$\bar{\nu}_\sigma - \bar{\nu}_T = 24\ \mathrm{cm}^{-1}$, we find that $\nu_\sigma - \nu_T > \nu_T$, so that the phonon-dispersion argument given above relating σ to ν_T^2 + constant is not expected to hold. The fact that Eq. (5) holds experimentally for KTN suggests that either the above arguments are overly restrictive or perhaps there could be an additional contribution to the constant term arising from the broad linewidth of the TO mode (e.g., 40 cm^{-1} in $KTaO_3$).[14] A more detailed analysis along these lines will be reported later.

In ABO_3 semiconductors the strong electron–TO-mode interaction which relates σ to ϵ is further evidence for a many-valley conduction-band model in these crystals. Detailed calculations of the interaction would require a knowledge of the charge distributions associated with the TO mode which are not presently available. The mobility temperature dependence expected for such an interaction is at present unknown. There are theoretical indications that the observed mobility temperature dependence may be associated with multiple-phonon processes.

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SELF-CONSISTENT CURIE-LAW CALCULATION FOR ANDERSON'S DILUTE-ALLOY MODEL

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The effects of correlations on the behavior of Anderson's single-orbital model of an impurity in a dilute alloy[1] have been studied extensively recently.[2] The model is most amenable to study using double-time Green's functions,[3] since taking exact account of the strong repulsion of opposite-spin electrons in the impurity "d" state precludes the use of diagrammatic expansions. When the chain of equations of motion is decoupled and solved, the d-state susceptibility, χ_d, is usually found to be temperature independent at reasonable temperatures. A Curie law has only been found in a treatment which uses the temperature-dependent occupation numbers for the uncoupled d state throughout, thus seeming to force this result,[4] and an unpublished calculation.[5] We shall show that a careful and systematic decoupling of the equa-

tions of motion enables one to solve for the d-state occupation numbers at the end of the calculation and find a Curie law. The processes which produce this behavior are formally quite different from those which yield a Curie law for the uncoupled d state.

The Hamiltonian for Anderson's model is[1]

$$H=\sum_\sigma \epsilon_{d\sigma} a_{d\sigma}^\dagger a_{d\sigma}+\sum_{k\sigma}\epsilon_{k\sigma}a_{k\sigma}^\dagger a_{k\sigma}+Un_{d+}n_{d-}+\sum_{k\sigma}(V_{kd}a_{k\sigma}^\dagger a_{d\sigma}+V_{kd}^* a_{d\sigma}^\dagger a_{k\sigma}), \quad (1)$$

where the d operators represent the localized orbital, the k operators the conduction band, and $\epsilon_{d\sigma}=\epsilon_d-\sigma_\mu \mathcal{H}$, etc.

In the physically interesting case, ϵ_d is negative (measured from the Fermi level), and U is large and positive. If the mixing potential V_{kd} is neglected, one finds for the up-spin d-state Green's function

$$G_{d+}(\omega)=\frac{1}{2\pi}\left[\frac{1-\langle n_{d-}\rangle}{\omega-\epsilon_{d+}}+\frac{\langle n_{d-}\rangle}{\omega-\epsilon_{d+}-U}\right]. \quad (2)$$

Although it is academic, one may substitute this in the formula[3]

$$\langle n_{d+}\rangle = i\int_{-\infty}^{\infty}[G_{d+}(\omega+i\eta)-G_{d+}(\omega-i\eta)]f(\omega)d\omega, \quad (3)$$

where $f(\omega)$ is the Fermi function, and find two equations relating $\langle n_{d+}\rangle$ and $\langle n_{d-}\rangle$. These yield a Curie law, but only after quantities of order unity cancel out, leaving quantities of order $\exp(\epsilon_d/kT)$. It has been suggested that the exact G_d should look like (2), but with the poles broadened by an imaginary term $2i\Gamma$.[6] If one calculates the populations using this form, he finds that the number of holes under the tail of the lower peak dominates the equations, and that χ_d remains small and temperature independent until the number of thermally produced holes near ϵ_d exceeds this, that is, until $\exp(\epsilon_d/kT)>\Gamma/-\epsilon_d$.

We have decoupled the equations of motion to obtain G_d exactly to order V^2, dropping terms of order V^4 and of order U^{-1}. This is the simplest physically interesting approximation. In our large-U limit, the upper peak of G_d is "out of sight" so that the portion of G_d we calculate violates the spectral-density sum rule. This does no harm, however, since virtual transitions to the two-d-electron state at intermediate stages are not excluded. In addition, we do not make the usual self-energy sum, but keep our expansion of G_d a strict one in powers of V^2. Doing so is crucial to obtain the correct behavior of the spectral density of G_d near the Fermi surface. Our approximation is very bad for $\omega\approx\epsilon_d$. In most many-body problems, one is chiefly interested in the behavior of Green's functions near their poles and must make self-energy sums. In this case, however, the exact behavior of G_d for $\omega\approx\epsilon_d$ is irrelevant.

We shall display only two of the most important equations of motion in their decoupled form:

$$(\omega-\epsilon_{d+})G_{d+}=\frac{1}{2\pi}(1-\langle n_{d-}\rangle)\left[1+\sum_k \frac{|V_{kd}|^2}{(\omega-\epsilon_{k+})(\omega-\epsilon_{d+})}\right]-\sum V_{kd}^*\langle\langle a_{d-}^\dagger a_{k-}a_{d+}|a_{d+}^\dagger\rangle\rangle, \quad (4)$$

$$(\omega-\epsilon_{k+})\langle\langle a_{d-}^\dagger a_{k-}a_{d+}|a_{d+}^\dagger\rangle\rangle=(\tfrac{1}{2}\pi)[\langle a_{d-}^\dagger a_{k-}\rangle-(1-\langle n_{d-}\rangle)\langle n_{k-}\rangle V_{kd}/(\omega-\epsilon_{d+})]. \quad (5)$$

The off-diagonal expectation value in (5) is evaluated to lowest order in V using a relation similar to (3), and introduces a term proportional to $(1-\langle n_{d+}\rangle)$ to the right-hand side of (5). Our final expression for G_d is

$$G_{d+}=\frac{1}{2\pi}(1-\langle n_{d-}\rangle)\left[\frac{1}{(\omega-\epsilon_{d+})}+\sum_k\frac{|V_{kd}|^2(1+\langle n_{k-}\rangle)}{(\omega-\epsilon_{k+})(\omega-\epsilon_{d+})^2}\right]-\frac{1}{2\pi}(1-\langle n_{d+}\rangle)\sum_k\frac{|V_{kd}|^2[f(\epsilon_{d-})-f(\epsilon_{k-})]}{(\omega-\epsilon_{k+})(\omega-\epsilon_{d+})(\epsilon_{d-}-\epsilon_{k-})}. \quad (6)$$

It may be seen that each k sum in (6) gives a discontinuity in the imaginary part of G_d at $\omega=0$, but that these cancel exactly (for $\langle n_{d+}\rangle=\langle n_{d-}\rangle$). Carrying out self-energy sums at an earlier stage might have led to an erroneous prediction of a discontinuous imaginary part and logarithmic real part for

G_d in order V^2, since all the contributing terms would not have been treated on an equal footing.

Substituting (6) in (3), setting $|V_{kd}|^2$ and the density of states equal to their values ρ and V^2 at the Fermi surface, and assuming $\mu\mathcal{H} \ll kT$ and $f(\epsilon_{d\sigma}) = 1$, we obtain

$$\langle n_{d+}\rangle = (1-\langle n_{d-}\rangle)\left[1-\rho V^2\int_{-\infty}^{\infty}\frac{1-f^2(\epsilon)+2\mu\mathcal{H}f'(\epsilon)}{(\epsilon-\epsilon_d)^2}d\epsilon\right]-(1-\langle n_{d+}\rangle)\rho V^2\int_{-\infty}^{\infty}\frac{[1-f(\epsilon)]^2}{(\epsilon-\epsilon_d)^2}d\epsilon. \quad (7)$$

The lack of convergence of the integrals at $\epsilon = \epsilon_d$ involves terms of order $\exp(\epsilon_d/kT)$ and is entirely negligible. (It could have been removed completely by dividing the energy range and doing self-energy sums near $\omega = \epsilon_d$.) At large ϵ the integrals converge, and thus our result does not depend on bandwidth. Assuming $kT/-\epsilon_d \ll 1$, the integrals may be evaluated exactly,[7] and we obtain

$$\langle n_{d+}\rangle = (1-\langle n_{d-}\rangle)\{1-(\rho V^2/-\epsilon_d)[1+(kT/-\epsilon_d)-2(\mu\mathcal{H}/-\epsilon_d)]\}-(1-\langle n_{d+}\rangle)(\rho V^2/-\epsilon_d)[1-(kT/-\epsilon_d)], \quad (8)$$

and a corresponding equation for $\langle n_{d-}\rangle$.

At $T = \mathcal{H} = 0$, these equations are identical, and $\langle n_{d+}\rangle - \langle n_{d-}\rangle$ is indeterminate. For finite magnetic field and temperature, we find

$$\langle n_{d+}\rangle + \langle n_{d-}\rangle = 1-(\rho V^2/-\epsilon_d). \quad (9)$$

In the equation for $\langle n_{d+}\rangle - \langle n_{d-}\rangle$, the leading terms are of order V^2, and higher order terms must be dropped to be consistent with our decoupling procedure. This yields an unmodified Curie law for χ_d,

$$\chi_d = \mu[\langle n_{d+}\rangle - \langle n_{d-}\rangle]/\mathcal{H} = \mu^2/kT. \quad (10)$$

The Curie law is "driven" in our treatment by temperature and magnetic field excitations in the small d-state tail at the Fermi surface, rather than by those at ϵ_d as in the case of the uncoupled spin. In a self-consistent calculation such as this, it is apparently necessary to decouple to order V^4 to obtain the V^2 corrections to χ_d[4] consistently.

The band-state Green's function is modified by a term proportional to $V^2 G_d$, as may be shown exactly. In the present calculation, there is no modification of the band electron susceptibility because of the "compensation principle."[1] The demonstrated relation between the Kondo and Anderson models[8] suggests that in a perturbation calculation, Kondo singularities[9] should appear in order V^6 in the band Green's function, and hence in order V^4 in G_d.[4] However, the demonstrated inability of our V^2 decoupling to give V^2 modifications in a self-consistent calculation of χ_d suggests that a V^6-decoupled self-consistent calculation is necessary to properly describe the expected log term in χ_d.[4]

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