INFRARED CATASTROPHE IN FERMI GASES WITH LOCAL SCATTERING POTENTIALS

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We prove that the ground state of a system of N fermions is orthogonal to the ground state in the presence of a finite range scattering potential, as $N\to\infty$. This implies that the response to application of such a potential involves only emission of excitations into the continuum, and that certain processes in Fermi gases may be blocked by orthogonality in a low-T, low-energy limit.

Kohn and Majumdar[1] have recently pointed out that there is no singular point for finite λ of some properties—notably the electron density and energy—of a many-body system consisting of a free noninteracting Fermi gas plus a single local scattering potential of strength $\lambda V(r)$ and finite range a. This is true even at the point where V becomes strong enough to begin discontinuously to form a bound state.

We describe here another rather different and somewhat unexpected aspect of this type of continuity. When λ is big enough to form a bound state, the overlap integral between the ground state with the potential, and thus with an electron in the bound state, and any state described entirely in terms of free plane waves, including the ground state of the unperturbed system, is at best of order $N^{-1/2}$ (since it necessarily contains the free-bound overlap which contains the volume to the $-\frac{1}{2}$ power). We show that for any λ this overlap is of order $N^{-\epsilon}$, $\epsilon > 0$, and thus in principle still 0: The ground states are orthogonal.

While wave functions and overlap integrals are often of little consequence in many-body systems, this one is at least related to the response to a sudden application of the potential V, and indicates that that response involves only the emission of low-energy excitations into the continuum, as well as that the truly adiabatic application of such a potential to such a system is impossible. Of course, orthogonality as the full interaction is turned on is expected, and can be dealt with; here the problem is pinpointed by the fact that the perturbation is infinitesimal in a real sense. Other physical implications of the result will be discussed later.

The proof is rather straightforward. For simplicity, but without changing the result, we place our system in a spherical box of radius R and consider only the $l=0$ scattering states. The unperturbed state is a determinant of spherical waves of which the $l=0$ representatives are

$$\varphi_0^{\,n}(r) = N_n \frac{\sin \kappa_n r}{\kappa_n r}; \quad \kappa_n = \frac{\pi n}{R}; \quad E_n = \frac{\hbar^2}{2m}\kappa_n^{\,2} < \epsilon_{\mathrm{F}}. \tag{1}$$

In the presence of a potential V causing a finite phase shift $\delta(E)$ for $l=0$ waves, the new wave functions are, asymptotically,

$$\psi_0^{\,n}(r) \sim N_n' \frac{\sin\{\kappa_n r - \delta(E_n)[1-(r/R)]\}}{\kappa_n r}. \tag{2}$$

The overlap integral between typical members of the two sets near the Fermi surface is

$$A_{nn'} = 4\pi \int_0^R r^2 dr\, \varphi_0^{\,n}(r) \psi^{n'}(r)$$

$$\simeq \frac{2\pi N_n N_{n'}}{\kappa_n \kappa_{n'}} \frac{\sin\delta_{n'}}{\kappa_n - \kappa_{n'} + \delta/R},$$

neglecting central-cell corrections, which, it will be obvious in what follows, are not important and only serve to increase the nonorthogonality in any case. Setting

$$N_n = \kappa_n/(2\pi R)^{1/2},$$

we obtain

$$A_{nn'} = \frac{\sin\delta_{n'}}{\pi(n-n')+\delta}. \tag{3}$$

Summing the squares of $A_{nn'}$ over n checks the normalization of (2), using a well-known sum for $\csc^2\delta$. The overlap integral between determinants made up of states $\varphi(1)$ and $\psi(2)$ is easily seen to be

$$S = \det_{\substack{E_n < E_{\mathrm{F}} \\ E_n' < E_{\mathrm{F}}}} |A_{nn'}|. \tag{4}$$

To evaluate this write the states $\psi_{n'}$ as

$$\psi_{n'} = \sum_{E_n < E_F} A_{nn'}\varphi_n + \sum_{E_n > E_F} A_{nn'}\varphi_n. \qquad (5)$$

Clearly we may omit the second term without changing (4), and we may multiply and divide by a factor to make the first part normalized by itself:

$$S = [\prod_{n'} (1 - \sum_{E_n > E_F} |A_{nn'}|^2)^{1/2}] \times \det |A_{nn'}(1 - \sum_{E_{n''} > E_F} |A_{n''n'}|^2)^{-1/2}|.$$

Now the determinant is the determinant of the components, in an orthonormal basis set, of a set of vectors of unit length, which is the volume of the N-dimensional parallelepiped formed by them and is thus ≤ 1. Usually it will be close to 1.

Thus

$$S \leq \prod_n (1 - \sum_{E_{n'} > E_F} |A_{nn'}|^2)^{1/2}.$$

This is a divergent product: The associated sum is

$$\frac{1}{\pi^2} \sum_{\substack{n < n_f \\ m > n_f}} \frac{\sin^2\delta}{(n - m + \delta)^2} \simeq \frac{\sin^2\delta}{\pi^2} \ln M,$$

where

$$\frac{\hbar^2}{2m}\left(\frac{\pi M}{R}\right)^2 = \Delta \qquad (6)$$

is an energy where δ has fallen to small values. Thus $M \sim$ the radius of the box in atomic units $\sim N^{1/3}$, and

$$S \leq \sim e^{-(\sin^2\delta \ln N^{1/3})/\pi^2} = N^{-\sin^2\delta/3\pi^2}, \qquad (7)$$

where δ is taken at the Fermi surface.

Generalizing to all angular momenta, we have

$$S \leq \exp\left[-\left(\sum_l \frac{2l+1}{\pi^2} \sin^2\delta_l\right) \ln N^{1/3}\right] \leq N^{-\sum [(2l+1)/3\pi^2] \sin^2\delta_l}.$$

Note that the seriousness of this catastrophe is enormously dependent on ths strength of the scattering. For $\delta \sim 0.1$, we get $N^{-1/3000} \sim 1$ even for a very big box; for $\delta \sim \frac{1}{2}\pi$, i.e., resonance, we expect very strong orthogonality, especially for $l > 1$. Note that the perturbed ground state is also orthogonal to all states with any finite number of excitations as $N \rightarrow \infty$. The total energy of excitation is, however, finite rather than $\sim N$.

Where is this "catastrophe" likely to appear physically? Characteristically, the orthogonality integral enters when a transition occurring in one system affects another: the Mössbauer effect, optical transitions accompanied by phonon emission and absorption, self-trapping, etc. For instance, the "zero-phonon" line always involves the ground-state–ground-state overlap for the original and perturbed systems of lattice vibrations (which incidentally is quite finite). What we have shown is that the "zero-quasiparticle" line does not exist for the Fermi system. More generally, this phenomenon affects not only overlap integrals, which enter matrix elements of operators for transitions in other systems coupled to the Fermi sea, but also matrix elements internal to the electronic system such as spin matrix elements in the local-spin problem. For instance, if we were to try to do the Kondo local-spin problem by starting from a diagonalized Ising $S_z s_z$ interaction and doing perturbation theory on the spin-flip elements, we would find that these matrix elements were renormalized to zero by the present phenomenon.

A preliminary calculation of the actual shape of the spectrum of final states indicates that nontheless there is an (integrable) singularity at the zero-energy point, with $\rho(E)$ proportional to $E^{-1+\epsilon}$. Thus this case is truly intermediate between a continuum such as the "one-phonon" band and a line spectrum. It is not clear in what case optical or other transitions in a metal are sharp enough to demonstrate the effect.

Another candidate is tunneling. An electron tunneling into a localized state may change the effective potential of the localized state for opposite-spin electrons radically, and thus encounter an orthogonality block for tunneling at the Fermi surface. As turned out to be the case for phonon interactions, however, this question must be handled with care. We believe this theorem is related to Fermi-surface anomalies both in tunneling and in impurity resistance,[2,3] and a paper on this application is being prepared.

I am grateful for discussions with W. F. Brinkman, D. R. Hamann, and W. L. McMillan. That

some such theorem might exist was called to the attention of my subconscious about a year ago by J. J. Hopfield.

[1]W. Kohn and C. Majumdar, Phys. Rev. 138, A1617 (1965).
[2]J. M. Rowell and L. Y. L. Shen, Phys. Rev. Letters 17, 15 (1966).
[3]B. R. Coles, Phys. Letters 8, 243 (1964). M. P. Sarachik, to be published; I am grateful to Mrs. Sarachick for seeing her preliminary data.

MÖSSBAUER EVIDENCE FOR A SPIN-COMPENSATED STATE IN DILUTE Fe-Cu ALLOYS

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There has been considerable recent interest in the existence and nature of the bound state[1-9] which is thought to be formed in certain dilute alloys between localized magnetic impurity moments and conduction-electron spins below some critical temperature characteristic of the alloy. In their recent communication, Daybell and Steyert[10] presented evidence based on low-temperature resistivity and susceptibility measurements for the formation of such a bound state consistent with some quenching of the localized moment associated with very dilute Fe in Cu. The results of Mössbauer experiments on dilute Fe in Cu in high external magnetic fields (42-136 kOe) are presented here as evidence for significant destruction of the bound state by magnetic fields for which $\mu H_0 \sim kT_K$ where kT_K is on the order of the energy change associated with the formation of the bound state. The fact that the Mössbauer hyperfine spectrum reflects the electronic environment within atomic dimensions of the ^{57}Fe nucleus enables us to make some conjectures as to the singlet nature of the bound state.

The hyperfine interaction in dilute Fe in Cu alloys has been reported by Kitchens, Steyert, and Taylor[11] using the Mössbauer technique in external magnetic fields up to 62 kOe and at temperatures down to 0.4°K. They noted significant deviations from pure paramagnetic behavior and interpreted their results in terms of a model due to Housley and Dash,[12] who introduced a phenomenological interaction between the localized Fe spin and conduction-electron spin-density waves. Measurements at higher fields ($H_0 = 110$ kOe) were reported by Blum, Freeman, and Grodzins.[13] In the ideal paramagnetic case the hyperfine field $H_{\rm hf}$ is proportional to a Brillouin function characterized by the parameters J, g, and $H_{\rm sat}$[14]:

$$H_{\rm hf} = H_{\rm sat} B_J(g\mu_{\rm B} H_0/kT), \tag{1}$$

where J is the total angular momentum associated with the paramagnetic moment, g is the g factor, and $H_{\rm sat}$ is the magnitude of the hyperfine field for sufficiently large values of H_0/T. The sign of $H_{\rm hf}$ for Fe in Cu is negative, i.e., opposite to the direction of the magnetic moment. In the simplest cases the value of $H_{\rm sat}$ has been shown to be proportional to the magnitude of the moment localized on the impurity site and does not change as a function of applied magnetic field, neglecting small Knight-shift contributions.[14] In the Fe-Cu system, however, for the fields and lowest temperatures used ($42 \leq H_0 \leq 136$ kOe; $T \simeq 1.1$°K), we find that although the effective localized moments are fully polarized in the sense that decreasing T does not change the value of the observed hyperfine field, the magnitude of the saturation hyperfine field $|H_{\rm sat}|$ does depend upon the magnitude of the externally applied field, and, as shown in Figs. 1 and 2, increases monotonically as H_0 increases. The experiments were performed using several sources of ^{57}Co plated onto pure (99.999 %) copper foil, annealed in hydrogen at 850°C for several hours and quenched to room temperature. The experimental results are essentially independent of the source used. Source strengths varied from 10 to 100 mCi and the impurity concentration (Fe + Co) is estimated from 100 to 1000 ppm for the various sources.

In view of the recent resistivity and susceptibility results,[10] our Mössbauer data may be explained on the basis of a spin-compensated state appearing at low temperatures and fields