(such as In), we note that application of the theory of Ref. 1 shows that the shift of T_c will depend on the orientation of the crystal with respect to the surface of the plate and that a study of the mfp effect for samples of varying orientation may be used to unfold the anisotropic-pairing interaction. In fact, some of the scatter in the data in Fig. 1 seems to be related to variation in crystal orientation. Using Ref. 1, the angular dependent part of ΔT_c would seem to be about 30% of the total. This part of ΔT_c should be measurable, to 10% accuracy, if the scatter in the data can be reduced by a factor of 3.

Finally, we note that Naugle and Glover[14] have recently reported a $1/d$-type depression of T_c, for thin films of amorphous materials. The total ΔT_c, as well as the slope $(\Delta T_c/d^{-1})$ that they observe, are in good agreement with the Maskowitz-Kadanoff[2] theory, leading to the interesting speculation that they are seeing the mfp effect. However, it is difficult to see how the amorphous materials they use could have any of the gap anisotropy required to observe an mfp effect. Also, they note that the resistances per square ($R_{\square}$) of their films are proportional to $1/d$ and that the films appear to have no ordered structure beyond tens of angstroms. These results imply that the mfp is much smaller than their film thicknesses so that the sample boundary would not determine l. We must conclude at the present time that, although similar phenomena, our data and those of Naugle and Glover are not necessarily due to the same effect.

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PHYSICAL REVIEW B VOLUME 3, NUMBER 1 1 JANUARY 1971

Self-Consistent Hartree-Fock Calculation of the Dielectric Function of an Electron Gas

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The dielectric function of the electron gas has been calculated in the self-consistent Hartree-Fock approximation. Results are presented and compared with that obtained in random-phase-approximation and Hubbard theories.

In the study of the uniform electron gas, knowledge of the wave number and frequency-dependent dielectric function $\epsilon(q, \omega)$ has proved to be extremely useful. Physical properties of the system, such as the dynamic form factor $S(q, \omega)$ and the ground-state energy E_0, are expressible in terms of $\epsilon(q, \omega)$.

The most commonly used expression for the dielectric function is calculated[1] by using the self-consistent Hartree method or the random-phase approximation (RPA). In the diagrammatic perturbation theory,[2] this is equivalent to the summation of bubble diagrams. It gives a good description of plasma oscillations and long-range screening effects. Otherwise, its validity is restricted to very dense systems [$r_S \ll 1$, where, in terms of the density n and Bohr radius a_0, $r_S = (\frac{3}{4}\pi n a_0^3)^{1/3}$], since local-field corrections due to the Coulomb hole and exchange effects are neglected in this approximation.

Various attempts have been made to improve upon the RPA. We mention only a few of these. Hubbard[3] tried to estimate the effects of exchange. He considered only a subset of exchange diagrams, and in order to obtain a simple expression, he approximated the Coulomb interaction in the exchange term by $\delta(\vec{r})4\pi e^2/(q^2+k_F^2)$. His calculation also violated particle conservation.

Singwi and co-workers[4] proposed a method of accounting for local-field corrections. Their numerical calculation is based on an ansatz, which one can also make for classical fluids, relating the two-particle distribution function to the one-particle distribution and the pair-correlation function. The connection between their procedure and perturbation theory is unclear, so that one does not know what corrections have been included. It is probably worth pointing out that although, unlike the results from the RPA and the Hubbard method, physically plausible results for the pair-correlation function $g(r)$ were obtained by Singwi *et al.*[5] at metallic densities; their results for the spin-up–spin-up pair-correlation function remained unphysical throughout the range of metallic densities.

It is of interest to carryout a calculation of the dielectric function in the self-consistent Hartree-Fock approximation (SHF). In this, one sums up all ladder-bubble diagrams self-consistently, using the Hartree-Fock single-particle energy for the electrons. Such a calculation should provide a more accurate description of exchange effects than that due to Hubbard. It is well defined in that one knows exactly which terms in the perturbation series are considered, and it is self-consistent in that conservation laws are satisfied. The resulting integral equation in this approximation has recently been considered by Langreth,[6] who has obtained a variational solution of the problem by using a very simple trial function. We will discuss this approximate result later. In this work we report results of a numerical calculation of $\epsilon_{\text{SHF}}(q,\omega)$.

We will now briefly sketch the derivation of the dielectric function at zero temperature in the SHF. The electron Green's function is defined by

$$G_{\sigma\sigma'}(1,1') = -i\langle T\,\psi_\sigma(1)\,\psi^\dagger_{\sigma'}(1')\rangle\,, \tag{1}$$

where T is the time-ordering operator, and $\psi_\sigma(1)$ and $\psi^\dagger_\sigma(1)$ destroy and create, respectively, an electron of spin σ at the space-time point 1. In the absence of an external field, the Green's function depends only on the difference 1-1′, is diagonal in the spin index, and is independent of spin. Henceforth, we suppress the spin index. In the wave vector and frequency space, the Dyson equation for $G(\vec{k}\omega)$ is

$$G(\vec{k}\omega) = G^0(\vec{k}\omega) - G^0(\vec{k}\omega)\Sigma(\vec{k}\omega)G(\vec{k}\omega), \tag{2}$$

where $G^{(0)}(\vec{k}\omega)$ is the Green's function for the noninteracting particles. In the Hartree-Fock approximation, the self-energy Σ is frequency independent, and is given by

$$\Sigma(\vec{k}) = \int\frac{d^3k'}{(2\pi)^3}\int\frac{d\omega'}{2\pi}\,G(\vec{k}',\omega')\,V(\vec{k}-\vec{k}')$$
$$= -\int_{k\le k_F}\frac{d^3k'}{(2\pi)^3}\,V(|\vec{k}-\vec{k}'|), \tag{3}$$

where $V(k)$ is the interaction potential. We take $V(k)$ to be the statically screened Coulomb interaction, i.e.,

$$V(k) = 4\pi e^2/(k^2+q_S^2), \tag{4}$$

where q_S^{-1} is the screening length. Following Langreth,[6] we take q_S^{-1} to be the Fermi-Thomas screening length.

In using Eq. (4) for the exchange-interaction potential, we have gone somewhat beyond the Hartree-Fock approximation. We note that if no screening were introduced in Eq. (4), the self-energy would have a singularity at the Fermi surface. Furthermore, the correct exchange potential should be the self-consistent potential, that is $V_{\text{Coulomb}}(q)/\epsilon(q,\omega)$. Our method is perhaps the simplest way of approximating this screening effect.

The dielectric function $\epsilon(q,\omega)$ is obtained by considering the response of the system to an external field of wave number q and frequency ω. In order to satisfy particle conservation, it is necessary to sum the bubble-ladder diagrams shown in Fig. 1. In the figure, the electron Green's function is denoted by solid lines, the screeened Coulomb interaction by wavy lines, and the unscreened Coulomb interaction by dotted lines. If we call the shaded bubble $L(q,\omega)$, we see the ef-

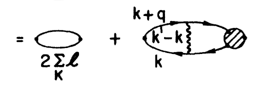

FIG. 1. Diagrammatic representation of the SHF approximation. The solid lines are renormalized electron propagators. The dotted line is the bare Coulomb interaction. The wavy line is the statically screened interaction.

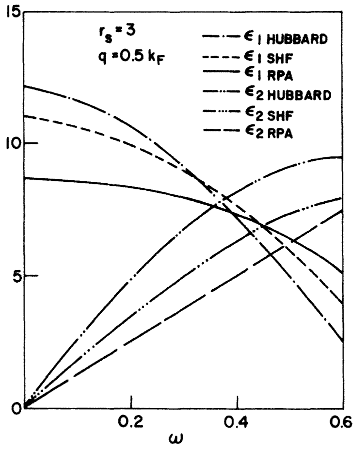

FIG. 2. Real part (ϵ_1) and the imaginary part (ϵ_2) of the dielectric function for $r_S=3$, $q=0.5k_F$.

fective interaction is given by

$$V_{\mathrm{eff}}(q,\omega)\equiv\frac{4\pi e^2}{q^2\epsilon(q,\omega)}=\frac{4\pi e^2/q^2}{1-(4\pi e^2/q^2)L(q,\omega)}\;.$$

Thus, the dielectric function is given by

$$\epsilon(q,\omega)=1-(4\pi e^2/q^2)L(q,\omega). \tag{5}$$

From Fig. 1, we also find

$$L(q,\omega)=2\int\frac{d^3k}{(2\pi)^3}\,\tilde{L}(\vec{k},\vec{q},\omega), \tag{6a}$$

$$\tilde{L}(\vec{k},\vec{q},\omega)=l(\vec{k},\vec{q},\omega)$$

$$\times\left(1-\int\frac{d^3k'}{(2\pi)^3}\,V(|\vec{k}-\vec{k}'|)\;\tilde{L}(\vec{k}',\vec{q},\omega)\right)\;, \tag{6b}$$

$$l(\vec{k},\vec{q},\omega)=\int\frac{d\omega'}{2\pi}\,G(\vec{k},\omega')\;G(\vec{k}+\vec{q},\omega+\omega').$$

Equations (2)–(6) form a closed set of equations from

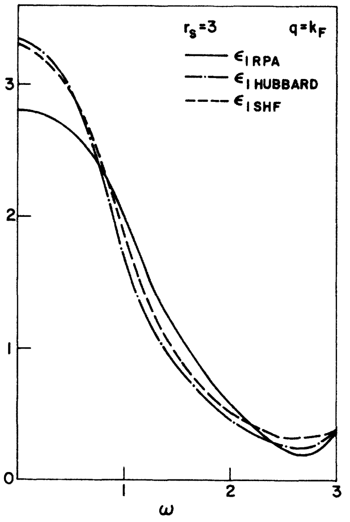

FIG. 3. Real part of the dielectric function for $r_S=3$, $q=k_F$.

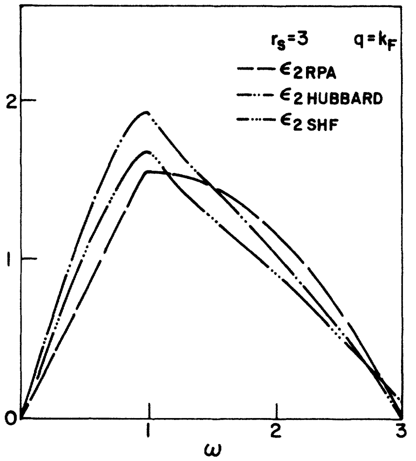

FIG. 4. Imaginary part of the dielectric function for $r_S=3$, $q=k_F$.

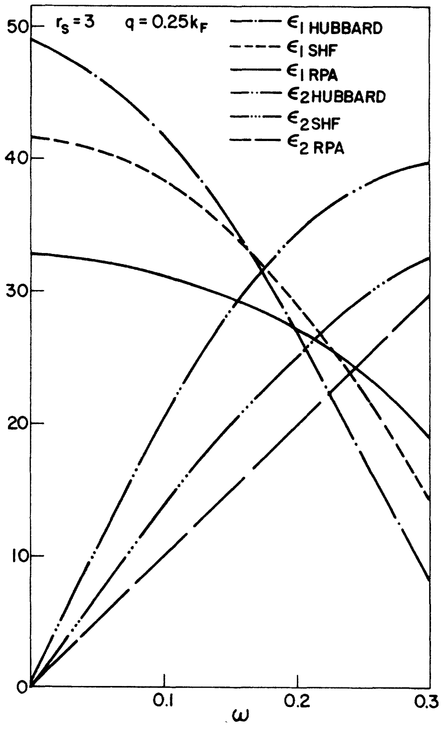

FIG. 5. Dielectric function for $r_S=3$, $q=0.25k_F$.

which $\epsilon(q, \omega)$ may be determined.

Because the system is homogeneous, $\tilde{L}$ is a function of k, q, ω, and $\vec{k}\cdot\vec{q}$ only. By fixing the direction of $\vec{q}$, one of the angular integrations in Eq. (6b) can be done immediately. Thus, we have to solve the integral equation

$$\tilde{L}(k, \mu, q, \omega) = l(k, \mu, q, \omega)\left[1 - \int dk' \int d\mu' \, k'^2 V(k, \mu, k', \mu') \, L(k', \mu', q, \omega)\right] , \tag{7}$$

with

$$V(k, \mu, k', \mu') = \frac{e^2/\pi}{[(k^2 + k'^2 - 2kk'\mu\mu' + q_S^2)^2 - 4k^2k'^2(1-\mu^2)(1-\mu'^2)]^{1/2}} , \tag{8}$$

$$l(k, \mu, q, \omega) = \frac{f((E\,(k^2+q^2+2kq\mu)^{1/2}) - f\,(E(k))}{E((k^2+q^2+2kq\mu)^{1/2}) - E(k) - \hbar\omega - i\delta} , \tag{9}$$

where $E(k) = \hbar^2k^2/2m + \Sigma(k)$ is the single-particle Hartree-Fock energy, $f(E)$ is the zero-temperature Fermi function, and

$$\mu = \vec{k}\cdot\vec{q}/kq, \quad \mu' = \vec{k}'\cdot\vec{q}/k'q .$$

The dielectric function is then obtained by using Eqs. (5) and (6a).

It should be pointed out that the above procedure is equivalent to calculating the dielectric response of a system for which the Hamiltonian is essentially the Hartree-Fock Hamiltonian of the free-electron gas. The only difference is that in the exchange part we have used the Yukawa rather than the bare Coulomb potential.

The integral equation (7) has been solved by iteration. δ function and principal-value integrals are involved. The iterative process was carried out until two successive values of $\epsilon(q, \omega)$ agreed to better than 1%. The results for the dielectric function are presented in Figs. 2–5. The values of $\epsilon - 1$ are expected to be accurate to ± 2%. For comparison, we have also plotted the real and imaginary parts of ϵ_{RPA} and $\epsilon_{\mathrm{Hubbard}}$. The Hubbard dielectric function is calculated by using Eq. (4) rather than the bare Coulomb potential in estimating the exchange terms. We point out that our calculation shows that the static dielectric constant is larger than the corresponding value for the RPA but smaller than that for the Hubbard dielectric functions.

Finally, we compare our results with that of Langreth. Equation (6b) for $\tilde{L}/l$ is equivalent to minimizing the following functional:

$$\begin{aligned} F(\tilde{\Lambda}(k, q, \omega)) = &- \sum_k \sum_{k'} \tilde{\Lambda}(k, q, \omega) l(k, q, \omega) \\ &\times V(|k - k'|) l(k', q, \omega) \tilde{\Lambda}(k', q, \omega) \\ &- \sum_k \tilde{\Lambda}^2(k, q, \omega) l(k, q, \omega) \\ &+ 2\sum_k \tilde{\Lambda}(k, q, \omega) l(k, q, \omega), \end{aligned} \tag{10}$$

where

$$\tilde{\Lambda}(k, q, \omega) \equiv \tilde{L}(k, q, \omega)/l(k, q, \omega), \quad l \neq 0.$$

As a trial solution, Langreth chose $\tilde{\Lambda}$ to be constant in k. This gives

$$\begin{aligned} \tilde{\Lambda}(q, \omega) = \sum_k l(k, q, \omega) \bigg/ \bigg(&\sum_k l(k, q, \omega) + \sum_k \sum_{k'} l(k, q, \omega) \\ &\times V(|k - k'|) l(k', q, \omega) \bigg). \end{aligned} \tag{11}$$

Our exact calculation showed that $\tilde{\Lambda}$ varies significantly between $k = 0$ and $k = 2k_F$ (e.g., for $q = 0.5k_F$ and $\hbar\omega = 0.25E_F^0$, where E_F^0 is the Fermi energy, $\mathrm{Re}\tilde{\Lambda}$ decreases from 1.27 at $k = 0$ to 1.12 at $k = 2k_F$, while $\mathrm{Im}\tilde{\Lambda}$ varies between 0.16 and 0.068). However, it is very significant to point out that the evaluation of the variational expression for $\epsilon(q, \omega)$ gave values within 1% of our exact numerical calculation, for all values of q and ω calculated. Thus, we find that the simple variational solution is very good indeed.

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Superconductivity and Spin Fluctuations in the *Ir*-Ni, *Ir*-Co, and *Ir*-Fe Alloy Systems*

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The superconducting transition temperatures of *Ir*-Ni, *Ir*-Co, and *Ir*-Fe alloys have been measured in the temperature interval 0.10–0.040 °K. It is shown that the rates of change of lnT_c with impurity concentration for these systems provide quantitative evidence that localized spin fluctuations are responsible for the suppression of superconductivity when these rates are compared with the rates of increase of the specific-heat coefficient γ and the susceptibility χ.

I. INTRODUCTION

Spin fluctuations are believed to be responsible for suppressing superconductivity in numerous alloy systems on the right end of the 4*d* and 5*d* transition-metal series.[1,2] However, solid evidence that this is the case is difficult to come by. We have found that very small concentrations of Ni, Co, and Fe in Ir rapidly destroy the latter's superconductivity. Because the suppression of superconductivity is strictly an impurity effect, certain theoretical simplifications can arise which permit a quantitative comparison between theory and experiment.

II. EXPERIMENTAL

Temperatures as low as 0.035 °K were obtained by adiabatic demagnetization, using a cryostat similar in construction to several reported elsewhere.[1] Superconductivity was detected by the low-frequency mutual inductance method. The temperature was measured with a 100-Ω $\frac{1}{2}$-W Speer carbon resistor which was calibrated to within a few millidegrees Kelvin with the aid of the known transition temperatures of certain high-purity superconductors and also with cerium magnesium nitrate (CMN).

One of the principal experimental difficulties was sample preparation. Samples were about 200 mg and were prepared by arc-melting 99.999%-pure starting material in an argon arc furnace. The melting point of iridium is close to the boiling points of iron, cobalt, and nickel. Consequently, the weight loss of the volatile impurity during arc melting can be considerable. This makes it difficult to determine the sample composition for such small samples and small impurity concentrations. The *Ir*-Fe samples were prepared after first preparing a master alloy containing 2.1-at.% Fe. The master was then broken up and further diluted with iridium to obtain the final samples. Fortunately, the master can be prepared with less than a few percent iron weight loss by careful arc melting. It is reasonable to assume that there is negligible iron weight loss upon further dilution and that the composition can be determined from the weights of the starting materials. However, there was a 30% cobalt weight loss in the preparation of a 3.9% cobalt master. The starting material for the *Ir*-Co alloys prepared from this master was weighed on a Mettler balance with a limiting accuracy of 0.01 mg before and after arc melting, and the composition determined by attributing any further weight loss to the volatile cobalt impurity. For these alloys, a 10% error in composition is still possible. For the *Ir*-Ni alloys as well, the composition was determined by assigning any weight loss to the nickel impurity. The problem of determining the composition is less severe because the nickel concentration in alloys of interest is higher.

III. RESULTS

The experimental results are given in Table I and Figs. 1 and 2. The iridium used was obtained from the United Mineral Corp. It was quoted to be 99.999% pure with calcium (1 ppm), silicon (5 ppm), and sodium (2 ppm) as the principal impurities. Its transition temperature T_c was 0.105 °K and the transition width ΔT_c for 90% of the transition was 0.004 °K. Surprisingly, adding iron to iridium reduces the transition width, so that the width of the 0.033%-Fe alloy was only about half a millidegree. The error in the compo-