of the response function. It accounts for the phenomena observed in systems with a potentially soft mode. RPA and classical theories are very inaccurate for such systems. Because of the simple and general nature of the approximation scheme in the correlation theory it may be considered as a generalization of the RPA with a wide range for applications.

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Scaling Theory of Interacting Disordered Fermions

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A scaling theory for the interacting disordered fermion problem is constructed by extending the perturbation in coupling constant to second order. A scaling hypothesis produces a set of scaling equations which incorporates both localization and interaction. The resulting exponents are compared with experiments and further experimental tests of the theory are proposed.

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Many disordered electronic systems undergo a metal-to-insulator transition as the amount of disorder is increased. In the past few years, increasing evidence has accumulated that the nature of the transition is governed by two aspects of the problems: (i) Anderson localization, i.e., the behavior of a single-electron wave function in the presence of a random potential and (ii) the interaction among electrons in the presence of disorder. By now, a scaling theory of the Anderson-

localization problem is well established. We can view the development of this theory in three stages. First, Abrahams *et al.*[1] showed by perturbation theory in $(\epsilon_F\tau)^{-1}$, where τ is the elastic scattering time, that a logarithmic correction to the conductivity exists in two dimensions (2D)

$$\sigma = \sigma_0[1 + t\ln(\omega/\Lambda)]. \quad (1)$$

In Eq. (1) the cutoff frequency $\Lambda = \tau^{-1}$ and $t = (4\pi^2 g)^{-1}$ where $g = \epsilon_F\tau/2\pi$ is the conductance per square per spin in 2D in units of $e^2/\hbar$. Next, it was shown by Gorkov, Khmel'nitskii, and Larkin[2] that the next leading term, $t^2\ln(\omega/\Lambda)$, has vanishing coefficient, and consequently a scaling theory with t as the sole scaling variable is consistent. Finally, Wegner[3] mapped the Anderson-localization problem to a field-theory model whose scaling behavior can be established with use of conventional renormalization-group methods. While the localization problem is in a satisfactory state, it deals only with noninteracting particles. It turns out that for electrons interacting with a potential $v(q)$ in the presence of weak impurity scattering, i.e., $H_I = \frac{1}{2}\sum_q v(q)\rho_q\rho_{-q}$, ρ_q being the density operator, the fact that density fluctuations are diffusive leads to singularities in 2D,[4,5]

$$P = P_0[1 + (\lambda_1 - s\lambda_2)\ln(\omega/\Lambda)], \quad (2)$$

where P stands for the conductivity σ, the single-particle density of states N_1, or the coefficient γ of the linear T term in the specific heat, and ω is the frequency or the temperature T, whichever is larger. In Eq. (2), s is the spin degeneracy, $\lambda_1 = v(0)N_{10}t$, and $\lambda_2 = F\lambda_1$ where F is a factor which depends on the interaction range such that $F \to 0$ or 1 for long- or short-range (compared with k_F^{-1}) interactions. The situation for the dynamically screened Coulomb interaction is more complicated, but in this paper we shall concentrate on the static interaction only. Our strategy is to extend the results of Gorkov, Khmel'nitskii, and Larkin[2] to include interactions, namely we calculate to order $\ln^2(\omega/\Lambda)$ and deduce the properties of the scaling theory without knowing the underlying field theory.

It is known that the logarithmic correction in Eq. (1) is destroyed when time-reversal symmetry is broken, a situation which is realized experimentally by the application of a magnetic field.[6] We shall first present the results in this limit. The spin susceptibility χ for $d = 2$ is given by[7]

$$\tilde{\chi}/\chi_0 = 1 - \lambda_2\ln(\omega/\Lambda) - \lambda_1\lambda_2\ln^2(\omega/\Lambda). \quad (3)$$

For $d > 2$, $\ln(\omega/\Lambda)$ is replaced by $[(\omega/\Lambda)^{\epsilon/2} - 1]/(\epsilon/2)$. For the single-particle density of states and the conductivity, the $\lambda^2\ln^2$ terms turn out to vanish. We note that the perturbation is in powers of λ; i.e., v and t always occur as a product. Our next step is to *assume* that a scaling theory exists with λ_1 and λ_2 as the scaling variables. Specifically, upon reducing the cutoff energy Λ to Λ', we can find new variables λ_1' and λ_2' such that

$$P(\omega/\Lambda,\lambda_1,\lambda_2)Z_P(\Lambda'/\Lambda,\lambda_1,\lambda_2) = P(\omega/\Lambda',\lambda_1',\lambda_2'), \quad (4)$$

for any physical quantity P that scales.[8] By assuming that N_1 and $\tilde{\chi}$ satisfy Eq. (4) we obtain the scaling equations

$$d\lambda_1/d\ln\Lambda = (\tfrac{1}{2}\epsilon)\lambda_1 - \lambda_1^2 + 4s\lambda_1\lambda_2 - (s^2 - s)\lambda_2^2, \quad (5)$$

$$d\lambda_2/d\ln\Lambda = (\tfrac{1}{2}\epsilon)\lambda_2 + \lambda_2^2 + 2\lambda_1\lambda_2, \quad (6)$$

where $\epsilon = d - 2$. The vanishing $\ln^2$ result for the conductivity serves as a test of our scaling hypothesis. We shall restrict our analysis to the case of repulsive interaction, such that λ_1 and λ_2 are both positive. Equation (6) shows that λ_2 scales towards weak coupling and becomes irrelevant. We obtain the fixed point $\lambda_1^* = \epsilon/2$, $\lambda_2^* = 0$ with an eigenvalue of $-\epsilon/2$. Furthermore, for any quantity that scales, we can write down the Lie equation which requires knowing only the linear logarithmic term[8]:

$$d\ln\sigma/d\ln\omega = \lambda_1 - s\lambda_2, \quad (7)$$

and similarly for N_1 and χ. Thus, at the transition we predict that both σ and N_1 vanish like $(\omega/\Lambda)^{\lambda_1^*} = (\omega/\Lambda)^{(d-2)/2}$. If we are a distance δn from the critical point (δn may be the impurity concentration from the critical value, for instance), and $\lambda_1 < \lambda_1^*$, we reach the metallic limit when the energy scale reaches $\Delta/\Lambda = (\delta n)^{2/\epsilon}$, beyond which point the conductivity stays constant. Thus, we predict that

$$\sigma \sim (\Delta/\Lambda)^{\epsilon/2} \sim (\delta n)^1. \quad (8)$$

Interestingly, this prediction is the same as the pure localization theory[1] and is characteristic of a one-parameter scaling theory. We should mention that the vanishing $\ln^2$ term for N_1 and the scaling exponents have been obtained independently by Castellani *et al.*[9]

We now proceed to discuss the full problem including the localization contributions. Technically, the $t\ln$ term in Eq. (1) comes from summing maximally crossed diagrams, and we must now

include such diagrams in the first-order interaction-theory calculations. The results are

$$N_1/N_{10} = 1 + (\lambda_1 - s\lambda_2)\ln(\omega/\Lambda) - t(\lambda_1 - s\lambda_2)\ln^2(\omega/\Lambda), \quad (9)$$

$$\sigma/\sigma_0 = 1 + (t + \lambda_1 - s\lambda_2)\ln(\omega/\Lambda) - \tfrac{3}{2}t(\lambda_1 - s\lambda_2)\ln^2(\omega/\Lambda), \quad (10)$$

$$\chi/\chi_0 = \tilde{\chi}/\chi_0 + \tfrac{1}{2}t\lambda_2\ln^2(\omega/\Lambda). \quad (11)$$

We now proceed as before except that we add an additional scaling variable t and assume that N_1, χ, and σ scale. The following scaling equations are obtained.

$$d\lambda_1/d\ln\Lambda = R_1 - 2\lambda_1 t + s\lambda_2 t, \quad (12)$$

$$d\lambda_2/d\ln\Lambda = \lambda_2(\tfrac{1}{2}\epsilon + \lambda_2 + 2\lambda_1 - t), \quad (13)$$

$$dt/d\ln\Lambda = t[\tfrac{1}{2}\epsilon - t - 3(\lambda_1 - s\lambda_2)], \quad (14)$$

where R_1 denotes the right-hand side of Eq. (5). We note that the localization fixed point $t^* = \epsilon/2$, $\lambda_1^* = \lambda_2^* = 0$ is unstable to λ. The fixed point that controls the metal-insulator transition is the one located at $t^* = \epsilon/5$, $\lambda_1^* = \epsilon/10$, $\lambda_2^* = 0$. Furthermore, for repulsive interaction λ_2 always scales towards zero. Thus, a two-parameter scaling theory results. The eigenvalue which characterizes the flow away from the fixed point is found to be $-\epsilon/2$.

We can again write down the Lie equation for σ, N_1, and χ:

$$d\ln\sigma/d\ln\omega = t + \lambda_1 - s\lambda_2, \quad (15)$$

$$d\ln N_1/d\ln\omega = \lambda_1 - s\lambda_2, \quad (16)$$

$$d\ln\chi/d\ln\omega = -\lambda_2. \quad (17)$$

Comparison of Eqs. (14) and (15) reveals the important fact that unlike the localization problem, $\sigma\Lambda^{\epsilon/2}$ does not satisfy the same scaling equation as t^{-1}. Thus, the conductance is *not* the scaling variable in the presence of interactions.

In the critical region we have

$$\sigma \sim (\omega/\Lambda)^{t^* + \lambda_1^* - s\lambda_2^*} \approx (\omega/\Lambda)^{3(d-2)/10}$$

$$N_1 \sim (\omega/\Lambda)^{(d-2)/10}.$$

Again, ω is frequency or T, whichever is greater. Away from the critical point we have a characteristic energy scale $\Delta/\Lambda \sim (\delta n)^{2/\epsilon}$, which is the scale at which we scale to the weak-coupling limit (metal). At this stage, we can do perturbation theory, i.e., we can use Eqs. (1) and (2) but with renormalized parameters. We therefore obtain

$$N_1(\omega) = N_1(0)[1 + (\omega/\Delta)^{\epsilon/2}], \quad \omega < \Delta \quad (18)$$

$$\sigma(\omega) = \sigma(0)[1 + (\omega/\Delta)^{\epsilon/2}], \quad \omega < \Delta \quad (19)$$

where $N_1(0) \sim (\Delta/\Lambda)^{\epsilon/10} \sim (\delta n)^{0.2}$ and $\sigma(0) \sim (\Delta/\Lambda)^{3\epsilon/10} \sim (\delta n)^{0.6}$. For $\omega > \Delta$, the critical behavior $N_1 \sim (\omega/\Lambda)^{\epsilon/10}$ and $\sigma \sim (\omega/\Lambda)^{3\epsilon/10}$ are restored. In general, the behavior of other scaling quantities whose leading logarithmic corrections are known (Hall constant,[6] thermopower, etc.) is determined by similar arguments and will be discussed elsewhere.

On the insulating side of the transition, scaling is towards strong coupling. The insulating region is reached on a scale $\Lambda = \Delta$. The dielectric constant ϵ_1 can be estimated by noting that $\epsilon_1 = \sigma''/\omega$ where σ'' is the imaginary part of the conductivity. By the Kramers-Kronig relation, $\sigma'' \sim (\omega/\Lambda)^{3\epsilon/10}$ in the critical region. Thus, we obtain for the dielectric constant

$$\epsilon_1 = (\Delta/\Lambda)^{(0.3\epsilon - 1)} = (\delta n)^{(0.6\epsilon - 2)/\epsilon}. \quad (20)$$

To the extent that we have a two-parameter scaling theory, our general picture is similar to that of McMillan.[10] Equations (18) and (19) are generic to any scaling theory which scales to weak coupling and were first written down by McMillan. However, the exponents and the relationship between exponents that we obtain are very different. McMillan has assumed that the screening constant is given by $K^2 = 4\pi e^2 s N_1$ and the conductivity is related to the diffusion constant by $\sigma = e^2 s N_1 D$. One of us argued elsewhere[11] that in both cases N_1 should be replaced by $dn/d\mu$ which contains no singularity. The erroneous use of the density of states shows up in the relationship between the exponents for the conductivity, N_1, and the dielectric constant which disagrees with the present work.

We now discuss some comparison with experiments. Very close to the metal-insulation transition in Si:P, it is found[12] that on the metallic side $\sigma \sim (\delta n)^{0.5}$, while on the insulating side ϵ_1 diverges with about twice the exponent. The conductivity exponent 0.5 is far from unity predicted for the pure localization model but compares well with 0.6 obtained here. The ratio of the ϵ_1 and σ exponents is predicted to be $2\frac{1}{3}$ if we set $\epsilon = 1$, and the agreement with experiments is acceptable. Our theory also predicts that near the transition, the conductivity should behave as $T^{1/2}$ for $T < \Delta$ as shown in Eq. (19) and the coefficient of the $T^{1/2}$ term should diverge as $(\delta n)^{-2/5} \sim \sigma^{-2/3}$ near the

transition. Experimentally, a $T^{1/2}$ term was observed in very metallic samples[13] and interpreted according to the first-order perturbation theory, Eq. (2). The sign indicates that λ_2 dominates over λ_1. As the transition is approached, the sign of the $T^{1/2}$ term is observed to change.[13] We may now understand this as the scaling of λ_2 to zero. We also point out that our theory predicts that if the conductivity is measured in the presence of a sufficiently large magnetic field (cyclotron frequency large compared with Δ) the time-reversal symmetry-breaking model is appropriate. The observed $\sigma \sim (\delta n)^{0.5}$ behavior should change over to a linear behavior in the vicinity of the transition.

It is worth mentioning that according to Eq. (17), the spin susceptibility should grow with decreasing temperature and then saturate to a constant value when λ_2 scales to zero. A rise in χ has been observed in Si:P on the metallic side of the transition.[14] However, on the insulating side χ diverges like $T^{\alpha-1}$, $\alpha < 1$. This has been interpreted as the freezing out of singlet pairs of localized spins.[15] The relation of this behavior on the insulating side to the present theory in the critical region remains to be clarified.

Tunneling and conductivity measurements have been performed on amorphous alloys such as Au_xGe_{1-x}[16] and Nb_xSi_{1-x}.[17] In contrast with the Si:P data, the conductivity in Nb_xSi_{1-x} was found to vanish linearly with concentration near the transition.[17] The tunneling data were analyzed according to Eq. (18). For $\omega > \Delta$, an $\omega^{1/3}$ behavior was reported,[17] somewhat different from the $\omega^{0.1}$ we predict. A possible reason for this discrepancy is that dynamic screening is important for the density of states (in 2D we know that dynamic screening produces $\ln^2$ corrections already in first order[6]). An intriguing possible explanation of the conductivity exponent is that spin-flip scattering becomes important near the transition and provides the time-reversal symmetry-breaking mechanism to convert the conductivity exponent from 0.6 to 1. We have also worked out the spin-orbit scattering case and it may serve the same purpose.

Finally, we make several comments on the theory: (i) At the fixed point $\lambda^* = 0.1\epsilon$, $t^* = 0.2\epsilon$, we have $vN_1 = \frac{1}{2}$. Thus, strictly speaking it is not legitimate to do perturbation in v. Parts of such corrections amount to replacing v by some Fermi-liquid coupling constant. This also raises the possibility of spin-dependent coupling, which we have ignored. (ii) There exist maximally crossed diagram contributions to lowest order in $Fvt \ln(\omega/\Lambda)$.[5,6,18] However, it has been shown[18] that such terms are renormalized to zero which justifies our ignoring them. (iii) We have also calculated the specific heat $c_v = \gamma T$ and obtained

$$\gamma/\gamma_0 = N_1/N_{10} + \tfrac{1}{2}(\lambda_1^2 - 2s\lambda_1\lambda_2 + \lambda_2^2)\ln^2(T/\Lambda). \quad (21)$$

The presence of the extra terms in Eq. (21) indicates that λ/λ_0 and N_1/N_{10} do not both scale, i.e., satisfy Eq. (4). At first sight, our choice of N_1/N_{10} as the scaling quantity seems arbitrary. Here we must be guided by some physical consideration, namely N_1 is expected to vanish at the transition whereas γ should remain finite. This is because even on the insulating side there exist low-lying particle-hole excitations which contribute to the specific heat.[19] This is in fact observed experimentally.[20] The constant term means that γ does not satisfy Eq. (4), but subtraction terms analogous to those for the free energy in critical phenomena are needed. We have further justification for choosing N_1 as the scaling quantity because it is consistent with the scaling of the conductivity.

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First-Principles Calculation of Stress

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A generalization of the virial theorem is presented for all components of the average stress tensor of arbitrary systems of interacting particles. Explicit expressions are given for local-density-functional calculations and the method is tested by *ab initio* pseudopotential calculations on silicon. Accurate determinations are made of lattice constant, bulk moduli, second-, third-, and fourth-order elastic constants, and the internal strain parameter ζ. Agreement with experiment is very good, except for ζ.

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In this Letter we present a general expression for the average stress tensor in an arbitrary system of interacting particles. We term this result the stress theorem, since it is a generalization of the quantum-mechanical virial theorem[1,2] and since it is closely related to the force theorem originally derived by Ehrenfest[3] (now often referred to as the Hellmann-Feynman theorem[4]). This form is used to derive an explicit, practical expression for the stress tensor of a periodic solid within the local-density-functional (LDF) framework. The combined force and stress theorems completely determine the equation of state of the crystal, i.e., external stresses and forces as a function of strains and internal atomic displacements. We apply the expression to silicon, using the *ab initio* pseudopotential method, to derive the equilibrium lattice constant and bulk moduli from calculations of both total energy and pressure. Elastic constants, higher-order elastic constants, the internal strain parameter ζ, and the TO(Γ) phonon frequency are derived by applying anisotropic strains and atomic displacements to the unit cell.

The stress tensor, introduced into quantum mechanics by Schrödinger[5] and Pauli,[6] can be derived in a many-body form with a scaling procedure due to Fock.[2] The total energy is

$$E_{\rm tot}=\langle H_{\rm int}+V_{\rm ext}\rangle=\langle\textstyle\sum_i p_i^{\,2}/2m_i+V_{\rm int}+V_{\rm ext}\rangle, \quad (1)$$

where i labels the particles, and $V_{\rm int}$ denotes general interactions between the particles; $V_{\rm ext}$, the external potentials; and angular brackets, the expectation value. Introducing a uniform scaling of the particle coordinates $\vec{r}_i$ by an infinitesimal strain tensor, $r_{i\alpha}\to r_{i\alpha}+\sum_\beta \epsilon_{\alpha\beta} r_{i\beta}$, the desired result follows from the variational property that a "stretching of the ground state"[2] does not change $E_{\rm tot}$ to first order. The stationarity of $E_{\rm tot}$ with respect to $\epsilon_{\alpha\beta}$ leads to the result that the total internal stress tensor $T_{\alpha\beta}$, given by

$$T_{\alpha\beta}=\partial\langle H_{\rm int}\rangle/\partial\epsilon_{\alpha\beta}$$
$$=-\textstyle\sum_i\langle p_{i\alpha}p_{i\beta}/m_i-r_{i\beta}(\nabla_{r_i}V_{\rm int})_\alpha\rangle, \quad (2)$$

must be balanced by the stress due to the external potential in order for the system to be in equilibrium. The average stress is denoted by