Disorder–enhanced electron correlations near the crystalline–amorphous transition

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The static density response $\chi(0,q)$ of a disordered electron sea in the presence of Coulomb interaction is calculated for a situation where diffusive relaxation dominates other decay processes. It is argued that this condition is realized near the crystalline–amorphous transition of certain binary alloys. Below a critical temperature, $\chi(0,q)$ exhibits a powerlaw divergence at the Fermi surface ($q = 2k_F$). It causes a systematical phase shift of the Friedel oscillations as well as an enhancement of their amplitude. The spatial decay exponent of the Friedel oscillations is also modified. Our results are consistent with experiments and are relevant for understanding the stability of the amorphous state against crystallization.

A large class of strongly disordered, noble–polyvalent metal alloys exhibit a crystalline to amorphous transition (CAT) as a function of doping[1]. This transformation goes hand in hand with the formation of a structure–induced pseudogap in the electronic density of states (DOS) at the Fermi energy ε_F and a maximum of the electrical resistivity. In the amorphous phase, the spatial density distribution of ions, although homogeneous on average, shows strong shell–like correlations. This is evidenced by a pronounced peak in the structure factor $S(q)$ at a wave number $q = q_o = 2\pi/a$, where a is the spacing between shells of ions formed around an arbitrary central ion. Remarkably, the wave length $\lambda_F = \pi/k_F$ of the Friedel oscillations of the electron density $\rho(r)$ coincides with a at the CAT [1]. This has led several authors [1, 2, 3] to conjecture that the CAT is triggered by the ions being bound in the minima of the Friedel potential. The experimental results [1] then require that, at the CAT, the Friedel oscillations are phase shifted by $\varphi = \pi/2$ w.r.t. a clean electron sea, and that their amplitude is enhanced in order to dominate the thermal energies at the typical experimental temperature of $T = 77K$.

We show [4] that quantum interference of Coulomb interaction and impurity scattering can cause both an amplitude enhancement and the observed systematical phase shift of the Friedel oscillations. It is intimately related to a novel instability of the disordered electron sea towards formation of concentrical charge density oscillations in $d = 3$ dimensions.

As a necessary and sufficient condition for this effect to occur the diffusive transport rate $1/\tau_{tr}$ of the electron system must be large compared to the single–particle relaxation rate $1/\tau_{qp}$. In the amorphous systems at hand strong backscattering occurs near the CAT because the impurity scattering T-matrix $t(q)$, proportional to $S(q)$, is peaked at a momentum transfer $q = q_o$ which matches $2k_F$ ("Bragg reflection", see above). This generically leads to an enhancement of $1/\tau_{tr}$ [5]. It may be calculated quantitatively for strong disorder from the impurity Bethe–Salpeter-Equation incorporating particle number conservation [6, 4] and shows a strong enhancement over $1/\tau_{qp}$. The calculation reproduces the observed pseudogap of the DOS (Fig. 1).

Accordingly, we let $\tau_{tr}^{-1} \gg \tau_{qp}^{-1}$ in evaluating the electronic density response $\chi(\omega = 0, q)$ *near the crystalline–amorphous transition.* Because of the diffusive motion of the electrons, the effective Coulomb interaction $\bar{v}_q(z, Z)$ between electrons with complex frequencies z and $z + Z$ acquires a long–ranged, retarded part [7, 8],

$$\bar{v}_q(z,Z) = \frac{v_q}{\epsilon^{RPA}(Z,q)}\Gamma^2(z,Z,q), \qquad v_q = \frac{4\pi e^2}{q^2},$$

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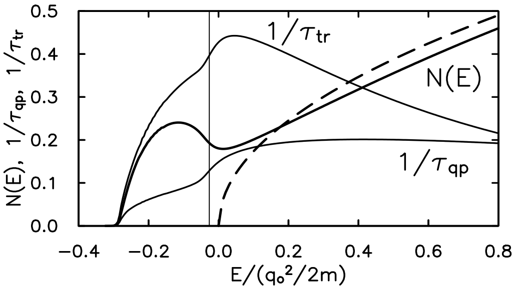

Figure 1: τ_{qp}^{-1}, τ_{tr}^{-1} (units of $q_o^2/2m$), and the DOS $N(E)$ (arb. units) as a function of energy for a T-matrix peaked at $q = q_o$. A quadratic bare band $\varepsilon_p = p^2/2m$ is assumed. $---$: clean DOS. Vertical line: position of the Fermi level ε_F for $2k_F = q_o$.

where $\epsilon^{RPA}(Z,q)=1+2\pi i\,\sigma\,/(Z\,\mathrm{sgn}Z''+iq^2D)$ is the disordered RPA dynamical dielectric function and the diffusion vertex is

$$\Gamma(z,Z,q)=\begin{cases}\frac{i/\tau_{tr}\ \mathrm{sgn}Z''}{Z+iq^2D\ \mathrm{sgn}Z''} & \text{if } z''(z+Z)''<0\\ 1 & \text{otherwise.}\end{cases}$$

$D=1/3\,v_F^2\tau_{tr}$, $\sigma=ne^2\tau_{tr}/m$ and $''$ denote the diffusion constant, the Drude conductivity and the imaginary part, respectively. The leading correction to the RPA vertex gives a contribution to the polarization $\Pi(0,q)$ the most divergent part of which is [4]

$$\Pi^{(1)}(0,q)=\frac{-3\sqrt{3/2}\;I(1)}{128(\varepsilon_F\tau_{tr})^{7/2}}\int \mathrm{d}\nu \frac{1/(4T)}{\cosh^2\frac{\nu}{2T}}\frac{\mathrm{sgn}(x-1)}{\sqrt{|x-1|}},$$

where $x=q/2k_F$ and $I(1)\simeq 11.8(2mk_F/(2\pi)^2)$. This directly implies a peak of $\chi(0,q)=\Pi(0,q)/(1-v_q\Pi(0,q))$ at $q=2k_F$, which, due to the vanishing denominator, turns into a powerlaw divergence at a critical transport rate $1/\tau_{tr,c}(T)$ *even for non-zero single-particle relaxation rate* $1/\tau_{qp}\ll 1/\tau_{tr}$ *and finite* T. By Fourier transforming $\chi(0,q)$ it is seen that the peak structure leads to density oscillations $\rho^{(1)}(r)\propto\sin(2k_Fr)/r^{(d-1)}$ superimposed on the conventional oscillations $\rho^{(0)}(r)\propto\cos(2k_Fr)/r^d$, i.e. to an effective phase shift φ, which approaches $\pi/2$ as the weight of the peak and, therefore, the amplitude of the oscillations diverges at $1/\tau_{tr}=1/\tau_{tr,c}$ (Fig. 2) [4]. Near this point the Friedel potential dominates other energy scales present in the system and can bind the ions in its minima. Thus, identifying this point with the CAT explains both the matching of the ionic spacing with λ_F and the measured phase shift from one single quantum effect. The powerlaw decay of the oscillations crosses over to an exponential decay for distances larger than R_o,

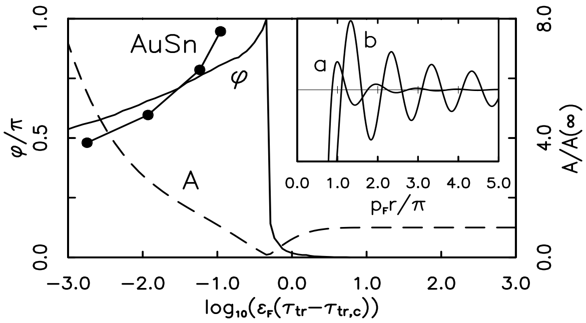

Figure 2: Phase shift φ and amplitude A of the 1st maximum of $\rho(r)$ as a function of $\varepsilon_F(\tau_{tr}-\tau_{tr,c})$; $\varepsilon_F\tau_{tr,c}=1.217$. Also shown are experimental data [1] for the shift of the nearest neighbor distance $2\pi(a/\lambda_F-1)$ of ions in amorphous AuSn ($\bullet$), where τ_{tr} is determined from conductivity measurements, $\sigma=C\tau_{tr}$. C is the only adjustable parameter. The inset shows $\rho(r)$ (arb. units) as a function of distance r from an impurity ion (a) in the clean case and (b) for $\varepsilon_F\tau_{tr}=1.23$.

where $R_o\simeq v_F/2\;(\tau_{qp}^{-1}+T)^{-1}$ for the conventional Friedel oscillations and $R_o\equiv\xi\simeq v_F/(2\sqrt{7})(\tau_{qp}^{-1}+T)^{-1}(1-\tau_{tr}^{-1}/\tau_{tr,c}^{-1})^{-1/2}$ for the quantum corrections $\rho^{(1)}$. I.e. the transition is characterized by long-range correlations and a diverging correlation length ξ.

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