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density of the wave function is larger at the positions of the second-nearest phosphorus neighbors than at the positions of the first-nearest neighbors.

The hyperfine interaction determined here for $^{207}Pb^{3+}$ in both YPO_4 and $LuPO_4$ is the largest ever determined for Pb^{3+} in solids,[5] and indicates that these particular orthophosphates have a strong ionic character. By comparison with the free atom value of 2.60 cm^{-1}, however,[6] it is evident that the wave function is still distorted to a large extent. Trivalent lead is apparently stabilized in the substitutional rare-earth site by the solid-state chemical restraints of the host lattice. This situation is similar to the stabilization of divalent rare-earth ions in the divalent alkaline-earth halides. In the present case, however, no irradiation or electrochemical reduction was necessary.

[1]L. A. Boatner, G. W. Beall, M. M. Abraham, C. B. Finch, P. G. Huray, and M. Rappaz, *Scientific Basis for Nuclear Waste Management* (Plenum, New York, 1980), Vol. II.

[2]*The Encyclopedia of the Chemical Elements*, edited by C. A. Hampel (Reinhold, New York, 1968), p. 712; C. M. Gramaccioli and T. V. Segalstad, Am. Mineral. 63, 757 (1978).

[3]R. C. Ewing, in *Proceedings of the Workshop on Ceramic and Glass Radioactive Waste Forms*, edited by D. W. Readey and C. R. Cooley, ERDA Report No. 770102 (National Technical Information Service, Springfield, Va., 1977), p. 139.

[4]R. S. Feigelson, J. Am. Ceram. Soc. 47, 257 (1964).

[5]B. Andlauer, J. Schneider, and W. Tolksdorf, Phys. Rev. B 8, 1 (1973). The largest hyperfine constant reported in Table I of this paper is 1.382 cm^{-1}.

[6]A. L. Schawlow, J. N. P. Hume, and M. F. Crawford, Phys. Rev. 76, 1876 (1949).

Anderson Localization in $d \leq 2$ Dimensions: A Self-Consistent Diagrammatic Theory

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A diagrammatic theory is presented for the density response function of a system of independent particles moving in a random potential in terms of a current relaxation kernel $M(\vec{q},\omega)$ (essentially the inverse of the diffusion coefficient). In the presence of time-reversal invariance, $M(\vec{q},\omega)$ is shown to have infrared divergencies in $d \leq 2$ dimensions. A self-consistent treatment of the divergent terms yields a finite static electric polarizability α, a dynamical conductivity $\sigma(\omega) \propto \omega^2$ ($\omega \to 0$), and a finite localization length in $d \leq 2$ for arbitrarily weak disorder.

It is well known that a quantum-mechanical particle moving in a random potential will be localized either if the potential fluctuations are strong enough[1] at a given particle energy or else if the particle energy is low enough at given disorder,[2] giving rise to an Anderson transition. Very recently a number of authors[3-8] have proposed that the particles in $d \leq 2$ dimensions are always localized, although for weak disorder in $d = 2$ localization is extremely weak.[3,7,8] In this Letter we want to address this question from the point of view of a standard diagrammatic analysis.

Rather than studying the localization behavior of single-particle states, we focus on a directly measurable physical quantity, the density response function $\chi(\vec{q}, \omega)$ ($\vec{q}$, wave vector; ω, frequency of a density fluctuation). The dynamical conductivity $\sigma(\omega)$ and electrical polarizability $\alpha(\omega)$ are obtained by taking the limit

$$\sigma(\omega) = -i\omega\alpha(\omega) = e^2 \lim_{q \to 0} (-i\omega/q^2)\chi(\vec{q}, \omega),$$

where n and m are the number density and the mass of electrons.

It is instructive to calculate $\chi(\vec{q}, \omega)$ from a simple hydrodynamic model in order to get an idea of what behavior to expect for small q, ω. By regarding the system as a fluid subject to effective macroscopic forces by the random scatterers, the local density $n(\vec{r}, t)$ and current density $\vec{j}(\vec{r}, t)$ obey a continuity equation $\partial_t n(\vec{r}, t) + \text{div} \vec{j}(\vec{r}, t) = 0$

and a relaxation equation

$$\partial_t \vec{j}(\vec{r},t) + \frac{1}{m}\nabla P(\vec{r},t)$$

$$= -\frac{1}{\tau}\vec{j}(\vec{r},t) - \omega_0^2 \int^t dt' \vec{j}(\vec{r},t') + \frac{1}{m}\nabla\mu^{\text{ext}}. \qquad (1)$$

The first term on the right-hand side of (1) describes the relaxation of the current density with a rate $1/\tau$, due to the frictional force the fluid experiences while streaming past the scattering centers. The second term accounts for the restoring force felt by the particles in the localized regime (oscillator frequency ω_0). The last term represents an external chemical potential. Converting the pressure gradient into a density gradient by $\nabla P = [n/\chi^T(0,0)]\nabla n$, where $\chi^T(0,0)$ is the (isothermal) static compressibility, the system of equations is closed. Taking the Fourier transform one finds, for $\chi(\vec{q},\omega) = \delta n(\vec{q},\omega)/\delta\mu^{\text{ext}}(\vec{q},\omega)$,

$$\chi(\vec{q},\omega) = \frac{-q^2 n/m}{\omega^2 + \omega M(\vec{q},\omega) - q^2 n/m\chi^T(\vec{q},0)}$$

$$\simeq \frac{iD(\vec{q},\omega)q^2}{\omega + iD(\vec{q},\omega)q^2}\chi^T(\vec{q},0), \quad \text{for } \omega \ll M, \quad (2)$$

where we have introduced a complex current relaxation kernel $M(\vec{q},\omega)$ and a generalized diffusion coefficient $D(\vec{q},\omega)$:

$$M(\vec{q},\omega) = \frac{i}{\tau} - \frac{\omega_0^2}{\omega} = i\frac{n}{m\chi^T}\frac{1}{D(\vec{q},\omega)}. \qquad (3)$$

To be general we here allow for a q dependence of M and $\chi(\omega=0)$.

In the nonlocalized regime, characterized by a vanishing restoring force ($\omega_0 = 0$), the relaxation

kernel takes the familiar form, $M = i/\tau$ and $\sigma(0) = e^2 n\tau/m$. In the localized regime, however, M is seen to diverge as $-1/\omega$, leading to a finite static polarizability $\alpha(0) = e^2 n/m\omega_0^2$ and a dynamic conductivity $\text{Re}\sigma(\omega) = (e^2 n/m\omega_0^4\tau)\omega^2$. The localization length r_0 may be obtained[6] via the q-dependent static (isolated) susceptibility $\chi(\vec{q},0) \simeq \chi^T(0,0)[q^2 r_0^2/(1+q^2 r_0^2)]$ as $r_0 = [n/m\omega_0^2\chi^T(0,0)]^{1/2} \simeq v_f/\omega_0$. It is quite clear that the $-1/\omega$ divergence of the relaxation kernel $M(\omega)$ is the signature of localization in the response-function formalism.[9]

We will now derive (2) in the limit of small q and ω from a microscopic theory, including an explicit expression for $M(\vec{q},\omega)$ which diverges for $\omega\to 0$. We then show by using a self-consistent generalization how these give rise to the behavior $M\propto -1/\omega$ for arbitrarily weak disorder in $d \leq 2$ dimensions.

We consider a system of independent electrons at zero temperature [Fermi momentum and energy p_F and E_F, density of states, $n(E)$] interacting with randomly distributed scattering centers [density, n_1; Fourier transform of scattering potential, $V(q)$]. $\chi(\vec{q},\omega)$ can be expressed in terms of impurity averages of pairs of retarded and advanced single-particle Green's function $G^{R,A}(\vec{p},\vec{p}';E)$ as[10,11]

$$\chi(\vec{q},\omega) = \omega\sum_{\vec{p},\vec{p}'} R_{\vec{p},\vec{p}'}(\vec{q},\omega) + n(E_F) + O(\omega), \qquad (4)$$

where $R_{\vec{p},\vec{p}'}(\vec{q},\omega) = (-1/2\pi i)\langle G^R(\vec{p}_+,\vec{p}_+'; E_F+\omega) \times G^A(\vec{p}_-,\vec{p}_-';E_F)\rangle_{\text{imp}}$ and $\vec{p}_\pm = \vec{p}\pm\vec{q}/2$, etc. $R_{\vec{p},\vec{p}'}(\vec{q},\omega)$ obeys the generalized kinetic equation[9] (Bethe-Salpeter equation)

$$\{\omega - \vec{p}\cdot\vec{q}/m - \Sigma_{\vec{p}_+}^R(E_F+\omega) + \Sigma_{\vec{p}_-}^A(E_F)\}R_{\vec{p},\vec{p}'}(q,\omega) = \Delta G_p[(1/2\pi i)\delta_{\vec{p},\vec{p}'} - \sum_{\vec{p}''}U_{\vec{p},\vec{p}''}(\vec{q},\omega)R_{\vec{p}'',\vec{p}'}(\vec{q},\omega)], \qquad (5)$$

where $\Delta G_p = G_{\vec{p}_+}^R(E+\omega) - G_{\vec{p}_-}^A(E)$. Here $G_{\vec{p}}^{R,A} = \{E - p^2/2m - \Sigma_{\vec{p}}^{R,A}(E)\}^{-1}$ is the averaged single-particle Green's function, $\Sigma_{\vec{p}}$ is the self-energy and $U_{\vec{p},\vec{p}'}$ is the irreducible vertex.

Summing (5) and $\vec{p}$ and $\vec{p}'$, one finds the analog of the continuity equation (1),

$$\omega\sum_{\vec{p},\vec{p}'} R_{\vec{p},\vec{p}'} - q\sum_{\vec{p},\vec{p}'}(\vec{p}\cdot\vec{q}/m)R_{\vec{p},\vec{p}'}(\vec{q},\omega) = -n(E_F) + O(\omega). \qquad (6)$$

In deriving (6) we have made use of the Ward identity

$$\Sigma_{\vec{p}_+}^R(E+\omega) - \sum_{\vec{p}_-}^A(E) = \sum_{\vec{p}'}U_{\vec{p},\vec{p}'}(\vec{q},\omega)\Delta G_{\vec{p}'} \qquad (7)$$

which may be proven for each diagram observing the property

$$G_1^R G_2^R \cdots G_n^R - G_1^A G_2^A \cdots G_n^A = G_1^R \cdots G_{n-1}^R \Delta G_n^A + G_1^R \cdots G_{n-2}^R \Delta G_{n-1} G_n^A + \cdots.$$

The dependence of $R_{\vec{p},\vec{p}'}$ on $|\vec{p}|$ is dominated by the peak structure of ΔG_p at $|\vec{p}| \simeq p_F$. Expanding the angular variables keeping only $l=0$ and $l=1$ terms, as

$$\sum_{\vec{p}'}R_{\vec{p},\vec{p}'} \simeq -[2\pi i n(E_F)]^{-1}\Delta G_p \sum_{\vec{p},\vec{p}'}\{1 + d(\vec{p}\cdot\hat{q})(\vec{p}''\cdot\hat{q})/p_F^2)\}R_{\vec{p}'',\vec{p}'}$$

and again observing (7) one finds the "current relaxation equation"

$$[\omega + M(\vec{q}, \omega)] \sum_{p,p'} (\vec{p} \cdot \hat{q}/m) R_{\vec{p},\vec{p}'}(q, \omega) - q(2E/md) \sum_{p,p'} R_{\vec{p},\vec{p}'}(q, \omega) = 0. \tag{8}$$

Equations (6) and (8) together with (4) yield $\chi(q, \omega)$ as given by the phenomenological theory, Eq. (2). The current relaxation kernel $M(\vec{q}, \omega)$ is found to be given by

$$M(\vec{q}, \omega) = 2i\gamma + [id/2\pi n(E_F)p_F^2] \sum_{p,p'} (\vec{p} \cdot \hat{q}) \Delta G_p \, U_{\vec{p},\vec{p}'}(\vec{q}, \omega) \Delta G_{p'} (\vec{p}' \cdot \hat{q}) \tag{9}$$

with

$$\gamma = \mathrm{Im}\, \Sigma_{p_F}{}^A(E_F) \simeq \pi n(E_F) n_i \int (d\Omega_{\vec{p}'}/4\pi) \, |V(\vec{p}_F - \vec{p}_F')|^2.$$

Note that $\Sigma^{R,A}$ are smooth functions of the coupling constant and therefore can be approximated by the lowest-order expression.

Substituting the bare vertex $U^0(\vec{p} - \vec{p}') = n_i |V(\vec{p} - \vec{p}')|^2$ in place of $U_{\vec{p},\vec{p}'}$ in (9), one recovers the well-known result of weak-coupling transport theory,

$$M(\vec{q}, \omega) = i/\tau = in_i \sum_{\vec{p}'} 2\pi \delta(E_F - p'^2/2m) \, |V(\vec{p}_F - \vec{p}_F')|^2 [1 - (\hat{p} \cdot \hat{p}')].$$

Let us now turn to a discussion of infrared divergent contributions to $U_{\vec{p},\vec{p}'}$ and M, with the eventual goal to explaining a behavior of $M \propto -1/\omega$. The natural way in which infrared singularities may enter perturbation theory is via the singular nature of the density propagator [cf.(2)], which is a consequence of particle conservation. Summing up the particle-hole ladder diagrams [Fig. 1(a)] we obtain a (bare) diffusion propagator $\Gamma^0(\vec{q}, \omega) = 2i\gamma U_0/(\omega + iD_0 q^2)$ (q, ω small), where $D_0 = 2\tau E/md$ is the bare diffusion constant. Note that the integral on $\vec{q}$ of $\Gamma^0(\vec{q}, \omega)$ diverges in the limit $\omega \to 0$ in $d \le 2$ dimensions. In Fig. 1(b) the leading contribution (in term of γ/E) of this type of divergence to the irreducible vertex part $U_{\vec{p},\vec{p}'}$ is shown, obtained by adding vertex corrections to Γ^0. (The double counting of the lowest-order crossed diagram is of no consequence for the following). Substituting this into (9) and expanding in q and k, one finds the following divergent contribution to $M(\vec{q}, \omega)$:

$$M^D(\vec{q}, \omega) = -\frac{d}{p_F^2} U_0 \sum_{\vec{k}} \frac{q^2 + (\vec{k} \cdot \hat{q})^2}{\omega + iD_0 k^2} \simeq \frac{q^2}{2p_F^2} \frac{i}{\tau} F_d(\omega), \, d = 1, 2, \quad \text{as } \omega \to 0, \tag{10}$$

where $F_1(\omega) = (2/\pi)(i/\omega\tau)^{1/2}$ and $F_2(\omega) = (1/2\pi E\tau) \ln(1/\omega\tau)$ (neglecting the momentum dependence of U_0).

This divergence appears to be the one previously found[7] within a mode-coupling approximation for $M(\vec{q}, \omega)$. A similar divergence occurs in the $q \neq 0$ current correlation function. Moreover we can prove that the diffusion pole never gives rise to any divergent contribution for $M(0, \omega)$.[9]
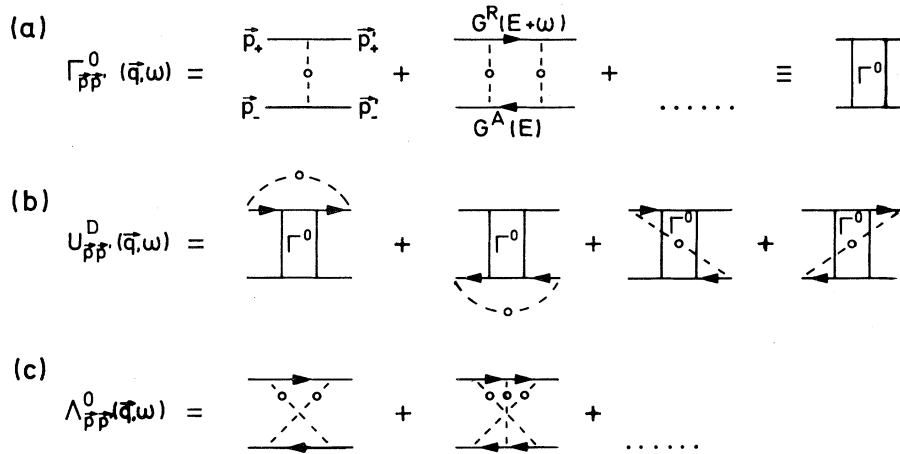

FIG. 1. (a) The diffusion propagator Γ^0, i.e., the sum of particle-hole ladder diagrams; (b) the leading diagrams of the irreducible vertex $U_{\vec{p},\vec{p}'}{}^D$ with respect to the divergence of Γ^0 for $\omega \to 0$; (c) Λ^0, the sum of maximally crossed diagrams.

There is, however, a further possibility of infrared divergencies in M even at $q = 0$, which has been noted first by Abrahams et al.[3]: in the presence of time-reversal invariance the diffusion pole is carried over to the particle-particle channel, giving rise to a singular structure

$$\Lambda_{\vec{p},\vec{p}'}^{0}(\vec{q},\,\omega) = 2i\gamma U_0/[\omega + iD_0(\vec{p} + \vec{p}')^2]$$

for $\vec{p}' \simeq -\vec{p}$ ($2k_F$ scattering), where Λ^0 is the sum of the maximally crossed diagrams [Fig. 1(c)]. Since the diagrams of Λ^0 are particle-hole irreducible, they contribute to $U_{\vec{p},\vec{p}'}^{-}$, and hence M, yielding a divergent contribution even at $q = 0$,

$$M^{2k_F}(0,\,\omega) = -2U_0 \sum_{\vec{k}}(1/\omega + i\,D_0k^2) \simeq (i/\tau)F_d(\omega), \quad \text{as } \omega \to 0. \tag{11}$$

The divergence is removed by the time-reversal invariance breaking fields, such as generated by spin-flip scattering.[12]

The result (10) and (11) is only meaningful as long as ω is not too small. Since according to (3) the diffusion coefficient D is related to M by $D(\vec{q},\,\omega) = D_0[(i/\tau)/M(\vec{q},\,\omega)]$ it is not justified to keep the diffusion constant D_0 in (10) and (11) fixed if M diverges. Replacing D_0 in (10) and (11) by $D(0,\,\omega)$ a self-consistent equation for $M(0,\,\omega)$ is obtained:

$$M(0,\,\omega) = \frac{i}{\tau} - 2U_0 \sum_{|\vec{k}| < k_0} \frac{1}{\omega + i/\tau_s - k^2(2E_F/md)/M(0,\,\omega)}. \tag{12}$$

Here we have introduced an upper cutoff k_0 of the order of the Fermi momentum p_F and a time-reversal–invariance–breaking term i/τ_s (τ_s spin-flip scattering time). The replacement $D_0 \to D$ in (12) is justified because of the identity satisfied by the complete vertex function

$$\Gamma_{\vec{p},\vec{p}'}(\vec{q}) = \Gamma_{(\vec{p}-\vec{p}'+\vec{q})/2,(\vec{p}'-\vec{p}+\vec{q})/2}(\vec{p}+\vec{p}')$$

in the case of time-reversal invariance. The $M(\vec{q},\,\omega)$ of Ref. 6 would correspond to a self-consistent generalization of (10). It has been shown in Ref. 7 that such a treatment gives rise to divergent contributions to $M(\vec{q},\,\omega)$ one order of U_0 smaller than the one in (12). We have identified these divergencies in terms of diagrams but are able to show[9] that these are cancelled by similar diagrams which are, however, not generated by the self-consistent generalization.

Let us now discuss the self-consistent solution of (12). In $d > 2$ dimensions (12) has the familiar solution $M(0,0) = i/\tau$ in the limit of small impurity concentration. In $d \leqslant 2$, if time-reversal invariance (obtained formally by putting $1/\tau_s = 0$) is assumed, M diverges in the limit $\omega \to 0$ as seen from the $\vec{k}$ integral in (12). The self-consistent solution has indeed the form $M(0,0) = i/\tau - \omega_0^2/\omega$ as required for a localized solution. Here $\omega_0^2 = (\pi/2)^2 E_F^2\lambda^2$ for $d = 1$ and $\omega_0^2 = 2E_F^2x_0^2 \exp(-1/\lambda)$ for $d = 2$, where $\lambda = n_i n\{V(q=0)/E_F\}^2$ is a dimensionless coupling parameter and $x_0 \equiv (k_0/p_F)$ is a cutoff parameter. The $d = 1$ result agrees with the exact solution[13,14] for the polarizability $\alpha(0)$

apart from a factor[14] of $\zeta(3) \simeq 1.20$ and for the dynamic conductivity as far as the coupling constant dependence is concerned (the level repulsion effect giving rise to a $(\ln\omega)^{d+1}$ factor in $\sigma(\omega)$ is not obtained by our present theory). In $d = 2$, ω_0 is seen to become exponentially small for small coupling λ, giving rise to an extremely large polarizability α and localization length r_0.

The effects of inelastic scattering at finite temperatures may be qualitatively incorporated in our theory by replacing ω by $\omega + i/\tau_{inel}$, where τ_{inel} is inelastic collision time. The leading-order correction to the weak coupling result $M = i/\tau$ is $\ln(\tau_{inel})$ ($d = 2$) and $(\tau_{inel})^{1/2}$ ($d = 1$) temperature dependence in the low-T resistance of a dirty metal film or wire. Such effects seem to have been observed[15,16] recently and have been interpreted[17] in terms of the $2k_F$ mechanism.

Further details on this work will be published elsewhere.[9]

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[1]P. W. Anderson, Phys. Rev. 109, 1492 (1958).

[2]N. F. Mott, Philos. Mag. 13, 989 (1966).

[3]E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. 42, 673 (1979).

[4]L. P. Gorkov, A. I. Larkin, and D. E. Khmelnitskii, Pis'ma Zh. Eksp. Teor. Fiz. 30, 248 (1979) [JETP Lett. 30, 228 (1979)].

[5]F. Wegner, Z. Phys. 35, 207 (1979).

[6]W. Götze, Solid State Commun. 27, 1393 (1978), and J. Phys. C 12, 1279 (1979), and to be published.

[7]W. Götze, P. Prelovšek, and P. Wölfle, Solid State Commun. 30, 369 (1979).

[8]P. B. Allen, to be published.

[9]D. Vollhardt and P. Wölfle, to be published.

[10]A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinskii, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Englewood Cliffs, N.J., 1969).

[11]S. V. Maleev and B. P. Toperverg, Zh. Eksp. Teor.

Fiz. 69, 1440 (1975) [Sov. Phys. JETP 42, 734 (1976)].

[12]D. E. Khmelnitskii, to be published.

[13]V. L. Berezinsky, Zh. Eksp. Teor. Fiz. 65, 1251 (1973) [Sov. Phys. JETP 38, 620 (1974)].

[14]A. A. Abrikosov and I. A. Ryshkin, Adv. Phys. 27, 147 (1978).

[15]G. J. Dolan and D. D. Osheroff, Phys. Rev. Lett. 43, 725 (1979).

[16]N. Giordano, W. Gilson, and D. E. Prober, Phys. Rev. Lett. 43, 725 (1979).

[17]P. W. Anderson, E. Abrahams, and T. V. Ramakrishnan, Phys. Rev. Lett. 43, 718 (1979).