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Electronic structure factor of disordered materials

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The dynamical structure factor of electrons in disordered systems is found to consist of two parts: One part is a disorder-induced elastic contribution with some form factor $S_e(\vec{q})$; the other one is related to the density relaxation spectrum. We evaluate $S_e(\vec{q})$ in perturbation theory and the density relaxation within the self-consistent current relaxation theory for two- and three-dimensional systems. For short-range potential fluctuations we find a peak in the static structure factor $S(\vec{q})$ at $q \cong 2k_F$.

I. INTRODUCTION

The dynamical structure factor $S(\vec{q},\omega)$ of electrons with wave vector $\vec{q}$ and frequency ω (Ref. 1) can be measured, for instance, by x-ray or light scattering. These techniques have been applied to investigate a great variety of physical phenomena (for a review see, e.g., Ref. 2). In particular, Coulomb-interaction effects in good conductors have been studied and a peak structure in the static structure factor $S(\vec{q})$, which is the frequency integral of $S(\vec{q},\omega)$, for q about twice the Fermi momentum k_F, has been found.[3]

In this paper we show that in disordered systems, characterized by a random potential, $S(\vec{q})$ has a nontrivial structure even for noninteracting electrons. In particular, there is an elastic contribution to $S(\vec{q},\omega)$ with form factor $S_e(\vec{q})$. Interpreting $S(\vec{q},\omega)$ as a scattering cross section,[1,2] this elastic peak reflects the indirect coupling of the radiation to the random potential via the conduction electrons. The elastic peak describes the analog of the scattering from static lattice distortions due to crystal imperfections.[4] A similar impurity-induced elastic peak was discussed in connection with magnetic scattering by Sacchetti.[5] In addition to this peak there is the usual contribution given by Kubo's density relaxation function $\Phi''(\vec{q},\omega)$ via the fluctuation-dissipation theorem.[6] To calculate $\Phi''(\vec{q},\omega)$ approximately we use the self-consistent current relaxation theory (SCCR).[7] To study the influence of the elastic peak on $S(\vec{q})$ we apply a lowest-order calculation for $S_e(\vec{q})$. In this way a disorder-induced peak in $S(\vec{q})$ at $q \cong 2k_F$ is found.

The shortcomings of the perturbation theory for $S_e(\vec{q})$ can be overcome by applying the coherent-potential approximation[8,9] (CPA) to this quantity. The resulting formulas, which yield the correct weak- and strong-coupling results for an Anderson Hamiltonian of disordered conductors[10] are given in the Appendix.

II. THE ELECTRONIC STRUCTURE FACTOR

Let us consider a d-dimensional zero-temperature gas of noninteracting, spinless electrons of density n. The density operator for wave vector $\vec{q}$ is given by

$$\rho(\vec{q}) = \sum_{\vec{k}} a^{\dagger}_{\vec{k}-\vec{q}/2} a_{\vec{k}+\vec{q}/2}$$

where a and $a^{\dagger}$ are the usual annihilation and creation operators for momentum eigenstates. The dynamical structure factor is given by[1]

$$S(\vec{q},\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} [\langle \rho^{\dagger}(\vec{q},t)\rho(\vec{q})\rangle]_{\mathrm{av}}/n \ . \quad (1)$$

Here the angular brackets denote the quantum-mechanical expectation value and the notation $[\ ]_{\mathrm{av}}$ denotes ensemble averaging. We decompose the density operator into its mean value and fluctuations:

$$\rho(\vec{q}) = \langle \rho(\vec{q})\rangle + \delta\rho(\vec{q}) \ .$$

Application of the fluctuation-dissipation theorem yields

$$S(\vec{q},\omega)=2\pi\delta(\omega)S_e(\vec{q})+(2/n)\omega\Theta(\omega)\Phi''(\vec{q},\omega)\ , \tag{2a}$$

where

$$S_e(\vec{q})=[\langle\rho^\dagger(\vec{q})\rangle\langle\rho(\vec{q})\rangle/n]_{\rm av}\ , \tag{2b}$$

and $\Phi''(\vec{q},\omega)$ denotes the absorptive part of Kubo's density relaxation function.[6]

For explicit calculations we choose the Edwards model[11] for electrons with Fermi energy $\epsilon_F=\hbar^2k_F^2/2m$ in a random potential $U(\vec{q})$, specified by the Hamiltonian

$$H=\sum_{\vec{k}}[\epsilon(\vec{k})-\epsilon_F]a_{\vec{k}}^\dagger a_{\vec{k}}+\sum_{\vec{q}}U(\vec{q})\rho^\dagger(\vec{q})\ , \tag{3}$$

where

$$\epsilon(\vec{k})=\hbar^2k^2/2m$$

with the effective electron mass m. Without loss of generality the random potential can be assumed to have a zero mean value: $[U(\vec{q})]_{\rm av}=0$. Applying standard perturbation theory then yields for $S_e(\vec{q})$ in the Born approximation, for $q\neq0$,

$$\begin{aligned}S_e(\vec{q})&=[\,|\,U(\vec{q})\,|^2]_{\rm av}g_0^2(q)/n\\&=c_iS_i(q)\,|\,u(\vec{q})\,|^2g_0^2(q)/n\ .\end{aligned} \tag{4}$$

Here c_i is the impurity concentration, $S_i(q)$ is the impurity structure factor, and $u(\vec{q})$ is the impurity electron pseudopotential. $g_0(q)$ is the wave-number-dependent compressibility of the free-electron gas; for $d=3$ $g_0(q)$ is the Lindhard function, while for $d=2$ it has been reported by Stern.[12] The preceding result is completely analogous to the corresponding formulas worked out before in connection with the lattice-distortion problem.[13]

If the random potential is so strong that the system undergoes an Anderson transition to an insulator,[10] the density relaxation spectrum $\Phi''(\vec{q},\omega)$ exhibits a zero-frequency peak due to the nonergodicity of the density fluctuations.[7] However, this feature of the Anderson insulator has no direct effect on the dynamical structure factor, as can be seen from Eq. (2a). The elastic peak in $S(\vec{q},\omega)$ appears no matter whether the system is a conductor or an insulator. In contrast to the usual Bragg peaks in crystals the form factor $S_e(\vec{q})$ of this disorder-induced elastic peak is a continuous function of momentum. By coupling to the random potential the electrons can transfer momentum without transferring energy. Thus a test field, probing $S(\vec{q},\omega)$, can transfer momentum without changing energy. A test particle can be scattered elastically by the static electronic density fluctuations created by the impurities.

III. RESULTS

According to Eq. (2a) the static structure factor consists of two parts:

$$S(\vec{q})=S_e(\vec{q})+S_{\rm in}(\vec{q}) \tag{5a}$$

with

$$S_{\rm in}(\vec{q})=\int_0^\infty d\omega\,\pi^{-1}\omega\Phi''(\vec{q},\omega)/n\ . \tag{5b}$$

We characterize the random potential by a strength parameter U and a momentum cutoff q_0:

$$[\,|\,U(\vec{q})\,|^2]_{\rm av}=U^2[(2\pi)^dd/(S_dq_0^d)]\Theta(q_0-q)\ , \tag{6}$$

where S_d is the surface of the d-dimensional unit sphere. To calculate $S(\vec{q})$ we use the SCCR. For given U and $\xi=2k_F/q_0$, $\Phi''(\vec{q},\omega)$ can be calculated by solving a transcendental equation.[7,14,15]

For a result shown in Fig. 1 we have chosen

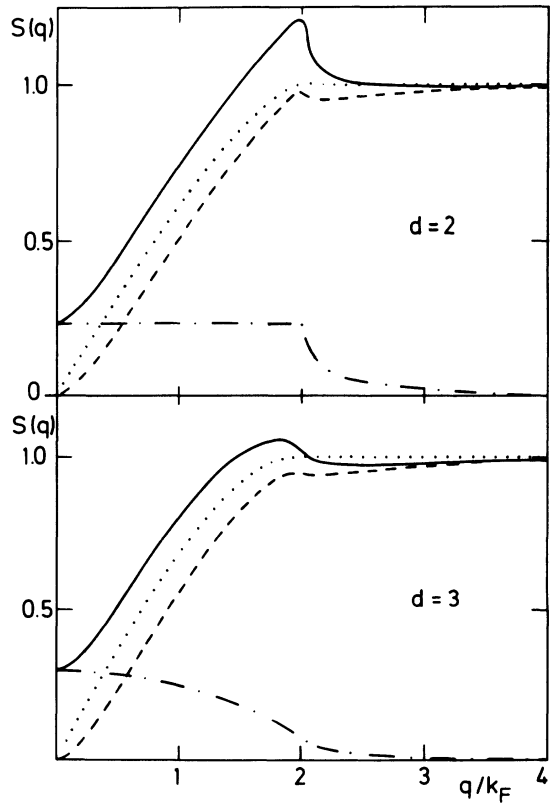

FIG. 1. Static structure factor in $d=2$ and $d=3$ for $\xi=0.5$ and $U/U_c=0.8$. The dotted lines are the free-electron results and the dashed, dashed-dotted, and solid curves represent $S_{\rm in}(q)$, $S_e(q)$, and $S(q)$, respectively.

$\xi=0.5$ and $U/U_c=0.8$ where U_c is the critical coupling for the metal-insulator transition. Since U is to be interpreted as a pseudopotential, it is reasonable still to rely on the lowest-order result for $S_e(\vec{q})$ for the coupling chosen.

For free electrons interference effects cause the structure factor to exhibit a nonanalytic small wave-number dependence

$$S_{\text{in}}(\vec{q})=sq/k_F$$

with $s=2/\pi$ and $s=\frac{3}{4}$ for $d=2$ and $d=3$, respectively. Owing to momentum relaxation the excitation spectrum $\Phi''(\vec{q},\omega)$ differs drastically from the one for free electrons. For small wave vectors a Green-Kubo identity

$$\Phi''(\vec{q},\omega)=-\rho_F/[\omega+q^2K(\omega)]$$

holds, where ρ_F is the density of states at the Fermi level, $\rho_F=g_0(q=0)$, and $-iK(\omega)$ is the frequency-dependent diffusiveness. For $U<U_c$ one gets

$$K(\omega\to 0)=iD$$

with diffusiveness D, while for $U>U_c$ one finds $D=0$ and $K(\omega\to 0)\propto\omega$.[7] Hence $S_{\text{in}}(\vec{q})$ approaches zero with horizontal slope:

$$S_{\text{in}}(q\to 0)=(\rho_F/\pi n)q^2\left[D\ln\{[1+(\Omega/q^2D)^2]^{1/2}\}+(1/\rho_F)\left[\int_0^{\Omega}d\omega\,\omega^{-1}[K''(\omega)-\rho_F D]+\int_{\Omega}^{\infty}d\omega\,\omega^{-1}K''(\omega)\right]\right]. \tag{7}$$

Here $\Omega>0$ is an arbitrary auxiliary frequency; for $U>U_c$ one can choose $\Omega=0$. According to the SCCR $S_{\text{in}}(\vec{q})$ is smaller than the corresponding free-electron expression for all values of q. $S_e(\vec{q})$ provides a broad background for $q\leq 2k_F$ dropping to zero for $q>2k_F$, and this leads to a peak in $S(\vec{q})$ at $q\cong 2k_F$. This peak is more pronounced for $d=2$ than for $d=3$ due to the different behavior of $g_0(q)$. The small oscillation in $S_{\text{in}}(q\cong 2k_F)$ is an artifact of the approximations since it stems from the nonanalyticity of $g_0(q)$ used in the SCCR. For $q\to 0$ the structure factor is given by $S_e(\vec{q})$ alone; this leads to a nonzero value of $S(q\to 0)$.

The anomalies shown in Fig. 1 are of comparable size to the ones discussed for interaction effects.[3] Therefore we consider it worthwhile to measure $S(\vec{q})$ for disturbed conductors. The model and the parameter value chosen to get the figure appear reasonable, since rather delicate conductivity measurements have been analyzed successfully on their basis.[16]

If the parameter ξ was chosen to be greater than unity, the peak in $S(\vec{q})$ would occur at $q=q_0$. In this case the peak strength strongly depends on the model potential, and the peak will be absent if there is no sharp cutoff in $[\,|\,U(\vec{q})\,|^2]_{\text{av}}$.

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APPENDIX: CPA EQUATIONS FOR $S_e(q)$

For the quantity $S_e(\vec{q})$ given by Eq. (2b) there is an exact representation

$$nS_e(q)=\int_{-\infty}^{\epsilon_F}d\omega_1\,\pi^{-1}\int_{-\infty}^{\epsilon_F}d\omega_2\,\pi^{-1}\sum_{\vec{k},\vec{p}}[G''_{\vec{k}-\vec{q}/2,\vec{k}+\vec{q}/2}(\omega_1)G''_{\vec{p}+\vec{q}/2,\vec{p}-\vec{q}/2}(\omega_2)]_{\text{av}}\,. \tag{8}$$

Here the G'' are anticommutator Green's functions

$$G''_{\vec{k},\vec{p}}(\omega)=\tfrac{1}{2}\int_{-\infty}^{\infty}dt\,e^{i\omega t}\langle\{a_{\vec{k}}(t),a_{\vec{p}}^{\dagger}\}\rangle\,, \tag{9a}$$

with the Hilbert-Stieltjes transform for complex frequency z,

$$G_{\vec{k},\vec{p}}(z)=\int_{-\infty}^{\infty}d\omega\,\pi^{-1}G''_{\vec{k},\vec{p}}(\omega)/(\omega-z)\,. \tag{9b}$$

For knowledge of $S_e(\vec{q})$ it is sufficient to know the function

$$H_{\vec{k},\vec{p}}(\vec{q};z_1,z_2)=[G_{\vec{k}-\vec{q}/2,\vec{p}-\vec{q}/2}(z_1)G_{\vec{p}+\vec{q}/2,\vec{k}+\vec{q}/2}(z_2)]_{\text{av}} \tag{10}$$

for all z_1, z_2, since

$$[G_{\vec{k}-\vec{q}/2,\vec{k}+\vec{q}/2}(z_1)G_{\vec{p}+\vec{q}/2,\vec{p}-\vec{q}/2}(z_2)]_{\mathrm{av}} = H_{(\vec{k}+\vec{p}-\vec{q})/2,(\vec{k}+\vec{p}+\vec{q})/2}(\vec{p}-\vec{k};z_1,z_2) . \tag{11}$$

For applying the CPA we use the Anderson Hamiltonian,[10] given by Eq. (3), with the dispersion of $\epsilon(\vec{k})$ for a simple cubic lattice and

$$U(\vec{q}) = (1/N)\sum_n e^{i\vec{q}\cdot\vec{R}_n}\epsilon_n . \tag{12}$$

Here n labels the N lattice sites $\vec{R}_n$ and the ϵ_n are random site energies with a distribution function $P''(\epsilon)$ whose Hilbert-Stieltjes transform shall be denoted by $P(z)$.

The coherent-potential approximation for $H_{\vec{k},\vec{p}}(\vec{q};z_1,z_2)$ (Ref. 9) results in an integral equation

$$H_{\vec{k},\vec{p}}(\vec{q};z_1,z_2) = G(\vec{k}-\vec{q}/2,z_1)G(\vec{k}+\vec{q}/2,z_2)\left[\delta_{\vec{k},\vec{p}} + L(z_1,z_2)(1/N)\sum_{\vec{l}} H_{\vec{l},\vec{p}}(\vec{q};z_1,z_2)\right] , \tag{13}$$

where

$$G(\vec{k},z) = -[z-\epsilon(\vec{k})+\Sigma(z)]^{-1} , \tag{14a}$$

$$L(z_1,z_2) = [t_n(z_1)t_n(z_2)]_{\mathrm{av}}/[1+[t_n(z_1)t_n(z_2)\pi F(z_1)\pi F(z_2)]_{\mathrm{av}}] , \tag{14b}$$

$$t_n(z) = [\epsilon_n+\Sigma(z)]/\{1+[\epsilon_n+\Sigma(z)]\pi F(z)\} , \tag{14c}$$

$$F(z) = (1/\pi N)\sum_{\vec{k}} G(\vec{k},z) . \tag{14d}$$

The self-energy $\Sigma(z)$ is to be determined from the CPA equation[8]

$$F(z) = P(-1/\pi F(z)-\Sigma(z)) . \tag{15}$$

The separable integral equation (13) can be easily solved to yield

$$H_{\vec{k},\vec{p}}(q;z_1,z_2) = \delta_{\vec{k},\vec{p}}G(\vec{k}-\vec{q}/2,z_1)G(\vec{k}+\vec{q}/2,z_2) + G(\vec{k}-\vec{q}/2,z_1)G(\vec{k}+\vec{q}/2,z_2) \times\{(1/N)L(z_1,z_2)/[1-L(z_1,z_2)\Pi(\vec{q};z_1,z_2)]\} \times G(\vec{p}-\vec{q}/2,z_1)G(\vec{p}+\vec{q}/2,z_2) \tag{16a}$$

with

$$\Pi(\vec{q};z_1,z_2) = (1/N)\sum_{\vec{k}} G(\vec{k}-\vec{q}/2,z_1)G(\vec{k}+\vec{q}/2,z_2) . \tag{16b}$$

Substitution of Eqs. (16) into Eq. (11) and evaluation of the discontinuities across the real axis yields $S_e(\vec{q})$ by Eq. (8). Similar CPA results have been obtained before for magnetic scattering.[5] Unfortunately, we could not find a practical procedure to evaluate the eight-dimensional integral entering Eq. (8).

Expanding the CPA equations up to the order $[|U(\vec{q})|^2]_{\mathrm{av}} = (1/N)[\epsilon_n^2]_{\mathrm{av}}$ yields again the lowest-order result, Eq. (4), while in the limit of completely localized electrons one gets the von Laue formula for diffuse scattering in solid solutions,[4]

$$S_e(\vec{q}) = 1-nV , \tag{17}$$

where V is the volume of the unit cell. So the CPA provides us with the correct result for $S_e(\vec{q})$ in both the weak- and strong-coupling limits.

We note in passing that Eqs. (16) also determine the generalized compressibility in CPA:

$$g(\vec{q}) = \int_{-\infty}^{\epsilon_F} d\omega\,\pi^{-1}\sum_{\vec{k},\vec{p}} H''_{\vec{k},\vec{p}}(\vec{q};\omega,\omega) . \tag{18}$$

In the weak-coupling limit at the lower band edge the resulting expression for $g(\vec{q})$ is identical to the one given by de Gennes.[17] We note further, that for a semicircle distribution,

$$P''(\epsilon) = [(2\pi[\epsilon^2]_{\mathrm{av}})]^{-1}(4[\epsilon^2]_{\mathrm{av}}-\epsilon^2)^{1/2}\Theta(4[\epsilon^2]_{\mathrm{av}}-\epsilon^2) ,$$

the CPA reduces to the much simpler self-consistent Born approximation. This holds for the one-particle

propagator $G(\vec{k},z)$ (Ref. 18) as well as for the two-particle function

$$H_{\vec{k},\vec{p}}(\vec{q};z_1,z_2) .$$

The latter statement can be easily proven from our Eq. (14b), which, for a semicircle distribution, reduces to

$$L(z_1,z_2)=[\epsilon^2]_{\text{av}} .$$

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