mathbf{K}\cdot\mathbf{L})\cos(\mathbf{Q}\cdot\mathbf{L}). \tag{57}$$

The sum over $\mathbf{L}$ is nonzero only if $\mathbf{K}\pm\mathbf{Q}$ is a reciprocal lattice vector. Consequently, the Fourier components of (56) are those given previously by (55), but the amplitudes are proportional to $f_{\mathbf{K}}$, the form factor of the scattering vector, rather than the form factor of the reciprocal lattice vector of which $\mathbf{K}$ is a satellite. For the rigid-spin model experimental determination of the wave vector $\mathbf{Q}$ is ambiguous to within any reciprocal lattice vector. However, a slight admixture of the flexible-spin model, which is required if $\mathbf{M}(\mathbf{r})$ is to be a continuous function, together with reasonable assumptions about the shape of $f_{\mathbf{K}}$ should allow $\mathbf{Q}$ to be determined uniquely. This will be illustrated in Sec. VIII for the case of chromium, which approximates the rigid-spin model.

It is evident that a systematic search for SDW neutron reflections would be extremely tedious, even with neutron beams of the highest available flux. Such experiments, however, would be of significant interest, at least for metals where weak antiferromagnetism is suspected. A search should not be confined to scans of lines in reciprocal space that pass through the origin. This would allow longitudinally polarized linear SDW's to go undetected. It is necessary to scan also lines in reciprocal space that pass through (nonzero) reciprocal lattice points. Furthermore, the experiments must, in general, be carried out at low temperatures since SDW amplitudes will approach zero at a critical temperature T_c (and remain zero at higher temperatures) as discussed in the following section.

Inelastic neutron (or x-ray diffuse) scattering may reveal indirectly the presence of SDW states. The phonon spectrum will be altered as a result of the energy gaps in the electron energy level spectrum caused by the periodic SDW exchange potential. Changes in the phonon frequencies are expected, of course, because the adiabatic readjustment of the electron gas during a lattice vibration plays an important role in determining its frequency. Kohn[19] has pointed out how such effects may be expected to leave an image of the Fermi surface in the phonon spectrum, solely from the sharpness of the Fermi surface in the paramagnetic state. Energy gaps across planes tangent to the Fermi surface would be expected to alter appreciably the frequencies of the modes with wave vector approximately equal (in magnitude and direction) to the wave vectors of the SDW's present, give or take a reciprocal lattice vector. The effect may show up as an additional kink or cusp (or both) in the phonon frequency spectrum. This phenomenon should differ from the one proposed by Kohn in that it is restricted to specific wave vector directions and should disappear abruptly at the critical temperature. A search for this effect by, say, temperature diffuse x-ray scattering in single crystal chromium is of considerable interest.

VII. TEMPERATURE DEPENDENCE OF SDW PARAMETERS

The formulation of the HF theory of a static SDW given in Sec. II is for an electron gas at 0°K, since it was tacitly assumed that the states in k space were either occupied or empty depending on their location with respect to the Fermi surface. At finite temperature occupation of higher energy one-electron levels by thermal excitation will occur, so the integral equation (14) must be appropriately generalized. The details of such a generalization are obvious, and it is our intention here to discuss only the important features that will result.

Occupation of one-electron levels of the upper energy branch of Fig. 1, together with a corresponding depletion of the lower branch, will cause the amplitude of a SDW to be smaller than its 0°K value. This arises from the fact that the spin polarization of a state of the upper branch is opposite (at every position) to the corresponding state of the lower branch. Consequently, the polarization contribution of upper branch states will tend to cancel that arising from the remaining lower branch electrons. Moreover, the exchange potential will be similarly reduced, so that the fractional polarization component of each state will be smaller, thereby causing a further reduction of the SDW amplitude, etc. Such effects will be greater the higher the temperature. The SDW amplitude $P(T)$ will therefore be a monotonic decreasing function with increasing T. It is reasonable to conjecture that P will approach zero continuously,

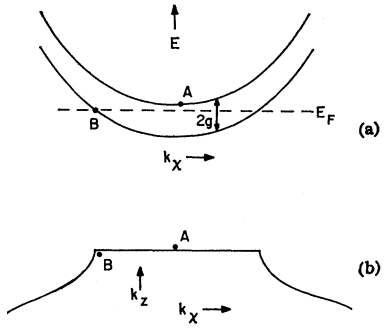

FIG. 6. Single-particle energy level spectrum, (a) on the plane in k space coincident with the SDW energy gap, and (b) the occupied region in k space near the plane of the gap. Observe the neck in the Fermi surface caused by the SDW exchange potential.

giving rise to a second order transition at a critical temperature T_c. Above T_c a nontrivial solution of the generalized integral equation will not exist.

It is an interesting coincidence that the structure of the integral equation (14) is similar to the integral equation that occurs in the Bardeen, Cooper, and Schrieffer (BCS) theory of superconductivity.[20] The similarity is perceived readily by comparing the integral equations that result in both theories when the relevant interactions are replaced by constants; compare (18) with Eq. (2.38) of reference 20. They are essentially identical, differing only in the shape of the integration volume. This similarity will also prevail with the generalized equations for finite T. On the basis of this analogy, one might guess that the SDW amplitude $P(T)$, as well as the SDW energy gap $2g$, will vary with T/T_c in a manner quite similar to the superconducting energy gap. Indeed, Swihart has shown[21] that the temperature variation of such parameters in the theory of superconductivity is quite insensitive to the form and strength of the interaction that appears in the kernel of the integral equation. Consequently, the similarity may be semiquantitative as well as qualitative. This conclusion is of course tentative since the SDW theory is complicated by several features not present in the superconductivity case. Nevertheless, the comparison for the case of Cr is quite satisfactory, as is shown in Sec. VIII.

One may anticipate on the basis of the foregoing analogy that the SDW energy gap $2g$ at 0°K is 3 or 4 times kT_c, as it is in superconductors. It is probable that the ratio should be somewhat larger for SDW's since $2g$ is not the minimum energy gap, as shown in Fig. 6(a), but the energy difference between states on opposite sides of the gap whose wave vectors have identical projections in the plane of the gap. The true thermal energy gap is the energy difference between points A and B of Fig. 6, and is necessarily smaller than $2g$. This minimum thermal gap may indeed be quite small because a SDW instability can be greater the smaller the magnitude of $\mathbf{Q}$, provided that the

[19] W. Kohn, Phys. Rev. Letters **2**, 393 (1959).

[20] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Phys. Rev. **108**, 1175 (1957).

[21] J. C. Swihart, IBM J. Research Develop. **6**, 14 (1962); Phys. Rev. **116**, 346 (1959).

states above the gap (near A) remain unoccupied. This feature can be seen from the deformation energy (22), which depends exponentially on μ, the gradient of ϵ_k at the Fermi surface. Therefore, in an electron gas for which μ is an increasing function of ϵ_k the SDW energy gaps will tend to "clamp down" tightly on the Fermi surface. On the other hand, if the Fermi surface lies beyond an inflection point in ϵ_k, this tendency to clamp down would not be so great.

The magnitude Q of the SDW wave vector will also be a function of temperature, as can be seen easily. When the energy gap decreases with increasing T, the periodic potential will be less able to sustain the repopulation of k space, which takes place predominantly near the gap at points such as B in Fig. 6. As a consequence the energy gaps will move apart with increasing T in order to accommodate the constant total number of electrons while keeping the fraction above the gap at a minimum. Also, the clamp-down effect discussed above will diminish with decreasing SDW amplitude, causing a further change in the repopulation and an additional increase of Q with T. Consequently, a detailed calculation should predict that Q will increase monotonically with increasing T. The fractional change of Q between 0°K and T_c will of course be larger the larger the fractional polarization P of the SDW at 0°K.

At T_c the magnitude of $\mathbf{Q}$ should equal the diameter of the Fermi surface (in the direction of $\mathbf{Q}$) that obtains for the paramagnetic state. This conclusion depends however on an assumption that only one unfilled energy band is participating appreciably in the SDW deformation. For if more than one band plays a significant role, it is difficult to anticipate the value of $\mathbf{Q}$ for which $\chi(\mathbf{Q},T)$ would first become singular as T is lowered through T_c. The reason that the Fermi surface diameter is the critical value for a single band is associated with the fact that the maximum in the Fourier transform, V_q, of the Coulomb interaction occurs at $q=0$. (And one expects this feature to remain even after correlation screening is appropriately accounted for.) Therefore, instabilities are maximized by keeping the highly deformed states as close together in k space as possible. This is almost self-evident from the structure of the integral equation (14). If Q is made smaller, states above the gap must be occupied, and their effect would cancel out the enhanced part of the exchange interaction between pairs of states just below the gap. The burden for enhancing exchange interactions would then fall upon pairs of states that have a larger average separation in k space, with a consequently smaller average value of V_q. In particular, for $Q=0$ (a ferromagnetic deformation), V_q must be averaged equally over all pairs of points around the entire Fermi surface, and this would lead to a relatively small average value. The foregoing considerations are, of course, qualitative in nature. A delicate instability might require a quantitative account of all factors before $Q(T_c)$ could be predicted reliably.

VIII. ANTIFERROMAGNETISM OF CHROMIUM

The antiferromagnetic state of chromium metal has recently received extensive study by single-crystal neutron diffraction techniques.[22–25] The wave vectors of the magnetization waves are parallel to the [100] directions of the bcc lattice. The wavelength is incommensurate with the lattice constant and varies continuously with temperature, as expected for a SDW state. The magnitude of the magnetization wave(s) is about a half Bohr magneton per atom. Several interpretations of this structure have been discussed,[22,26,27] assuming that Cr atoms have a localized moment (with a spin degree of freedom) in the metal. It is now apparent, however, that localized moments do not occur in Cr.

The excess entropy near the antiferromagnetic transition temperature ($T_c \approx 311$°K) would be about $\frac{1}{2}R \ln 2 \approx 0.7$ cal/deg, if the magnetization arose from localized moments. Such a large anomaly would be easily observed. Its apparent absence[28] had previously indicated that a collective electron mechanism is operating.[29,30] The heat capacity anomaly associated with the transition has now been observed[31] and the integrated (molar) entropy is

$$\Delta S = 0.0044 \text{ cal/deg.} \tag{58}$$

This very small value can be satisfactorily explained on the basis of a SDW mechanism.

The absence of localized moments has also been confirmed by the nonoccurrence of paramagnetic neutron scattering above the critical temperature.[32] The only sources of entropy, then, are the phonons and the electron gas. Changes in both contributions occur at the transition, but we shall consider only the latter one since the phenomenon is primarily electronic. The Sommerfeld constant γ has been measured[33] for Cr. Con-

[22] L. M. Corliss, J. M. Hastings, and R. J. Weiss, Phys. Rev. Letters **3**, 211 (1959).
[23] V. N. Bykov, V. S. Golovkin, N. V. Ageev, and V. A. Levdik, Doklady Akad. Nauk S.S.S.R. **128**, 1153 (1959); [translation: Soviet Phys.—Doklady **4**, 1070 (1960)].
[24] G. E. Bacon, Acta Cryst. **14**, 823 (1961).
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[26] T. A. Kaplan, Phys. Rev. **116**, 888 (1959).
[27] A. W. Overhauser and A. Arrott, Phys. Rev. Letters **4**, 226 (1960). The experiment proposed in this paper was based on the presumed existence of localized moments, which are now known not to occur in Cr. A field cooling effect is not anticipated on the basis of the current interpretation.
[28] J. E. Goldman, Revs. Modern Phys. **25**, 113 (1953).
[29] C. J. Gorter, Revs. Modern Phys. **25**, 113 (1953).
[30] A. B. Lidiard, Proc. Phys. Soc. (London) **A66**, 1188 (1953); J. C. Slater and G. F. Koster, Phys. Rev. **94**, 1498 (1954).
[31] R. H. Beaumont, H. Chihara, and J. A. Morrison, Phil. Mag. **5**, 188 (1960).
[32] M. K. Wilkinson (to be published).
[33] J. A. Rayne and W. R. G. Kemp, Phil. Mag. **1**, 918 (1956).

sequently, the electronic entropy at the transition temperature is,

$$S=\int_0^{311}\gamma T(dT/T)\approx 0.10 \text{ cal/deg.} \qquad (59)$$

Therefore, the entropy (58) associated with the antiferromagnetic transition is only 4% of the total Sommerfeld entropy at T_c. On the basis of the SDW model the entropy loss that occurs as a result of lowering the temperature below T_c arises from the truncation of the Fermi surface by the energy gaps of the SDW exchange potential. (Electron states adjacent to the gap will, for the most part, be completely occupied or completely empty and therefore will not contribute significantly to the entropy.) From the experimental data one would conclude that about 4% of the Fermi surface of Cr is truncated by energy gaps of magnetic origin in the antiferromagnetic state.

Now, the fraction of the Fermi surface that is truncated by energy gaps can be estimated independently in several ways. That portion of the Fermi surface truncated by energy gaps will not contribute to the electrical conductivity, since the normal component of electron velocity at an energy gap is zero. Therefore, SDW energy gaps should cause an abrupt resistivity increase as a result of the decrease in the effective number of current carriers. This conclusion assumes that the phase of the SDW(s) is locked to the lattice—a phenomenon that could result from paramagnetic impurities, inhomogeneous strains, etc. The electrical resistivity of Cr does indeed undergo an abrupt increase[34] below T_c, and the magnitude of the increase is about 5%. This estimate of the fractional truncation is in satisfactory agreement with the heat-capacity result. The comparison should be only semiquantitative, since truncation of the Fermi surface will tend to reduce the density of final states available to electron scattering processes. Consequently, the resistivity increase may be partly cancelled by decreased scattering rates. But changes in phonon frequencies, which do occur,[34] will enhance the thermal scattering. An accurate comparison would have to include all such effects, including the phonon contribution to the heat-capacity anomaly as well as another contribution from spin-wave excitations of the "giant" SDW.

A more interesting estimate of the fractional truncation derives from the coincidental mathematical similarity, discussed in Sec. VII, between the BCS theory and SDW theory. The temperature dependence of the fractional polarization P should compare with the energy gap parameter of the BCS theory. That it does so very well is shown in Fig. 7, for which the relative values of P were determined from the neutron diffraction intensity measurements of Shirane and Takei.[25] Therefore, it is reasonable to suppose that the ratio of energy gap to kT_c is about 3.5 for Cr. This would imply an energy gap of about 0.1 eV.

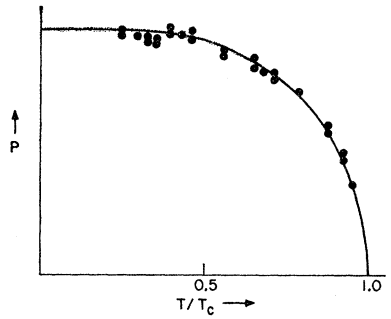

FIG. 7. Temperature dependence of the SDW amplitude P for a chromium single crystal. The experimental points are taken from Shirane and Takei (see reference 24). The small break near $T/T_c=0.4$ occurs at the spin-flip transition. The solid curve is the theoretical temperature dependence of the superconducting energy gap, after the BCS theory.

The largest possible area of each truncated face can now be estimated by setting the energy difference between points A and B of Fig. 6 to zero. If R_0 is the radius of the truncated face,

$$\hbar^2R_0^2/2m^*=0.1 \text{ eV}, \qquad (60)$$

where m^* is the effective mass. The fractional area of the Fermi surface truncated by energy gaps is

$$t=pR_0^2/4k_F^2, \qquad (61)$$

where p is the number of truncated faces. The diameter $2k_F$ of the Fermi surface is determined directly from the neutron diffraction scattering vector $\mathbf{Q}$, according to the argument given in Sec. VII. The observations indicate that for the [100] directions,

$$k_F\approx 1.1\times 10^8 \text{ cm}^{-1}. \qquad (62)$$

The effective mass can be estimated from the measured electronic heat capacity, but one must first know the total area of the Fermi surface. We have already assumed it to be spherical in writing (60) and (61). However, calculations by Lomer[35] indicate that the shape is somewhat fluted, and that the energy bands are essentially of d character. His estimate of the Fermi surface radius in the [100] directions is in agreement with (62). But he also finds that the relevant d band is doubly degenerate in that direction. There is an electron band and a hole band of approximately equal size, and their Fermi surfaces touch where they intersect the [100] axes. Taking both surfaces into account, one obtains from the Sommerfeld constant γ,

$$m^*\approx 1.5m. \qquad (63)$$

[34] H. Pursey, J. Inst. Metals **86**, 362 (1958); S. Arajs, R. V. Colvin, and M. J. Marcinkowski, J. Less-Common Metals **4**, 46 (1962); M. J. Marcinkowski and H. A. Lipsitt, J. Appl. Phys. **32**, 1238 (1961).

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The maximum radius of each truncated face, from (60), is therefore

$$R_0 \approx 0.2 \times 10^8 \text{ cm}^{-1}. \quad (64)$$

The number p of truncated faces is presumably six, since the linear SDW instabilities in each of the [100] directions are equal by symmetry. The polarization density that would result is given (crudely) by (44). From (61) the maximum fraction truncated by energy gaps is

$$t \approx 5\%. \quad (65)$$

This estimate is in excellent agreement with those derived from the entropy argument and the resistivity argument.

The SDW energy gaps will cause necks, Fig. 6(b), in the Fermi surface, and these should give rise to de Haas-van Alphen oscillations, magnetoacoustic oscillations, etc. Two de Haas-van Alphen periods have been observed[36] with orbits in (100) planes, confirming both the double degeneracy in the [100] directions pointed out by Lomer and the estimated size (64) of the necks.

Chromium undergoes an order-order transition at low temperature, which has been reported at about 155°K by some workers[23,24] and near 110°K by others.[25,37,38] Below this critical temperature the neutron reflections located on the cubic axes disappear, proving[37] that the magnetization waves are longitudinally polarized in the low temperature phase. Intensity studies[25,37] of the satellites of the (110) reciprocal lattice points indicate that the order-order transition is merely a change from longitudinal to transverse polarization of the linear SDW's. The absence of third harmonics[25] of the magnetization waves indicates that the magnetization density follows a cosine modulation, in conformity with the SDW model.

The polarization density given by (44), which describes qualitatively the magnetic ground state of Cr, would be reasonably accurate if the flexible-spin model were a good approximation here. However, the neutron-diffraction intensities that obtain in Cr can be interpreted only if the rigid-spin model is the appropriate approximation, as discussed below. This conclusion indicates that the electron energy bands which contribute to the polarization are d bands, as would be anticipated from Lomer's work on the location of the Fermi surface.

The neutron reflections that lie on the [100] axis in reciprocal space have approximately the coordinates,

$$\begin{aligned} Q_1 &\approx (0.96,0,0), \\ Q_2 &\approx (1.04,0,0). \end{aligned} \quad (66)$$

One of them is the satellite of the origin (0,0,0) and the other is the satellite of the (2,0,0) reciprocal lattice point. If the flexible-spin model applies, one of them would have an intensity corresponding to the form factor for zero scattering angle, as discussed in Sec. VI. The other would have an intensity corresponding to the form factor (squared) of a (2,0,0) scattering angle. Consequently, the intensities would differ by an order of magnitude or more. Actually, the intensity of Q_1 is only about 30% larger than the intensity of Q_2.[23–25] Therefore, one is forced to conclude that the rigid-spin model is the better approximation in Cr. And one should compare the observed intensities with that expected, say, for d-electron form factors in the rigid-spin approximation. The form factors for Mn^{++} d electrons have been measured[39] and, if applicable here, could account for only a 10% intensity difference between Q_1 and Q_2. In view of the fact that a slight admixture of the flexible-spin model is necessary in order that the magnetization density be a continuous function of position, which would add appreciable scattering intensity only to the satellites of the origin, the larger intensity difference observed can be easily interpreted. One would surmise, then, that the SDW wave vector $\mathbf{Q}$ is to be identified with Q_1 and not Q_2. (This conclusion is not absolutely certain, since a less centralized d-electron density distribution in the atomic cell, calling for a more rapidly falling form factor vs scattering angle, could reverse the assignment, assuming that loss in centralization is possible without compromising the rigid-spin hypothesis.)

The Cr^{53} nuclear resonance in Cr metal has recently been observed[40] above the critical temperature T_c. The resonance line broadens as the temperature is reduced near T_c and disappears gradually below T_c. This behavior is explained by the fact that the SDW wave length is incommensurate with the lattice. Consequently, the hyperfine fields at the nuclei arising from the magnetization density take on a wide, continuous spectrum of values. This type of behavior need not be characteristic of all SDW antiferromagnets, however, A small amplitude SDW state may have very low energy spin wave excitations, which would allow the hyperfine field direction to change rapidly at finite temperatures. Observation of the nuclear resonance in this case would be impaired only if the nuclear relaxation rate were comparable to or greater than the spin wave excitation frequencies. Otherwise the effect of the hyperfine fields would tend to a null time-averaged value.

Magnetomechanical damping at low frequencies ($\sim$1 cps) has been observed[41] in polycrystalline Cr wire by the torsion technique. The damping increases markedly with decreasing temperature below T_c, but the measurements were not extended below 200°K. A possible mechanism for this damping, suggested by de Morton,[41]

[36] D. Shoenberg (private communication).
[37] J. M. Hastings, Bull. Am. Phys. Soc. **5**, 455 (1960).
[38] M. K. Wilkinson, E. O. Wollan, and W. C. Koehler, Bull. Am. Phys. Soc. **5**, 456 (1960).
[39] L. Corliss, N. Elliot, and J. Hastings, Phys. Rev. **104**, 924 (1956).
[40] R. G. Barnes and T. P. Graham, Phys. Rev. Letters **8**, 248 (1962).
[41] M. E. de Morton, Phil. Mag. **6**, 825 (1961).

is antiferromagnetic domain wall motion. An alternative mechanism arises from the transverse polarization of the linear SDW's. Since each of the three SDW's can have two transverse polarization directions, there are eight energetically equivalent states which can become inequivalent as a result of elastic strain, and so give rise to anelastic transitions. (The wide variation of the spin-flip transition temperature from sample to sample, cited previously, indicates that there is a significant interaction between the SDW polarization modes and crystal imperfections, e.g., elastic strains.) This suggested mechanism can easily be subjected to experimental test. Below the spin-flip transition temperature there is just one magnetic state, since the SDW's are then longitudinally polarized. Therefore, it is of considerable interest to determine whether or not the large magnetomechanical damping found by de Morton disappears below the spin-flip transition temperature.

SDW theory provides a consistent and satisfactory interpretation of the magnetic phenomena in Cr. On the other hand it is not at all clear, from an *a priori* basis, why Cr should be unique in possessing large amplitude SDW's. The rapid variation of the transition temperature with small concentrations of alloying elements[34] suggests that it may be associated with a fortuitously favorable band configuration.

IX. ACCIDENTAL FERRIMAGNETISM

Metals with a SDW ground state are multiply periodic structures. There is no pure translation operation which leaves the system invariant, provided the SDW wave vectors are incommensurate with the reciprocal lattice vectors (times 2π). In the absence of magnetocrystalline interactions of sufficient strength, a commensurate relationship between the two types of wave vector would be accidental. Such a coincidence, however, could cause a bulk magnetization of the material to occur, analogous to that in ferrimagnetic materials.

A SDW is commensurate with the lattice if its wave vector $\mathbf{Q}$ satisfies

$$\mathbf{Q}=2\pi\mathbf{G}_0/p, \tag{67}$$

for some reciprocal lattice vector $\mathbf{G}$ and integer p. We shall take $\mathbf{G}_0$ to be the smallest vector satisfying this relation. Suppose for the sake of simplicity that $p=1$, and that the rigid-spin model applies. Then the moments in each primitive unit cell will all have the same phase, as defined by the SDW. Consequently, a net moment will arise. (Of course, if there are several identical atoms per primitive cell, the moment would be zero if $\mathbf{G}_0$ is a reciprocal lattice vector having zero x-ray structure factor. Also the moment could be zero for a monatomic Bravais lattice if each lattice site were at the node of a linear SDW. But such a situation seems unlikely energetically.) It is relatively easy to see that similar situations can prevail for $p>1$, especially if p is prime. For example, in thulium,[42] which has localized moments oriented by a linear SDW, $p=7$. Alternately, four hexagonal layers are polarized up and three down. It is not our purpose, here, to envision all conceivable structures and special requirements, but rather to cite a few examples and to discuss qualitatively some of the relevant features.

One would not, in general, anticipate a SDW instability in an electron gas with $\mathbf{Q}=2\pi\mathbf{G}$, since the periodic potential of the lattice will cause energy gaps in the conduction electron spectrum across the same planes in k space as the exchange potential of the commensurate SDW. It should be recalled that the SDW instability arises as a result of the approximate degeneracy between filled levels on one side and empty levels on the other side of the Fermi distribution. This near degeneracy would be destroyed by the periodic crystal potential, excepting the chance situation where the latter potential is very small. This might occur at a superlattice $\mathbf{G}$ of an ordered alloy, if the two species of atoms are, say, of equal valence. A different magnetic response of the two species could then cause a net moment per superlattice cell.

The remarkable ferromagnetism of ordered Sc-In alloys[43] near the Sc_3In composition may be an example of the foregoing phenomenon. The ferromagnetic state is observed only for In concentrations between 23.8 and 24.2 at.%. This very narrow range is hard to understand if the ferromagnetic mechanism is an ordinary alignment of local moments depending, though, on long-range lattice order, expecially since it does not occur at the stoichiometric composition. The proposed SDW mechanism would require that the ordered alloys are antiferromagnetic over a wide composition range, but that the wave vector $\mathbf{Q}$ happens to be coincident with the superlattice $\mathbf{G}$ only at 24% indium (presuming that the Fermi surface location varies with composition). This suggestion can, in principle, be checked by neutron diffraction. A somewhat similar phenomenon has been observed in $ZrZn_2$.[43,44]

Magnetocrystalline interactions that could force commensurateness of a SDW for $\mathbf{Q}$ near to, but not quite satisfying (67) is, of course, possible. It is perhaps surprising that Cr, with large amplitude linear SDW's, appears insensitive to the nearness of the (1,0,0) point in reciprocal space, even though $\mathbf{Q}$ is short of that point by only four percent. Similarly, the wave vectors of the spiral spin configurations in dysprosium and holmium,[45] which have a significant temperature variation, show no evidence of locking when they pass through sub-

[42] W. C. Koehler, J. W. Cable, E. O. Wollan, and M. K. Wilkinson, J. Appl. Phys. **33**, 1124 (1962).

[43] B. T. Matthias, A. M. Clogston, H. J. Williams, E. Corenzwit, and R. C. Sherwood, Phys. Rev. Letters **7**, 7 (1961).

[44] B. T. Matthias and R. M. Bozorth, Phys. Rev. **109**, 604 (1958).

[45] M. K. Wilkinson, W. C. Koehler, E. O. Wollan, and J. W. Cable, J. Appl. Phys. **32**, 20S, 48S (1961).

multiples of the reciprocal lattice vectors. Locking does occur for the linear spin wave configurations in erbium[46] and thulium.[42] For both cases, $p=7$. But the energetic cause is easy to understand in these two cases. The magnetic interaction responsible for the ordered state is the $s-f$ exchange interaction between a linear SDW in the conduction electrons and the localized f electrons. This interaction is negligible for atoms at nodes of the linear SDW; and there will always be a significant fraction of lattice sites at or very near such nodes for an incommensurate linear SDW. This loss of interaction energy is avoided by a commensurate SDW wave vector. The phase of the SDW can adjust so that no lattice site is near a node. Consequently, a locking mechanism is provided. This cannot occur for a spiral spin wave configuration, since a spiral SDW has no nodes. It is interesting that the locking in erbium stops when a spiral component appears, as might be anticipated, since the (perpendicular) spiral component eliminates the nodes, even though the linear component remains.

[46] J. W. Cable, E. O. Wollan, W. C. Koehler, and M. K. Wilkinson, J. Appl. Phys. **32**, 49S (1961).

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Radiative Corrections to Decay Processes Mediated by Vector Bosons*

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The lowest order electromagnetic corrections to β and μ decay have been calculated in an intermediate vector-boson theory. Assuming universal coupling, the μ lifetime agrees with the experimental value if the boson's mass is chosen to be that of a K meson. The results are relatively insensitive to the value chosen for the cutoff.

I. INTRODUCTION

THE lowest order radiative corrections to decays through a $(V-A)$ Fermi interaction have been calculated by Kinoshita and Sirlin and by Berman.[1] In a universal coupling theory these corrections affect the lifetime of the muon in two ways: in the contributions to the μ decay itself and in the contributions to the O^{14} decay. The latter decay determines the coupling constant to be used in all weak interactions. For universal coupling, the most recent experimental data indicate a significant discrepancy between the predicted and observed μ lifetimes.[2]

It has been suggested that decay processes be described not by a Fermi interaction but by two Yukawa-type interactions mediated by a vector boson.[3] The intermediate vector-boson (IVB) description reduces to the Fermi theory for infinite boson mass. We calculate below the lowest order electromagnetic corrections to μ and β decay in an IVB theory. We then determine the μ lifetime for universal coupling and compare it with the experimental value.

* Supported in part by National Science Foundation.
[1] S. M. Berman, Phys. Rev. **112**, 267 (1958); T. Kinoshita and A. Sirlin, *ibid.* **113**, 1652 (1959).
[2] J. W. Butler and R. O. Bondelid, Phys. Rev. **121**, 1770 (1961).
[3] See, e.g., T. D. Lee and C. N. Yang, Phys. Rev. **119**, 1410 (1960).

II. INTERACTION LAGRANGIAN AND CUTOFF DEPENDENCE

Consider the following type of interaction Lagrangian as a basis for all weak processes[4]:

$$L_1=ig\bar{\psi}_X\gamma_\mu\frac{(1+i\gamma_5)}{2}\psi_Y\phi^{\mu*}+\text{H.c.}, \tag{1}$$

where ψ_Y destroys a positively charged fermion Y, ϕ^μ creates a positively charged IVB, B^+, and the fermion X is neutral. g is a real, semiweak coupling constant. The electromagnetic field is introduced by replacing $\partial_\mu U^*$ in the free Lagrangian by $(\partial_\mu+ieA_\mu)U^*$. Here U^* is a charged field operator, and A_μ is the electromagnetic vector potential. Additional interactions corresponding to anomalous magnetic moments will not be considered here. The interaction Lagrangian is now of the form

$$\begin{aligned}L=L_1&-ie\bar{\psi}\gamma_\mu\psi A^\mu-ie(A_\mu\phi_\nu{}^*\partial^\mu\phi^\nu-A_\mu\phi_\nu{}^*\partial^\nu\phi^\mu\\&-\partial^\mu\phi_\nu{}^*A_\mu\phi^\nu+\partial_\nu\phi_\mu{}^*A^\mu\phi^\nu)\\&-e^2(A_\mu A^\mu\phi_\nu{}^*\phi^\nu-A_\mu A^\nu\phi^{\mu*}\phi_\nu),\end{aligned} \tag{2}$$

where e is positive, and ψ destroys a negatively charged fermion.

[4] We follow the notation of J. M. Jauch and F. Rohrlich, *Theory of Photons and Electrons* (Addison-Wesley Publishing Company, Inc., Reading, Massachusetts, 1955).