Spin Waves in an Interacting Electron Gas*

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Some previous results of the author in collaboration with H. Brooks are improved and corrected concerning the coefficient of q^2 in the spin-wave dispersion law in an electron gas interacting according to a Yukawa potential. A variational method of solution for the integral equation occurring in this theory is given which, besides giving the spin-wave energy correctly, also gives the spin-density-wave instability when extended suitably. Having uncovered the instability of the paramagnetic state, an alternative derivation of the new state is given by a Green's-function method. In an Appendix, a theory of spin-density waves in a Bloch electron system is outlined. The variational method given here seems to be of quite general use in solving similar problems in other contexts.

INTRODUCTION

OVERHAUSER'S[1] recent demonstration that a nonuniform static spin-density-wave state (SDW) is lower in energy than the uniform states (paramagnetic, P) in a Coulomb gas within the Hartree-Fock (HF) approximation has stirred a great deal of discussion in recent times. In fact, that such an SDW state may appear was suspected by Herring[2] when he discovered in the Coulomb gas a small region of densities (small within the approximations he was making) over which the ferromagnetic spin waves showed an instability. These investigations call for a good understanding of the nature of solutions to the spin-wave equation. The present paper is an attempt to make these concepts uniform through the help of a variational solution to such equations.

This paper is divided into three parts. We[3a] had earlier reported a calculation of the HF ground-state energy and of the spin-wave energy, in the long-wave limit in the random-phase approximation (RPA), of an electron gas interacting according to a Yukawa potential. The spin-wave energy was calculated as a function of the range of interaction and relative magnetization at $T=0°$K. In the first part we rectify our original solution to be in conformity with Herring,[2] by developing a variational solution to the equations in the long-wavelength limit. The Yukawa interaction is chosen because we have proved[3a,b] that in general the exchange interactions are screened by electron-electron interactions and so a Yukawa potential may well simulate most of the correlations in an interacting system. To be more precise, the exchange interactions are screened by a dynamic dielectric constant, which to the author's knowledge cannot be handled in any clear-cut manner without involving drastic assumptions, which make the conclusions rather dubious. The notations employed here are as in our previous work.[3a,b] It must be remarked that recently there have been many attempts to study spin waves in an interacting electron gas. Almost all these papers deal with a short-range interaction only and we refer the reader to Ref. 3b for a discussion of these. Having noted a possibility of an instability of the uniform ground state towards the formation of SDW, in the next part we discuss a similar variational principle to deal with zero frequency but finite wave vectors for spin waves. Using the solution of the noninteracting case as a trial function, we arrive at the condition for stability of static spin waves of finite wave vector, derived earlier by Iwamoto and Sawada[4] and Fukuda *et al.*[5] The finite-frequency and finite-vector case is also indicated. Recently, Fedders[6] has re-examined the SDW instability by employing a "t-matrix" method. [This t-matrix method, it should be pointed out, is not the same as the one used usually in the discussion of low-density problems. It is in fact, a variant of the random-phase-approximation (RPA) equations.] He has discussed also a variational method of the type introduced here, except that his is in terms of t-matrix components. The present work brings together the formulations of the long-wavelength spin-wave instability and static spin-wave instability. See, for a detailed discussion of these questions, the recent review article by Herring.[7] From this review article (Sec. Vc), it is found that there is a great deal of interest in the calculation of magnetic properties of a Yukawa gas. In the third part, we rederive the new state[1] by a Green's-function method.[3b] The inclusion of this derivation makes this article complete. This alternative derivation has a close resemblance to that of the gap equation for superconductors

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[2] C. Herring, Phys. Rev. **85**, 1003 (1952); **87**, 60 (1952).

[3a] A. K. Rajagopal and H. Brooks, *Proceedings of the International Conference on Magnetism, Nottingham, 1964* (The Institute of Physics and The Physical Society, London, 1965), p. 55.

[3b] A. K. Rajagopal, H. Brooks, and N. R. Ranganathan, Advanced Research Projects Agency Technical Report No. **11**, Harvard University, Cambridge, Massachusetts, 1964 (unpublished).

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[6] P. A. Fedders, Ph.D. thesis, Harvard University, Cambridge, Massachusetts, 1965 (unpublished); P. C. Martin and P. A. Fedders (unpublished).

[7] C. Herring, in *Magnetism*, edited by G. T. Rado and Suhl, (Academic Press Inc., New York, 1965), Vol. IIb.

by Nambu.[8] In the last section we summarize the results. In Appendix A we derive the equations for SDW states for Bloch electrons in a many-band complex based on a certain model. In Appendix B we take the opportunity of giving the complete set of equations describing the collective excitations in SDW systems. This serves as an addendum to our previous paper on the same subject in this journal[9] which contained only approximate equations specialized to short-range interactions.

LONG-WAVELENGTH SPIN WAVES

The correlation function

$$\chi_{+-}(11')=(1/i)\langle T(\hat{\sigma}_+(1)\hat{\sigma}_-(1'))\rangle, \qquad (1)$$

where $1=(\mathbf{r}_1t_1)$, T is Wick time ordering, and $\sigma_\pm=\sigma_x\pm i\sigma_y$ are the circular components of spin density, is related to the transverse spin susceptibility.[3a,b] $\hat{\sigma}$ stands for $\sigma-\langle\sigma\rangle$. Taking the space and time Fourier transforms we get after some manipulations,

$$\chi_{+-}(\mathbf{q},\omega)=-\int\frac{d^3\mathbf{q}_1}{(2\pi)^3}N_{\uparrow\downarrow}(\mathbf{q}_1\mathbf{q})\Gamma_{\uparrow\downarrow}(\mathbf{q}_1;\mathbf{q}\omega); \qquad (2)$$

$\chi_{+-}(\mathbf{q},\omega)$ is the generalized spin susceptibility, dependent on wave vector $\mathbf{q}$ and frequency ω; $N_{\uparrow\downarrow}(\mathbf{q}_1\mathbf{q})=n_F(\omega_\uparrow(\mathbf{q}_1+\mathbf{q}))-n_F(\omega_\downarrow(\mathbf{q}_1))$, with $n_F(x)$ standing for Fermi function; and $\omega_{\uparrow\downarrow}$ are the single-particle energies of the up- and down-spin states. $\Gamma_{\uparrow\downarrow}(\mathbf{q}_1;\mathbf{q}\omega)$ satisfies a certain integral equation to be quoted presently. The transverse spin susceptibility of physical interest involves a commutator in (1) instead of time ordering, and it is related to (2) by

$$\bar{\chi}_{+-}(\mathbf{q},\omega)=\lim_{\substack{\epsilon\to0^+\\(\epsilon,\,\text{real})}}\chi_{+-}(\mathbf{q},\omega+i\epsilon). \qquad (3)$$

In RPA including exchange processes, the equation satisfied by $\Gamma_{\uparrow\downarrow}$ is (we shall usually drop the subscript $\uparrow\downarrow$ from now on):

$$(\omega-\omega_{\uparrow\downarrow}(kq))\Gamma(k;q\omega)=-1+\int\mathcal{V}(k-k_1)N_{\uparrow\downarrow}(k_1q)\Gamma(k_1;q\omega)\frac{d^3k_1}{(2\pi)^3}. \qquad (4a)$$

The single-particle energies in the up- and down-spin states are

$$\omega_{\uparrow,\downarrow}(k)=|\mathbf{k}|^2/2m-\int\mathcal{V}(k-k_1)n_F(\omega_{\uparrow,\downarrow}(k_1))\frac{d^3k_1}{(2\pi)^3} \qquad (4b)$$

and

$$\omega_{\uparrow\downarrow}(kq)=\omega_\uparrow(k+q)-\omega_\downarrow(k). \qquad (4c)$$

Here $\mathcal{V}(k)$ is the Fourier transform of the interaction potential; its form is not specified here to keep the discussion quite general. For a general derivation of (4) employing Green's functions and variational derivative techniques, see Refs. 3(a) and 3(b). It was shown there that the bare $\mathcal{V}$ is in general screened by a generalized dynamic dielectric constant and hence in (4) we do not specify its form. [When $\mathcal{V}$ is dynamically screened, (4b) is an equation to be solved for ω, and there is an additional integration over frequency ω_1 in all the above; we imply it wherever necessary and do not explicitly exhibit it.] In what follows now and in most of the next section, unless mentioned, we treat $\mathcal{V}$ as statically screened; in the beginning of the next section when a generalized variational principle is developed we deal with a fully general interaction.

The purpose of the present section is to discuss the solution of Eq. (4a) by a variational method in the long-wavelength limit. First we let

$$\begin{gathered}\mathcal{V}(q-q_1)=(4\pi e^2/k_F^2)V(|q-q_1|),\\ y=k/k_F,\quad y_1=q_1/k_F,\quad x=q/k_F,\quad \omega=(k_F^2/2m)\nu,\\ \alpha=(4/9\pi)^{1/3}=0.521,\quad \alpha r_s/\pi=me^2/k_F,\\ k_F=\text{paramagnetic Fermi wave vector},\quad \hat{y}=(\theta,\phi),\end{gathered} \qquad (5)$$

where r_s is the effective electron-radius in the interacting system. Choosing x to be the z axis of a reference coordinate system so that $\cos\theta=(4\pi/3)^{1/2}Y_{10}(\theta,\phi)$, where Y_{lm} are the usual spherical harmonics, we write (4a) in the form:

$$\left\{\nu-x^2-2xy\left(\frac{4\pi}{3}\right)^{1/2}Y_{10}(\hat{y})+\left(\frac{\alpha r_s}{\pi^2}\right)\int d^3y_1V(|y-y_1|)N_{\uparrow\downarrow}(y_1;x)\right\}\Gamma(y;x\nu)$$
$$=-(2m/k_F^2)+(\alpha r_s/\pi^2)\int d^3y_1V(|y-y_1|)N_{\uparrow\downarrow}(y_1;x\nu)\Gamma(y_1;x\nu). \qquad (6)$$

To derive spin waves we need only consider the homogeneous part of (6), or the poles of (3) in the ω plane, and hence we drop the inhomogeneous term in Eq. (6). Let $x=0$ in the homogeneous equation; multiplying the resulting expression by $N_{\uparrow\downarrow}(y;0)$ and integrating over y, we find that a solution exists with

$$\nu=0\quad\text{and}\quad\Gamma(y;00)=\text{a constant}. \qquad (7)$$

[8] Y. Nambu, Phys. Rev. **117**, 648 (1960).
[9] A. K. Rajagopal, Phys. Rev. **137**, A1429 (1965).

Multiplying (6) through by $N_{\uparrow\downarrow}(y;x)$ and integrating over y, we get after some manipulation (we assume V to be symmetric here):

$$\nu=x^2+2x\left(\frac{4\pi}{3}\right)^{1/2}\int d^3y\,(2\pi)^{-3}yY_{10}(\hat{y})N_{\uparrow\downarrow}(y;x)\Gamma(y;x)\bigg/\int d^3y\,(2\pi)^{-3}N_{\uparrow\downarrow}(y;x)\Gamma(y;x). \tag{8}$$

Let us write

$$\begin{aligned}N_{\uparrow\downarrow}(y;x)&=N_{\uparrow\downarrow}(y;0)+\sum_{i=1}^{\infty}\sum_{l=0}^{\infty}x^iY_{l0}(\hat{y})N_{\uparrow\downarrow l}{}^{(i)}(y),\\ \Gamma(y;x)&=\Gamma^{(0)}+\sum_{j=1}^{\infty}\sum_{l'=0}^{\infty}\sum_{m'=-l'}^{+l'}x^jY_{l'm'}(\hat{y})\Gamma_{l'm'}{}^{(j)}(y).\end{aligned} \tag{9}$$

Only Y_{l0} appears in the expansion of $N_{\uparrow\downarrow}$, since the left-hand side is seen to contain only y. Working then to lowest order in x, we get

$$\nu\sim x^2+2x^2\left(\frac{4\pi}{3}\right)^{1/2}\left\{\frac{\int y^3N_{\uparrow\downarrow}(y;0)\Gamma_{10}{}^{(1)}(y)dy+\Gamma^{(0)}\int y^3N_{\uparrow\downarrow1}{}^{(1)}(y)dy}{4\pi\Gamma^{(0)}\int y^2N_{\uparrow\downarrow}(y;0)dy}\right\}. \tag{10}$$

Let us choose

$$\Gamma^{(0)}=(3/4\pi)^{1/2}(\alpha r_s/\pi). \tag{11}$$

Then (reverting to the original notation),

$$\omega_{\mathrm{SW}}\sim(q^2/2m\zeta)\{1+(\pi/\alpha r_s)S(\zeta)\}, \tag{12}$$

$$S(\zeta)=\int dy\,y^3N_{\uparrow\downarrow}(y;0)\Gamma_{10}{}^{(1)}(y). \tag{13}$$

Here ζ is the relative magnetization of the system. The above derivation shows that the spin-wave frequency in the long-wavelength limit is proportional to the square of the wave vector. We must point out that the first term in (12) arises purely from the kinetic motions of the electrons and the second term, which is proportional to $(\pi/\alpha r_s)$, comes from the readjustment of the system due to the interaction between electrons. Thus we see that in this limit the only term of interest is S, which is determined by solving the equation for $\Gamma_{10}{}^{(1)}$, which we proceed to formulate now. Quite generally we can write for potentials of the form $V(|y-y_1|)$,

$$V(|y-y_1|)=\frac{2\pi}{yy_1}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}Q_l(y;y_1)Y_{lm}(\hat{y})Y_{lm}{}^*(\hat{y}_1), \tag{14}$$

where

$$\frac{1}{yy_1}Q_l(y;y_1)=\int_{-1}^{+1}d\mu P_l(\mu)V(|y-y_1|). \tag{15}$$

Note that $Q_l(y;y_1)$ is symmetrical like $V(|y-y_1|)$.

[$P_l(\mu)$ is the usual Legendre polynomial of order l.] (15′)

Here Y_{lm}'s are such that

$$\int d\hat{y}\,Y_{lm}(\hat{y})Y_{l'm'}{}^*(\hat{y})=\delta_{ll'}\delta_{mm'} \tag{16}$$

and

$$\int d\hat{y}=\int_{-1}^{+1}d\mu\int_0^{2\pi}d\phi.$$

For the Yukawa potential, we find

$$Q_l(y;y_1)=Q_l\left(\frac{y^2+y_1{}^2+\xi^2}{2yy_1}\right), \tag{17}$$

where we have taken

$$V(|y|)=1/(|y|^2+\xi^2), \tag{18}$$

ξ is a dimensionless screening parameter, and

$$Q_l(x)=\frac{1}{2}\int_{-1}^{+1}\frac{P_l(\mu)d\mu}{x-\mu} \tag{19}$$

is the Legendre function of the second kind. The equation satisfied by $\Gamma_{lm}^{(1)}$ is then found to be (taking $\nu=\nu_2x^2$)

$$-2y\left(\frac{4\pi}{3}\right)^{1/2}Y_{10}(\hat{y})\Gamma^{(0)}+2\left(\frac{\alpha r_s}{\pi y}\right)\sum_{l'm'}Y_{l'm'}(\hat{y})\Gamma_{l'm'}^{(1)}(y)\int y_1N_{\uparrow\downarrow}(y_1;0)Q_0(y;y_1)dy_1$$
$$=2\left(\frac{\alpha r_s}{\pi y}\right)\sum_{l'm'}Y_{l'm'}(\hat{y})\int y_1N_{\uparrow\downarrow}(y_1;0)Q_{l'}(y;y_1)\Gamma_{l'm'}^{(1)}(y_1). \quad (20)$$

Multiplying this by $Y_{lm}^*(y)$ and integrating over y, we get

$$-2y\left(\frac{4\pi}{3}\right)^{1/2}\Gamma^{(0)}\delta_{l1}\delta_{m0}+2\left(\frac{\alpha r_s}{\pi y}\right)\left[\int dy_1y_1N_{\uparrow\downarrow}(y_1;0)Q_0(y;y_1)\right]\Gamma_{lm}^{(1)}(y)$$
$$=2\left(\frac{\alpha r_s}{\pi y}\right)\int dy_1y_1N_{\uparrow\downarrow}(y_1;0)Q_l(y;y_1)\Gamma_{lm}^{(1)}(y_1). \quad (20')$$

Note that for $l\neq1$, $m\neq0$, we get homogeneous equations for $\Gamma_{\uparrow\downarrow lm}^{(1)}$, which can therefore be taken to be zero without loss of generality. Also, only $\Gamma_{10}^{(1)}$ appears in the expression for ν_2 (or ω_{SW}) so that we need to consider only the equation for it. Using (11) for $\Gamma^{(0)}$, which now becomes trivial, we finally obtain

$$-y^2+\left[\int dy_1y_1N_{\uparrow\downarrow}(y_1;0)Q_0(y;y_1)\right]\Gamma_{10}^{(1)}(y)=\int dy_1y_1N_{\uparrow\downarrow}(y_1;0)Q_1(y;y_1)\Gamma_{10}^{(1)}(y_1). \quad (21)$$

From now on we write

$$\psi(y)=\Gamma_{10}^{(1)}(y_1). \quad (21')$$

Earlier[3a,b] we solved this equation for the case of a Yukawa potential by a series method. We will discuss this solution in comparison with Herring's[2] work and the present variational solution at the end of this section. At $T=0°\mathrm{K}$, we must point out that $N_{\uparrow\downarrow}(y;0)$ is the difference between two positive unit step functions,

$$N_{\uparrow\downarrow}(y;0)=n_F(\omega_\uparrow(y))-n_F(\omega_\downarrow(y))=\eta_+((1+\zeta)^{1/3}-y)-\eta_+((1-\zeta)^{1/3}-y), \quad (22)$$

where $\eta_+(x)$ is the positive unit step function. This then gives the limits of integration over y, in all the above expressions. Equation (21) may be written in a symmetrical form, thus

$$y^3+\varphi(y)\psi(y)=\int_b^a K(y,y_1)\psi(y_1)dy_1, \quad (23)$$

where

$$\varphi(y)=\int_b^a yy_1Q_0(y;y_1)dy_1,$$
$$K(y,y_1)=yy_1Q_1(y;y_1)=K(y_1,y), \quad (24)$$

since Q_1 is symmetric. Further

$$a=(1+\zeta)^{1/3} \text{ and } b=(1-\zeta)^{1/3}. \quad (24')$$

We now solve (23) by constructing a variational method. Consider the functional

$$J(\psi)=2\int_b^a y_1^3\psi(y_1)dy_1+\int_b^a\varphi(y_1)\psi^2(y_1)dy_1-\iint_b^a\psi(y_1)K(y_1y_2)\psi(y_2)dy_1dy_2. \quad (25)$$

The Euler equation corresponding to first-order variations in $\psi(y)$ is (23). Inserting (23) in this functional J, we arrive at

$$J_{\mathrm{ext}}(\psi)=\int_b^a y^3\psi(y)dy\equiv S(\zeta) \quad (26)$$

from (13). J_{ext} is the extremum of J for such ψ. This variational principle therefore gives an extremum on S and hence seems more reliable than our previous series solution. So far we have been discussing in general terms without specific reference to the form of V.

We now specialize our results to the Yukawa potential (18), in which case we have specifically

$$Q_0(y;y_1)=\tfrac{1}{2}\ln\left(\frac{\xi^2+(y+y_1)^2}{\xi^2+(y-y_1)^2}\right), \tag{27a}$$

$$Q_1(y;y_1)=\left[\left(\frac{y^2+y_1^2+\xi^2}{4yy_1}\right)\ln\left(\frac{(y+y_1)^2+\xi^2}{(y-y_1)^2+\xi^2}\right)-1\right]. \tag{27b}$$

And

$$\phi(y)=y^2\left[\left\{a+\left(\frac{\xi^2+a^2-y^2}{4y}\right)\ln\left(\frac{\xi^2+(a+y)^2}{\xi^2+(y-a)^2}\right)-\xi\left(\tan^{-1}\left(\frac{a+y}{\xi}\right)+\tan^{-1}\left(\frac{a-y}{\xi}\right)\right)\right\}-\{(a\leftrightarrow b)\}\right], \tag{27c}$$

$$K(yy_1)=\left[\tfrac{1}{4}(y^2+y_1^2+\xi^2)\ln\left(\frac{\xi^2+(y+y_1)^2}{\xi^2+(y-y_1)^2}\right)-yy_1\right]. \tag{27d}$$

We try as a trial function,

$$\psi(y)=Ay. \tag{28}$$

Then,

$$\begin{aligned}J(A)=\tfrac{2}{5}A(a^5-b^5)+A^2\{&\tfrac{1}{9}(a^3-b^3)^2-\tfrac{1}{4}\xi^2(a-b)(a^3-b^3)+(\xi^4/24)(a-b)^2\\&-\tfrac{1}{16}\xi^2(a^2-b^2)^2L(a,b)-\tfrac{1}{8}\xi^4[a^2L(a,a)+b^2L(b,b)-(a^2+b^2)L(a,b)]-(\xi^6/96)(L(a,a)+L(b,b)-2L(a,b))\\&+\tfrac{1}{3}\xi^3[a^3(T(a,a)-T(a,b)-T(-a,b))+b^3(T(b,b)-T(a,b)-T(-a,b))]\},\end{aligned} \tag{29}$$

$$L(a,b)=\ln\left(\frac{(a+b)^2+\xi^2}{(a-b)^2+\xi^2}\right),\quad T(a,b)=\tan^{-1}((b+a)/\xi). \tag{30}$$

Hence A is determined and thus

$$\omega_{\rm SW}\sim(q^2/2m\zeta)\{1+(\pi/\alpha r_s)\tfrac{1}{5}(a^5-b^5)A\}. \tag{31}$$

We must remark here that the linear term in (28) is itself sufficient to bring out all the main features of the calculation; as found by Herring,[2] the higher-order terms in powers of y in (28) do not give any more valuable information than the linear one, and even it gives a better numerical estimate of A only in the ferromagnetic (F) state. In the paramagnetic limit, however, it always gives the same result as that found by a ground-state condition to be discussed presently, as indeed it must.

We would like to remark here that Herring[2] had earlier developed an expression similar to (13) for the spin-wave frequency in the long-wavelength limit but only for the F state, both for the Coulomb gas ($\xi=0$) and for the Stoner gas ($\xi\to\infty$), based on a perturbation approach to the HF equations given earlier by Peng.[10] The author recently found, in response to a query by Herring and Brooks, that Peng's approach is equivalent to RPA quite generally[11] and so the equivalence of Herring's expression with (13) here is not surprising even though our methods are quite different.

The functional $J(\psi)$ introduced here makes S a *minimum* for the Yukawa and similar potentials when ψ is taken as a power series in y, and hence we arrive at a *lower bound* on $\omega_{\rm SW}$ (as S turns out to be negative).

We will now discuss this solution in the light of our previous result[3a,b] and Herring's result.[2] We follow Herring's[7] discussion of these problems. In the limit when $\xi\to\infty$, we have the Stoner model and we obtain from (29,30),

$$A_{\rm St}=-(3\xi^2/4\zeta),$$

$$\omega_{\rm SW}(\text{Stoner})=q^2/2m\zeta\left\{1-\frac{2}{5(K\theta'/\epsilon_F)}\left(\frac{a^5-b^5}{a^3-b^3}\right)\right\}, \tag{32}$$

where

$$K\theta'/\epsilon_F=\text{Stoner parameter}=\tfrac{4}{3}(\alpha r_s/\pi\xi^2). \tag{32'}$$ [3a,b]

In this limit, the equation for the spin waves can be solved exactly also, and indeed this coincides with the exact answer.[3a,b] Also, consideration of the stability of the HF ground state has shown that there are three types of states: P, F, and UF, the unsaturated ferromagnetic states, ($0<\zeta<1$). The spin waves are stable, i.e., $\omega_{\rm SW}>0$,[7] in the range of $K\theta'/\epsilon_F$ where the ground states are stable, and vice versa. This is in complete conformity with a theorem due to Thouless[12] and Fukuda,[13] which states: The stability of the HF ground state against any small deformation preserving the single-particle nature of the wave function ensures the

[10] H. W. Peng, Proc. Roy. Soc. (London) **A178**, 499 (1941).

[11] A. K. Rajagopal, Advanced Research Projects Agency Technical Report No. 15, Harvard University, Cambridge, Massachusetts, 1965 (unpublished).

[12] D. J. Thouless, Nucl. Phys. **21**, 225 (1960).

[13] N. Fukuda, Nucl. Phys. **44**, 553 (1963).

stability of the collective motions in RPA, and vice versa. This is not surprising, since Overhauser[1] had already shown that there are no SDW instabilities in the short-range gas. In this limit, many other general features of the spin waves in an electron gas can be explicitly computed, such as the existence of a maximum wave vector beyond which the spin waves are dynamically unstable, and so on; and these are dealt with in Refs. 3a,b. In the Coulomb limit ($\xi=0$), we have

$$A_c=(-9/5)[(a^5-b^5)/(a^3-b^3)^2],$$

$$\omega_{\mathrm{SW}}(\text{Coulomb})=(q^2/2m\zeta)\left[1-\frac{9\pi}{25\alpha r_s}\left(\frac{a^5-b^5}{a^3-b^3}\right)^2\right]. \quad (33)$$

For the F state ($\zeta=1$),

$$\omega_{\mathrm{SW}}{}^F(\text{Coulomb})\sim(q^2/2m)[1-5.4699/r_s], \quad (34)$$

and for the P state ($\zeta\sim0$),

$$\omega_{\mathrm{SW}}{}^P(\text{Coulomb})\sim(q^2/2m\zeta)[1-(\pi/\alpha r_s)]. \quad (35)$$

The differential stability condition for the Coulomb gas in HF is[3b]

$$(\alpha r_s/\pi)=\tfrac{1}{2}(a+b). \quad (36)$$

In the limit $\zeta\rightarrow0$, the coefficient of q^2 for ω_{SW} coincides with the corresponding result in (36). However, it must be remarked that the UF states are unstable in this case since they are states of relative maxima.[3a,b] Hence it was deduced that F states are stable in HF if

$$r_s>5.45\ (\approx0.9/\alpha) \quad (36')$$

by just comparing the P- and F-state energies.

Previously,[3a,b] we had reported a series solution for Γ. Using three terms in the series as an approximation, in the F state, we found,

$$\omega_{\mathrm{SW}}{}^{(3)}(\text{Coulomb})\sim(q^2/2m)(1-5.3447/r_s), \quad (37\text{a})$$

whereas Herring[2] obtained

$$\omega_{\mathrm{SW}}{}^{\mathrm{Herring}}(\text{Coulomb})\sim(q^2/2m)(1-5.485/r_s). \quad (38)$$

This series solution is now improved by taking 4, 5 terms in the series and we obtained, respectively,

$$\omega_{\mathrm{SW}}{}^{(4)}(\text{Coulomb})\sim(q^2/2m)(1-5.4106/r_s), \quad (37\text{b})$$

$$\omega_{\mathrm{SW}}{}^{(5)}(\text{Coulomb})\sim(q^2/2m)(1-5.4416/r_s). \quad (37\text{c})$$

If Herring's calculation is correct, then in view of the ground-state criterion (36′), the implication is that there is a small but finite range of densities between $r_s=5.45$ and 5.485, over which a static spin wave of finite q has a lower HF energy than either of the uniform states. Using a better solution would only give a value of r_s larger than 5.485, so that the range of densities depends on the approximation. The range is not very important but the indication of the instability is quite significant. Note that none of our solutions corresponding to series solutions, (37a,b,c), gives this instability (though they probably would if more terms were taken) whereas our new variational solution (34) does give it. In view of Overhauser's[1] discovery, the instability of the spin wave in the long-wavelength limit is not surprising; thus all these results are in concordance with each other and with the theorem of Thouless[12] and Fukuda[13] quoted earlier. Thus when $r_s<5.4699$ ($<\pi/\alpha$) there is an instability for $q\approx0$, and by continuity, when $r_s<5.4699+\eta$ (η is a positive number), there is still an instability for small but finite q. These are hints of the SDW instability, which is not pronounced for larger q. (I am grateful to Professor Paul Martin for this comment.) Thus Herring's calculation (38) is correct. The result (31) is valid for all ξ and ζ, and this was not reported in our earlier communication.[3a,b]

STATIC SPIN DENSITY WAVES

An alternative proof of Overhauser's[1] assertion that the SDW is more stable than the P state in an unscreened Coulomb gas in HF was given by Fukuda *et al.*[5] Amusia[14] has very recently proved that such an instability does not occur if the bare Coulomb interaction is screened, using a Landau-theoretic argument for a SDW. On the formal level, Fano[15] has quite recently shown that SDW states are exact in the same sense as the BCS superconductive states are. De Graaf and Luzzi[16,17] have very recently proposed a reformulation of SDW states in terms of the Landau theory of Fermi liquids. Iwamoto and Sawada[4] discussed only the instability of the P state towards the F state in a Yukawa gas. We[3a,b] dealt with this problem in greater detail than Iwamoto and Sawada[4] in that we investigated the stability problem for all magnetizations. We found that there exists a $\xi_{\max}$ below which the system is either F or P with UF being states of relative maxima just as in a Coulomb gas, and above $\xi_{\max}$ there are regions of all three magnetizations possible as in a Stoner gas. Very recently Fedders[6] has examined this problem for the existence of SDW states. He found that there exists a $\xi_{\max}$ below which SDW states are lower in energy than P states, just as in the Coulomb gas, and above which there are no SDW states at all, as in a Stoner gas—quite analogous to our result. For Thomas-Fermi screening we both found that the system remains in the P state. Fedders has also examined the case of the dynamically screened interaction, although not so completely. He suspects from his rough estimates that SDW states almost certainly are not present, in quite the same manner as Amusia[14] concluded from his Landau theory. In view of SDW states, it is natural to ask whether our variational principle can be generalized so as to indi-

[14] M. Ya. Amusia, Phys. Letters **16**, 254 (1965).
[15] G. Fano, Nuovo Cimento **38**, 597 (1965).
[16] A. M. De Graaf and R. Luzzi, Nuovo Cimento **38**, 285 (1965).
[17] A. M. De Graaf and R. Luzzi, Phys. Letters **16**, 256 (1965).

cate this instability. We now construct a variational principle for the spin-wave problem valid for finite q,ω and derive therefrom the SDW instability also.

Let us consider Eq. (4a) for Γ, and construct a variational solution for it. Let us note that for all q,ω in general, Γ and χ_{+-} are complex. The complex conjugate Γ^* satisfies an equation similar to Eq. (4a). We treat ω here as a real parameter. Then consider the functional,

$$J(\Gamma,\Gamma^*)=\int(\omega-\omega_{\uparrow\downarrow}(kq))\Gamma^*(k;q\omega)\Gamma(k;q\omega)N_{\uparrow\downarrow}(kq)\frac{d^3k}{(2\pi)^3}+\int N_{\uparrow\downarrow}(kq)$$
$$\times(\Gamma(k;q\omega)+\Gamma^*(k;q\omega))\frac{d^3k}{(2\pi)^3}-\int\int\mathcal{V}(k-k_1)N_{\uparrow\downarrow}(k_1q)\Gamma(k_1;q\omega)N_{\uparrow\downarrow}(kq)\Gamma^*(k;q\omega)\frac{d^3k_1d^3k}{(2\pi)^6}. \quad (39)$$

Treating Γ^* and Γ as independent, the Euler equation corresponding to variations of Γ^* is the equation (4a) for Γ. Similarly we get the corresponding equation for Γ^* when Γ is varied. Thus Γ and Γ^* are extremum solutions of the variational problem with J as the Lagrangian. Substituting these in Eq. (39) we arrive at

$$J_{\text{ext}}(\Gamma,\Gamma^*)=-\tfrac{1}{2}[\chi_{+-}(q,\omega)+\chi_{+-}^*(q\omega)]. \quad (40)$$

The above variational principle will now be applied to the special case where $\omega=0$, so that we study the static spin susceptibility. If $\chi_{+-}(q,\omega=0)>0$ for some finite q, then there appears an SDW instability. In this case, Γ and χ_{+-} are real. The above functional is just

$$J(\Gamma)=\int(\omega-\omega_{\uparrow\downarrow}(kq))N_{\uparrow\downarrow}(kq)\Gamma^2(k,q)\frac{d^3k}{(2\pi)^3}$$
$$+2\int N_{\uparrow\downarrow}(kq)\Gamma(k;q)\frac{d^3k}{(2\pi)^3}-\int\int\mathcal{V}(k-k_1)N_{\uparrow\downarrow}(k_1q)N_{\uparrow\downarrow}(kq)\Gamma(k_1;q)\Gamma(k;q)\frac{d^3kd^3k_1}{(2\pi)^6} \quad (39')$$

and

$$J_{\text{ext}}(\Gamma)=-\chi_{+-}(q,0). \quad (41)$$

In Appendix B of Fedders'[6] thesis a similar variational procedure is given involving his t matrices. Following Herring[7] (Sec. 3) we assert that $\chi_{+-}(q,0)>0$ is necessary for stable spin waves for any q but with zero frequency. Iwamoto and Sawada[4] and Fukuda *et al.*[5] have developed a variational estimate of the existence of a SDW by examining the stability of the P state towards static spin-density fluctuations and do not give a corresponding expression for the susceptibility. We will derive from the above a similar estimate, valid for all magnetizations and finite temperatures, unlike the authors quoted here.[4,5,16,17] De Graaf *et al.*[17] have also calculated the spin susceptibility using the Landau theory. To this end let us assume $\lambda(q)\Gamma(k;q0)$ to be a trial function and vary λ. Then we find

$$\chi_{+-}(q,\omega=0)=\frac{-\int N_{\uparrow\downarrow}(kq)\Gamma(k;q)\frac{d^3k}{(2\pi)^3}}{(k_F^2/8\pi^2m)[N(q\zeta)-(\alpha r_s/\pi)(D_1(q\zeta)-D_2(q\zeta))]}, \quad (42)$$

where N, D_1, and D_2 are similar to those derived by Iwamoto *et al.*,[4] except that this expression is valid for a general potential of interaction V just as in (5), including screening. Thus,

$$N(q\zeta)=\int(|y+x|^2-y^2)N_{\uparrow\downarrow}(yx)\Gamma^2(y;x)\frac{d^3y}{2\pi},$$
$$D_1(q\zeta)=\int\int V(|y-y_1|)N_{\uparrow\downarrow}(y_1x)N_{\uparrow\downarrow}(yx)\Gamma^2(y_1;x)\frac{d^3yd^3y_1}{2\pi^3}, \quad (43)$$
$$D_2(q\zeta)=\int\int V(|y-y_1|)N_{\uparrow\downarrow}(y_1x)N_{\uparrow\downarrow}(yx)\Gamma(y_1;x)\Gamma(y;x)\frac{d^3yd^3y_1}{2\pi^3},$$

using the notation defined in (5). The static spin wave then is unstable if $\chi_{+-}(q,\omega=0)\leq 0$, and this happens if

$$\left(\frac{\alpha r_s}{\pi}\right)\leq\left[\frac{N(q\zeta)}{D_1(q\zeta)-D_2(q\zeta)}\right]. \tag{44}$$

For $\zeta=0$ this condition is the same as that derived by Iwamoto and Sawada,[4] with Γ replaced by the noninteracting solution, namely $[1/(|y+x^2|-|x|^2)]$. The same procedure could be used here to investigate the Yukawa case; for the results we refer the reader to Fedders,[6] whose work we have described already.

We must point out here that the instability of the ground state towards the formation of SDW states is only one part of the problem. Once this instability is discovered, and all the effort so far has been directed towards this, we must examine the properties of this new state. This is done in the next section by a Green's-function method.[3b]

GREEN'S-FUNCTION DESCRIPTION OF SDW STATES

In this section we follow closely the procedure given in Ref. 3b. An alternative derivation of Overhauser's[1] equations by a canonical-transformation method has been recently given by Yan Shi.[18] This was employed by the author[9] to study the collective properties of SDW systems. Here we outline another derivation of the Overhauser equations based on a Green's-function technique. In Appendix A we generalize this procedure to include certain SDW correlations among band electrons. In Appendix B, we describe the collective states in SDW systems in a more general form than was given originally.[9] The derivation given here includes dynamic screening also. We define a 2×2 matrix Green's function with components (following Ref. 3b):

$$G_{\sigma\sigma'}(11')=(1/i)\langle T(\psi_\sigma(1)\psi_{\sigma'}{}^\dagger(1'))\rangle \quad (\sigma,\sigma'=\uparrow,\downarrow)$$

in the usual notation.[3b] From Eq. (2.1.28)[3b] we have the equation for the inverse G^{-1}:

$$G^{-1}(11')=\left\{i\frac{\partial}{\partial t_1}+\frac{\nabla_1{}^2}{2m}-V(1)\right\}\delta^{(4)}(1-1')+i\int d^4\bar{4}\,V(1;\bar{4}1')G(\bar{4}1'), \tag{45}$$

where

$$V(1;\bar{4}1')=\int d^4\bar{3}\,\mathcal{V}(1-\bar{3})\Gamma_0(\bar{4}1';\bar{3}). \tag{46}$$

[A positive background is assumed and this cancels the direct Coulomb term in (45).] $\mathcal{V}(1-1')$ is the bare interaction; Γ_0 is a vertex part corresponding to density fluctuations and is related to the dielectric constant of the system. In the k space the last term in (45) takes the form

$$\int\frac{d^4k_1}{(2\pi)^4}\frac{\mathcal{V}(k-k_1)}{\epsilon(k-k_1)}G(k_1)\Lambda_0(k;k-k_1),$$

where ϵ is a generalized dielectric constant involving a modified vertex part Λ_0, whose integral equation may be found in Refs. 3a and 3b. In RPA, $\Lambda_0=-1$ and ϵ is the usual RPA dielectric constant, thus exhibiting the usual dielectric screening of the exchange. From now on we shall not retain the dielectric constant but shall subsume it in the definition of the interaction potential. The equation (45) is a 2×2 matrix equation (i.e., G, Γ_0, and Λ_0 are matrices) and we will not make it more specific unless necessary. (ϵ is a scalar.)

The symmetry-breaking solutions of (45) will now be shown to lead to Overhauser's[1] equations. Overhauser derived them only for HF states, a case which obtains in our formulation if we take $\Gamma_0(12;3)=-\delta^{(4)}(1-2)\times\delta^{(4)}(1-3)$. In (45) $V(r)$ is the one-particle periodic potential, which is not considered here but is taken into account in Appendix A. Following Overhauser,[1] we associate a plane wave of the form $\exp(i\mathbf{k}\cdot\mathbf{r})$ with the up-spin electron and $\exp(i(\mathbf{k}+\mathbf{Q})\cdot\mathbf{r})$ with the down-spin electron. Here $\mathbf{Q}$ is a measure of the breaking of the translation symmetry. Correspondingly, we define

$$\begin{aligned}
G_{\uparrow\uparrow}(11')&=\int\frac{d^3\mathbf{k}'}{(2\pi)^3}e^{i\mathbf{k}'\cdot(\mathbf{r}_1-\mathbf{r}_{1'})}G_{\uparrow\uparrow}(\mathbf{k}';t_1-t_{1'}),\\
G_{\downarrow\downarrow}(11')&=\int\frac{d^3\mathbf{k}'}{(2\pi)^3}e^{i(\mathbf{k}'+\mathbf{Q})\cdot(\mathbf{r}_1-\mathbf{r}_{1'})}G_{\downarrow\downarrow}(\mathbf{k}';t_1-t_{1'}),\\
G_{\uparrow\downarrow}(11')&=\int\frac{d^3\mathbf{k}'}{(2\pi)^3}e^{i\mathbf{k}'\cdot\mathbf{r}_1-i(\mathbf{k}'+\mathbf{Q})\cdot\mathbf{r}_1'}G_{\uparrow\downarrow}(\mathbf{k}';t_1-t_{1'}),\\
G_{\downarrow\uparrow}(11')&=\int\frac{d^3\mathbf{k}'}{(2\pi)^3}e^{i(\mathbf{k}'+\mathbf{Q})\cdot\mathbf{r}_1-i\mathbf{k}'\cdot\mathbf{r}_1'}G_{\downarrow\uparrow}(\mathbf{k}';t_1-t_{1'}).
\end{aligned}\tag{47}$$

Then Eq. (45) with (RPA) screened potential takes the form (we use a four-dimensional notation; here we have taken Fourier transforms in time also)

$$G^{-1}(k)=\begin{pmatrix}\omega-\epsilon_\uparrow(k) & -g_{\uparrow\downarrow}(k)\\ -g_{\downarrow\uparrow}(k) & \omega-\epsilon_\downarrow(k)\end{pmatrix}, \tag{48}$$

[18] Yan Shi, Dokl. Akad. Nauk SSSR **153**, 798 (1963) [English transl.: Soviet Phys.—Doklady **8**, 1171 (1964)].

where

$$\begin{aligned}
\epsilon_\uparrow(k)&=k^2/2m+i\int \mathcal{V}(k-k')G_{\uparrow\uparrow}^<(k'\omega')e^{i\omega'0^+}d^3k'd\omega'/(2\pi)^4,\\
\epsilon_\downarrow(k+Q)&=|\mathbf{k}+\mathbf{Q}|^2/2m+i\int \mathcal{V}(k-k')G_{\downarrow\downarrow}^<(k'\omega')e^{i\omega'0^+}d^3k'd\omega'/(2\pi)^4,\\
g_{\uparrow\downarrow}(k)&=i\int \mathcal{V}(k-k')G_{\uparrow\downarrow}^<(k'\omega')e^{i\omega'0^+}d^3k'd\omega'/(2\pi)^4,\\
g_{\downarrow\uparrow}(k)&=i\int \mathcal{V}(k-k')G_{\downarrow\uparrow}^<(k'\omega')e^{i\omega'0^+}d^3k'd\omega'/(2\pi)^4.
\end{aligned}\tag{49}$$

Thus inverting we arrive at

$$G(k,\omega)=\frac{1}{[\omega-\omega_+(k)][\omega-\omega_-(k)]}\begin{pmatrix}\omega-\epsilon_\downarrow(k+Q) & g_{\uparrow\downarrow}(k)\\ g_{\downarrow\uparrow}(k) & \omega-\epsilon_\uparrow(k)\end{pmatrix},\tag{50}$$

where

$$\omega_\pm(k)=\tfrac{1}{2}(\epsilon_\uparrow(k)+\epsilon_\downarrow(k+Q))\mp[\tfrac{1}{2}(\epsilon_\uparrow(k)-\epsilon_\downarrow(k+Q))^2+g_{\uparrow\downarrow}(k)g_{\downarrow\uparrow}(k)]^{1/2}.\tag{51}$$

Casting the terms in (50) into partial fractions and defining

$$\begin{aligned}
\cos^2\theta_k&=\left[\frac{\omega_+(k)-\epsilon_\downarrow(k+Q)}{\omega_+(k)-\omega_-(k)}\right]=\frac{g_{\uparrow\downarrow}(k)g_{\downarrow\uparrow}(k)}{(\omega-\epsilon_\uparrow(k))^2+g_{\uparrow\downarrow}(k)g_{\downarrow\uparrow}(k)},\\
\cos^2\theta_k\,\sin^2\theta_k&=\frac{g_{\uparrow\downarrow}(k)g_{\downarrow\uparrow}(k)}{(\omega_+(k)-\omega_-(k))^2}=\frac{g_{\uparrow\downarrow}(k)g_{\downarrow\uparrow}(k)}{4[([\epsilon_\uparrow(k)-\epsilon_\downarrow(k+Q)]/2)^2+g_{\uparrow\downarrow}(k)g_{\downarrow\uparrow}(k)]}.
\end{aligned}\tag{52}$$

(The simplified forms at the end of (52) are obtained after some manipulations); we obtain the Green's function describing Overhauser states:

$$G(k\omega)=\begin{pmatrix}[\cos^2\theta_k g_+(k\omega)+\sin^2\theta_k g_-(k\omega)] & \cos\theta_k\,\sin\theta_k(g_{\uparrow\downarrow}(k)/g_{\downarrow\uparrow}(k))^{1/2}(g_+(k\omega)-g_-(k\omega))\\ \cos\theta_k\,\sin\theta_k(g_{\downarrow\uparrow}(k)/g_{\uparrow\downarrow}(k))^{1/2}(g_+(k\omega)-g_-(k\omega)) & [\sin^2\theta_k g_+(k\omega)+\cos^2\theta_k g_-(k\omega)]\end{pmatrix}.\tag{53}$$

Here

$$g_\pm(k\omega)=1/(\omega-\omega_\pm(k)).\tag{54}$$

These, substituted back in (49), give

$$\begin{aligned}
\epsilon_\uparrow(k)&=k^2/2m-\int\frac{d^3k'}{(2\pi)^3}\mathcal{V}(k-k')\{\cos^2\theta_{k'}n_F(\omega_+(k'))+\sin^2\theta_{k'}n_F(\omega_-(k'))\},\\
\epsilon_\downarrow(k+Q)&=|\mathbf{k}+\mathbf{Q}|^2/2m-\int\frac{d^3k'}{(2\pi)^3}\mathcal{V}(k-k')\{\sin^2\theta_{k'}n_F(\omega_+(k'))+\cos^2\theta_{k'}n_F(\omega_-(k'))\},\\
g_{\uparrow\downarrow}(k)&=\int\frac{d^3k'}{(2\pi)^3}\mathcal{V}(k-k')\left(\frac{g_{\uparrow\downarrow}(k')}{g_{\downarrow\uparrow}(k')}\right)^{1/2}\cos\theta_{k'}\,\sin\theta_{k'}[n_F(\omega_+(k'))-n_F(\omega_-(k'))],\\
g_{\downarrow\uparrow}(k)&=\int\frac{d^3k'}{(2\pi)^3}\mathcal{V}(k-k')\left(\frac{g_{\downarrow\uparrow}(k')}{g_{\uparrow\downarrow}(k')}\right)^{1/2}\cos\theta_{k'}\,\sin\theta_{k'}[n_F(\omega_+(k'))-n_F(\omega_-(k'))],
\end{aligned}\tag{55}$$

$n_F(x)$ is the usual Fermi function. If we take $g_{\uparrow\downarrow}=g_{\downarrow\uparrow}=g$, and assume that only $\omega_+(k)$ is occupied, and $T=0°$K, then we recover all of Overhauser's[1] results. Moreover, this generalizes the original Overhauser results for finite temperatures, nonzero magnetizations (Overhauser had up and down spins equally populated to start with), and a larger class of interaction potentials. We may point out here that if we put $\mathbf{Q}=0$ in these equations, we recover a variant of Stoner's results[3b] as indeed we must. Another point worth mentioning is that if we take the limit of small g, we arrive at the static spin-wave equation (homogeneous counterpart), as is also to be expected.

For the sake of completeness we derive here the expression for the total energy of the system, $\langle H\rangle/\Omega_0$, in the SDW state using the Green's function (53).

$$\langle H\rangle/\Omega_0=\int\frac{d^3q}{(2\pi)^3}\bigg[\bigg(\frac{q^2}{2m}\cos^2\theta_q+\frac{|q+Q|^2}{2m}\sin^2\theta_q\bigg)n_F(\omega_+(q))+\bigg(\frac{q^2}{2m}\sin^2\theta_q+\frac{|q+Q|^2}{2m}\cos^2\theta_q\bigg)n_F(\omega_-(q))\bigg]$$

$$-\frac{1}{2}\int\int\frac{d^3qd^3q'}{(2\pi)^6}\mathcal{V}(q-q')\Big\{[\cos^2\theta_q n_F(\omega_+(q))+\sin^2\theta_q n_F(\omega_-(q))][\cos^2\theta_{q'} n_F(\omega_+(q'))+\sin^2\theta_{q'} n_F(\omega_-(q'))]$$

$$+[\sin^2\theta_q n_F(\omega_+(q))+\cos^2\theta_q n_F(\omega_-(q))][\sin^2\theta_{q'} n_F(\omega_+(q'))+\cos^2\theta_{q'} n_F(\omega_-(q'))]+2\bigg(\frac{g_{\uparrow\downarrow}(q)g_{\downarrow\uparrow}(q')}{g_{\downarrow\uparrow}(q)g_{\uparrow\downarrow}(q')}\bigg)^{1/2}$$

$$\times\cos\theta_q\sin\theta_q\cos\theta_{q'}\sin\theta_{q'}[n_F(\omega_+(q))-n_F(\omega_-(q))][n_F(\omega_+(q'))-n_F(\omega_-(q'))]\Big\}\,. \quad (56)$$

Treating θ_q in this expression as a variational parameter, one recovers the condition on $\tan2\theta_q$ which is equivalent to (52). We now summarize our results obtained so far.

SUMMARY

The spin-wave frequency in the long-wavelength limit is here shown to be proportional to the square of the wave vector for a large class of interaction potentials (not dynamically screened). The long-wavelength limit of the spin-wave frequency previously reported by us[3a,b] is recalculated by a variational method of solution of the equation describing the spin waves for electrons interacting according to a Yukawa potential. This calculation corrects the previous one and extends it to include all magnetizations and the dependence on range of interaction. The present result also gives the correct limit for the P state. In the Coulomb limit ($\xi=0$) the results are in concordance with Herring's[2] results for the F state. The long-wavelength spin-wave instability in the Coulomb gas already shows the possibility of SDW-type states, as they are static spin-waves of finite wave vector. A variational method for the same spin-wave equation for the static case but with finite wave-vector is developed, quite similar to the long-wavelength case. As a special case of this we rederive and extend a result derived earlier for the P-state instability by Iwamoto and Sawada.[4] The SDW states are then described by means of a 2×2 matrix Green's function,[3b] thus giving an alternative derivation of Overhauser's[1] equations, which can also be derived by a canonical-transformation method.[18] The Green's-function method given here is quite similar to Nambu's theory[8] for superconductivity. The present derivation is quite general and includes the screened interactions as well as general interaction potentials. In Appendix A we derive the corresponding results for Bloch electrons based on intraband SDW correlations only. This result has since been extended[19] to include all inter-band correlations for a two-band complex. Fedders[6] has attempted a similar model but involving very drastic approximations concerning the matrix elements of the interaction potential, whereas the model[19] considered by us is more general. Fedders applies his model to chromium, unlike Overhauser,[1] who treats chromium on an essentially one-band model. In Appendix B, the general equation in RPA describing the collective states in SDW systems is written out,[9] which is valid for general interaction potentials, whereas the previous derivation was specifically concerned with delta-function interactions and involved some approximations. This forms an addendum to our previous paper.[9]

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APPENDIX A

In this Appendix we derive the Overhauser equations for the case when we have electrons in a periodic potential. All the results given here are formal and it is hoped that they will be useful in the realistic situations. As in the text of this paper, we *assume* that the electrons with spin up and wave vector $\mathbf{k}$ in band l is associated only with the one of spin down in the *same band* but with wave vector $(\mathbf{k}+\mathbf{Q})$. With this pre-

[19] A. K. Rajagopal and H. Brooks, Advanced Research Projects (unpublished).

scription, the following redefinitions of (47) are made:

$$
\begin{aligned}
G_{\uparrow\uparrow}(11') &= \sum_{l'} \int_{\mathrm{I\,BZ}} \frac{d^3k'}{(2\pi)^3} b_{l'k'}(1) b_{l'k'}^*(1') G_{\uparrow\uparrow}(l'k';t_1-t_{1'}),\\
G_{\downarrow\downarrow}(11') &= \sum_{l'} \int_{\mathrm{I\,BZ}} \frac{d^3k'}{(2\pi)^3} b_{l',k'+Q}(1) b_{l',k'+Q}^*(1') G_{\downarrow\downarrow}(l'k';t_1-t_{1'}),\\
G_{\uparrow\downarrow}(11') &= \sum_{l'} \int_{\mathrm{I\,BZ}} \frac{d^3k'}{(2\pi)^3} b_{l'k'}(1) b_{l',k'+Q}^*(1') G_{\uparrow\downarrow}(l'k';t_1-t_{1'}),\\
G_{\downarrow\uparrow}(11') &= \sum_{l'} \int_{\mathrm{I\,BZ}} \frac{d^3k'}{(2\pi)^3} b_{l',k'+Q}(1) b_{l'k'}^*(1') G_{\downarrow\uparrow}(l'k';t_1-t_{1'}).
\end{aligned}
\tag{A1}
$$

Then a calculation similar to the one outlined in text follows and we give here only the final results. In the above, $b_{l\mathbf{k}}(\mathbf{r})$ is the Bloch function for electron in band l and with wave vector $\mathbf{k}$. We introduce the notation $\epsilon_l(\mathbf{k})$ for the energy of the electron with wave vector $\mathbf{k}$ and in band l. I BZ in the above indicated first Brillouin zone. We also introduce the notation,

$$
\mathcal{V}_{l_3\mathbf{k}_3l_4\mathbf{k}_4}{}^{l_1\mathbf{k}_1l_2\mathbf{k}_2} = \int\!\!\int d^31\,d^32\, b_{l_1\mathbf{k}_1}^*(1) b_{l_2\mathbf{k}_2}^*(2) \mathcal{V}(1-2) b_{l_3\mathbf{k}_3}(2) b_{l_4\mathbf{k}_4}(1).
\tag{A2}
$$

We obtain after some manipulations:

$$
\omega_l^{\pm}(\mathbf{k}) = \left(\frac{\epsilon_{l\uparrow}(\mathbf{k})+\epsilon_{l\downarrow}(\mathbf{k}+\mathbf{Q})}{2}\right) \mp \left[\tfrac{1}{2}(\epsilon_{l\uparrow}(\mathbf{k})-\epsilon_{l\downarrow}(\mathbf{k}+\mathbf{Q}))^2 + g_{\uparrow\downarrow}(l\mathbf{k}) g_{\downarrow\uparrow}(l\mathbf{k})\right]^{1/2},
\tag{A3}
$$

$$
G(l\mathbf{k};\omega) = \begin{bmatrix}
[\cos^2\theta_{l\mathbf{k}} g_+(l\mathbf{k};\omega) + \sin^2\theta_{l\mathbf{k}} g_-(l\mathbf{k};\omega)] & \cos\theta_{l\mathbf{k}}\sin\theta_{l\mathbf{k}} \left(\dfrac{g_{\uparrow\downarrow}(l\mathbf{k})}{g_{\downarrow\uparrow}(l\mathbf{k})}\right)^{1/2} (g_+(l\mathbf{k};\omega) - g_-(l\mathbf{k};\omega)) \\
\cos\theta_{l\mathbf{k}}\sin\theta_{l\mathbf{k}} \left(\dfrac{g_{\downarrow\uparrow}(l\mathbf{k})}{g_{\uparrow\downarrow}(l\mathbf{k})}\right)^{1/2} (g_+(l\mathbf{k};\omega) - g_-(l\mathbf{k};\omega)) & [\sin^2\theta_{l\mathbf{k}} g_+(l\mathbf{k};\omega) + \cos^2\theta_{l\mathbf{k}} g_-(l\mathbf{k};\omega)]
\end{bmatrix},
\tag{A4}
$$

where

$$
g_{\pm}(l\mathbf{k};\omega) = 1/[\omega - \omega_l^{\pm}(\mathbf{k})],
\tag{A5}
$$

where $\theta_{l\mathbf{k}}$ is defined quite analogously to $\theta_{\mathbf{k}}$ in (52) of the text.

$$
\begin{aligned}
\epsilon_{l\uparrow}(\mathbf{k}) &= \epsilon_l(\mathbf{k}) - \sum_{l'} \int_{\mathrm{I\,BZ}} \frac{d^3k'}{(2\pi)^3} \mathcal{V}_{l\mathbf{k}l'\mathbf{k}'}{}^{l\mathbf{k}l'\mathbf{k}'} [\cos^2\theta_{l'\mathbf{k}'} n_F(\omega_{l'}^+(\mathbf{k}')) + \sin^2\theta_{l'\mathbf{k}'} n_F(\omega_{l'}^-(\mathbf{k}'))],\\
\epsilon_{l\uparrow}(\mathbf{k}+\mathbf{Q}) &= \epsilon_l(\mathbf{k}+\mathbf{Q}) - \sum_{l'} \int_{\mathrm{I\,BZ}} \frac{d^3k'}{(2\pi)^3} \mathcal{V}_{l\mathbf{k}+\mathbf{Q}l'\mathbf{k}'+\mathbf{Q}}{}^{l\mathbf{k}+\mathbf{Q}l'\mathbf{k}'+\mathbf{Q}} [\sin^2\theta_{l'\mathbf{k}'} n_F(\omega_{l'}^+(\mathbf{k}')) + \cos^2\theta_{l'\mathbf{k}'} n_F(\omega_{l'}^-(\mathbf{k}'))],\\
g_{\uparrow\downarrow}(l\mathbf{k}) &= \sum_{l'} \int_{\mathrm{I\,BZ}} \frac{d^3k'}{(2\pi)^3} \mathcal{V}_{l\mathbf{k}+\mathbf{Q}l'\mathbf{k}'}{}^{l\mathbf{k}l'\mathbf{k}'+\mathbf{Q}} \left(\frac{g_{\uparrow\downarrow}(l'\mathbf{k}')}{g_{\downarrow\uparrow}(l'\mathbf{k}')}\right)^{1/2} \cos\theta_{l'\mathbf{k}'}\sin\theta_{l'\mathbf{k}'} [n_F(\omega_{l'}^+(\mathbf{k}')) - n_F(\omega_{l'}^-(\mathbf{k}'))],\\
g_{\downarrow\uparrow}(l\mathbf{k}) &= \sum_{l'} \int_{\mathrm{I\,BZ}} \frac{d^3k'}{(2\pi)^3} \mathcal{V}_{l\mathbf{k}l'\mathbf{k}'+\mathbf{Q}}{}^{l\mathbf{k}+\mathbf{Q}l'\mathbf{k}'} \left(\frac{g_{\downarrow\uparrow}(l'\mathbf{k}')}{g_{\uparrow\downarrow}(l'\mathbf{k}')}\right)^{1/2} \cos\theta_{l'\mathbf{k}'}\sin\theta_{l'\mathbf{k}'} [n_F(\omega_{l'}^+(\mathbf{k}'')) - n_F(\omega_{l'}^-(k'))].
\end{aligned}
\tag{A6}
$$

The equation for $g_{\uparrow\downarrow}$, $g_{\downarrow\uparrow}$ may be written more explicitly thus:

$$
g_{\uparrow\downarrow}(l\mathbf{k}) = \sum_{l'} \int_{\mathrm{I\,BZ}} \frac{d^3k'}{(2\pi)^3} \mathcal{V}_{l\mathbf{k}+\mathbf{Q}l'\mathbf{k}'}{}^{l\mathbf{k}l'\mathbf{k}'+\mathbf{Q}} \frac{g_{\uparrow\downarrow}(l'\mathbf{k}')\{n_F(\omega_{l'}^+(\mathbf{k}')) - n_F(\omega_{l'}^-(\mathbf{k}'))\}}{[\omega_{l'}^+(\mathbf{k}') - \omega_{l'}^{-1}(\mathbf{k}')]}
\tag{A7}
$$

and a similar equation for $g_{\downarrow\uparrow}$. We shall not write down the expression for total energy corresponding to (56), because it is too complicated.

APPENDIX B

Recently we derived the collective excitations in SDW systems by a canonical transformation method[9] for the case when we have delta-function interactions in the random-phase approximation. We also decoupled the equations so that the transverse and longitudinal oscillations are not coupled. Here we give the complete set of equations in RPA. The notations are the same as in our previous paper.[9]

The complete equations of motion for

$$S_k^+(q)=A_{k+q}^\dagger B_k\,,\quad S_k^-(q)=B_{k+q}^\dagger A_k\,,\quad \rho_k^A=A_{k+q}^\dagger A_k\,,\quad \rho_k^B(q)=B_{k+q}^\dagger B_k\,, \tag{B1}$$

in the random-phase approximation are

$$\begin{aligned}S_k^+(q)=A_{-+}(kq)\textstyle\sum_{q_1}\{&[-\mathcal{V}(q)S_1(kq)S_1(q_1q)+\mathcal{V}(k-q_1)C_2(kqq_1)C_3(kq_1)]S_{q_1}^+(q)\\&+[\mathcal{V}(q)S_1(kq)C_1(q_1q)-\mathcal{V}(k-q_1)C_2(kqq_1)S_3(kq_1)]\rho_{q_1}^A(q)\\&+[\mathcal{V}(q)S_1(kq)C_1(q_1q)-\mathcal{V}(k-q_1)S_2(kqq_1)C_3(kq_1)]\rho_{q_1}^B(q)\\&+[\mathcal{V}(q)S_1(kq)S_1(q_1q)+\mathcal{V}(k-q_1)S_2(kqq_1)S_3(kq_1)]S_{q_1}^-(q)\}\,.\end{aligned}\tag{B2a}$$

$$\begin{aligned}S_k^-(q)=A_{+-}(kq)\textstyle\sum_{q_1}\{&[-\mathcal{V}(q)S_1(kq)S_1(q_1q)+\mathcal{V}(k-q_1)C_2(kqq_1)C_3(kq_1)]S_{q_1}^-(q)\\&+[-\mathcal{V}(q)S_1(kq)C_1(q_1q)+\mathcal{V}(k-q_1)S_2(kqq_1)C_3(kq_1)]\rho_{q_1}^A(q)\\&+[-\mathcal{V}(q)S_1(kq)C_1(q_1q)+\mathcal{V}(k-q_1)C_2(kqq_1)S_3(kq_1)]\rho_{q_1}^B(q)\\&+[\mathcal{V}(q)S_1(kq)S_1(q_1q)+\mathcal{V}(k-q_1)S_2(kqq_1)S_3(kq_1)]S_{q_1}^+(q)\}\,.\end{aligned}\tag{B2b}$$

$$\begin{aligned}\rho_k^A(q)=A_{++}(kq)\textstyle\sum_{q_1}\{&[-\mathcal{V}(q)C_1(kq)C_1(q_1q)+\mathcal{V}(k-q_1)C_2(kqq_1)C_3(kq_1)]\rho_{q_1}^A(q)\\&+[-\mathcal{V}(q)C_1(kq)C_1(q_1q)-\mathcal{V}(k-q_1)S_2(kqq_1)S_3(kq_1)]\rho_{q_1}^B(q)\\&+[\mathcal{V}(q)C_1(kq)S_1(q_1q)+\mathcal{V}(k-q_1)C_2(kqq_1)S_3(kq_1)]S_{q_1}^+(q)\\&+[-\mathcal{V}(q)C_1(kq)S_1(q_1q)-\mathcal{V}(k-q_1)S_2(kqq_1)C_3(kq_1)]S_{q_1}^-(q)\}\,.\end{aligned}\tag{B2c}$$

$$\begin{aligned}\rho_k^B(q)=A_{--}(kq)\textstyle\sum_{q_1}\{&[-\mathcal{V}(q)C_1(kq)C_1(q_1q)+\mathcal{V}(k-q_1)C_2(kqq_1)C_3(kq_1)]\rho_{q_1}^B(q)\\&+[-\mathcal{V}(q)C_1(kq)C_1(q_1q)-\mathcal{V}(k-q_1)S_2(kqq_1)C_3(kq_1)]\rho_{q_1}^A(q)\\&+[\mathcal{V}(q)C_1(kq)S_1(q_1q)+\mathcal{V}(k-q_1)S_2(kqq_1)C_3(kq_1)]S_{q_1}^+(q)\\&+[-\mathcal{V}(q)C_1(kq)S_1(q_1q)-\mathcal{V}(k-q_1)C_2(kqq_1)S_3(kq_1)]S_{q_1}^-(q)\}\,.\end{aligned}\tag{B2d}$$

Here

$$A_{\sigma\sigma'}(kq)=\left[\frac{n_F(\omega_\sigma(k))-n_F(\omega_{\sigma'}(k+q))}{\omega-\omega_\sigma(k)+\omega_{\sigma'}(k+q)}\right](\sigma,\sigma'=\pm) \tag{B3}$$

and

$$\begin{aligned}\cos(\theta_{k+q}-\theta_k)&=C_1(kq)\,, & \sin(\theta_{k+q}-\theta_k)&=S_1(kq)\,,\\ \cos(\theta_{k+q}-\theta_{q+q_1})&=C_2(kqq_1)\,, & \sin(\theta_{k+q}-\theta_{q+q_1})&=S_2(kqq_1)\,,\\ \cos(\theta_{q_1}-\theta_k)&=C_3(kq_1)\,, & \sin(\theta_{q_1}-\theta_k)&=S_3(kq_1)\,.\end{aligned}\tag{B4}$$

$\omega_\pm(k)$ has the same meaning as in (51) of the text. The approximations made in the paper[9] consist of dropping $\mathcal{V}(k-q_1)$ term (exchange) entirely, as well as dropping the $\rho^{A,B}$ terms in the $S^\pm$ equations and the $S^\pm$ terms in the $\rho^{A,B}$ equations. For $Q=0$, $g=0$, we recover from the above equations the RPA equations discussed earlier for the uniform states.[3b] From these equations it is easy to verify that there exist solutions with $\omega^{(0)}=\text{const}$, with $\rho_A(0)=\rho_B(0)=0$ and $\omega^{(0)}=0$, and with $S^{(\pm)}(0)\neq 0$. The next approximation is quite cumbersome, but the indications are that there are oscillations with $\omega\sim\text{const}$ (as in plasma modes) and $\omega\sim q$ (as in antiferromagnetic spin waves), for Coulomb interactions analogous to those obtained earlier by us[9]—when $\mathcal{V}(q)$ is of short range, and under quite drastic further restrictions. Dr. Yan Shi informs me that he arrived at results similar to those given in this Appendix in a paper he has published in the Proc. Armenian Acad. Sci. (USSR) **39**, 73 (1964).