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Can one expect a Kondo effect in quasiperiodic structures?

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Abstract. We show that electrons hopping over quasiperiodic tilings give rise to a modified Kondo effect, obeying a power-law behaviour in place of the standard logarithmic behaviour.

1. Introduction

In the usual description of the Kondo effect, it is assumed that the conduction electrons near the Fermi level can fill a single uniform energy band. However, there exists a variety of situations in which the assumption of a uniform density of states fails to provide the correct physical answer.

For instance, if one assumes a multiple band structure, the conduction electrons can overscreen the spin impurity resulting in an anomalous effect [1]. In $U_xY_{1-x}Pd_3$ alloys a quadrupolar Kondo effect with marginal Fermi-liquid behaviour has, in fact, been observed [2]. A different situation, in which the fermions occupy a band with a density of states going to zero with power-law behaviour near the Fermi energy, has been shown to give rise to a non-trivial zero-temperature phase transition at a finite coupling constant, in contrast to the zero-coupling constant transition of the ordinary case [3].

In this paper we consider electrons moving over a quasiperiodic structure, such as a quasiperiodic superlattice or a quasicrystalline tiling. It is now established that electron propagation over such structures is weaker than in the periodic case. Recent measurements on defect-free quasicrystals exhibit a behaviour close to the metal–insulator transition [4]. Various mechanisms can be responsible for the observed anomalously high resistivity, including a low density of carriers at the Fermi energy, band hybridization and critical energy eigenstates. We focus here on the latter property, i.e. on the fact, verified on quasiperiodic lattices, that the wavefunctions are neither Bloch states nor do they have an exponential decay at large distances, but instead have an algebraic decay.

In the simplest case of a 1D quasicrystal, e.g. the Fibonacci chain, all eigenstates are critical [5]; correspondingly, the energy spectrum has been shown rigorously to be singular continuous (see, e.g., [6]) with a total bandwidth decreasing with a power-law behaviour with respect to the system size.

Various numerical works refer to quasicrystalline tilings in 2D (see, e.g., [7] for the Penrose tiling (PT) and [8] for the octagonal tiling (OT)). Both PT and OT, together with quasiperiodic translational ordering, include topological disorder with coordination number varying from site to site. Since their Fourier transforms are invariant under non-crystallographic symmetry groups (pentagonal and octagonal, respectively), it is generally accepted that these tilings provide a realistic description of real quasicrystals.

It was shown in the OT case, in particular, that the Lebesgue measure of the spectrum, in contrast to the 1D case, is generally finite, but in spite of this there is evidence of a singular continuous behaviour. Quantum diffusion is characterized by a slower than ballistic spreading of the wavepacket with power-law behaviour in time. Consistently, it was shown that in the PT case the stationary states are critical: $\psi_E(r) \approx |v|^{-\beta}$ with the exponent β generally varying along the energy spectrum.

The observed conductive properties of 3D Al–Cu–Fe icosahedral phases have been interpreted satisfactorily in terms of weak localization theory: critical wavefunctions seem appropriate for describing the physical states of such systems.

Interestingly enough, it was observed that the perfectly quasicrystalline samples are more resistive than the disordered ones [9]. This effect was recovered in the OT upon introducing phasonic disorder with the following interpretation: the singular structure of the density of states is smeared out by the disorder, recovering a smooth density of states with extended wavefunctions.

Our aim here is to determine how the effective electron–electron interaction induced by the scattering with magnetic impurities is influenced by such anomalous behaviour. We will assume that the Fermi energy lies close to a power-law singularity of the density of states and that the wavefunctions there are critical.

2. Electronic lifetime

We consider the Kondo model associated with electrons hopping over a quasiperiodic tiling with N sites so that the unperturbed Hamiltonian H_0 already includes the underlying disorder of the lattice; the electrons have a contact interaction with N_i impurities having spin S. In the energy representation, the total Hamiltonian H is

$$H = \sum_{\epsilon,\lambda} \epsilon c^+_{\epsilon,\lambda} c_{\epsilon,\lambda} - \sum_{\epsilon,l} J(\epsilon, \boldsymbol{R}_l)[(c^+_{\epsilon,+}c_{\epsilon,+} - c^+_{\epsilon,-}c_{\epsilon,-})S^{(z)}_l + c^+_{\epsilon,+}c_{\epsilon,-}S^{(-)}_l + c^+_{\epsilon,-}c_{\epsilon,+}S^{(+)}_l] \tag{1}$$

where $l = 1, \ldots, N_i$. The magnitude of the interaction $J(\epsilon, \boldsymbol{R}_l)$ depends on the localized wavefunction ψ_l of the impurity at the site $\boldsymbol{R}_l$ as well as on the scattering wavefunction ψ_ϵ, $(H_0\psi_\epsilon = \epsilon\psi_\epsilon)$: $J(\epsilon, \boldsymbol{R}_l) = j_l|\psi_\epsilon(\boldsymbol{R}_l)|^2$.

We will hereafter disregard the site dependence of j_l $(j_l \equiv j)$. As usual, we consider low impurity concentration $c = N_i/N$, so that one can assume that the conduction electron scatters one impurity at a time. The scattering matrix, up to second order at the lth impurity, is (see, e.g., [10])

$$\begin{aligned} t^{(2)}_{\lambda'\lambda}(\xi, \boldsymbol{R}_l) &= -J(\boldsymbol{\sigma}\cdot\boldsymbol{S})_{\lambda'\lambda} + j^2|\psi_\xi(\boldsymbol{R}_l)|^2 \int_{-D}^{D} \mathrm{d}\xi'\, \tfrac{1}{2}\nu(\xi')|\psi_{\xi'}(\boldsymbol{R}_l)|^2 \\ &\quad \times \left[\frac{S(S+1)}{\xi-\xi'}\delta_{\lambda'\lambda} + \frac{2f(\xi')-1}{\xi-\xi'}(\boldsymbol{\sigma}\cdot\boldsymbol{S})_{\lambda'\lambda}\right] \\ &\approx -J(\boldsymbol{\sigma}\cdot\boldsymbol{S})_{\lambda'\lambda} + J^2 \int_{-D}^{D} \mathrm{d}\xi'\, \tfrac{1}{2}\nu(\xi') \left[\frac{S(S+1)}{\xi-\xi'}\delta_{\lambda'\lambda} + \frac{2f(\xi')-1}{\xi-\xi'}(\boldsymbol{\sigma}\cdot\boldsymbol{S})_{\lambda'\lambda}\right] \end{aligned} \tag{2}$$

$J \equiv J(\xi, \boldsymbol{R}_l)$.

Here $\nu(\xi')$ is the global density of states over a band having width $2D$ around the Fermi energy μ, $(\xi = \epsilon - \mu)$; $f(\xi)$ is the Fermi distribution (i.e. $2f(\xi) - 1 = -\tanh(\xi/(2T))$). The final approximate formula is responsible for the dominant contribution to the Kondo singularity. In fact, the integrand of the neglected term contains the factor $|\psi_\xi(\boldsymbol{R}_l)|^2 - |\psi_{\xi'}(\boldsymbol{R}_l)|^2/(\xi - \xi')$, which, independently of the explicit behaviour of the wavefunction in terms of the energy, gives rise to a weaker singularity than the one appearing in the right-hand side of equation (5) (see below).

As a further remark, one can think that the single impurity contribution becomes negligible if the wavefunction is centred away from the scattering site. This is certainly true if one deals with exponentially localized wavefunctions and the average impurity distance is larger than the localization length. However, as we will see, the wavefunctions in these systems are characterized by power-law decay so that their amplitude at a generic impurity site can be significantly different from zero.

In the case of a pure band spectrum one replaces $\nu(\xi)$ by $\nu(0)$ giving

$$\int_{-D}^{D} \mathrm{d}\xi' \frac{\nu(\xi')}{\xi - \xi'} = \nu(0) \log \left| \frac{1 + \xi/D}{1 - \xi/D} \right| \tag{3}$$

where ξ is taken outside the integration interval.

Notice, however, that (3) is still valid when ξ lies in the interval, provided $1/(\xi - \xi')$ is interpreted as $P(1/\xi - \xi')$.

For the second term we have

$$-\int_{-D}^{D} \mathrm{d}\xi' \tanh\left(\frac{\xi'}{2T}\right) \frac{\nu(\xi')}{\xi - \xi'} \approx 2\nu(0) \log\left(\frac{D}{\max(\xi, T)}\right). \tag{4}$$

Note that contribution (3) is usually negligible with respect to (4). Following the results obtained in [7] for PT and in [8] for OT, we assume that close to the Fermi energy the density of states is dominated by a power-law singularity: more precisely we let $\nu(\xi) \approx |\xi|^{\alpha-1}$ $(0 < \alpha < 1)$. From level statistics, as well as from anomalous diffusion analysis in [8], it was argued that, in general, the singularity in the density of states is energy dependent; in the 1D case this fact has been shown explicitly (see, e.g., [5]).

In the present context this implies a strong dependence of the modified Kondo behaviour on the energy region where the Fermi level is located. Equation (3) now takes the form

$$\int_{-D}^{D} \mathrm{d}\xi' \, |\xi'|^{\alpha-1} \frac{1}{\xi - \xi'} \approx 2\xi^{\alpha-1} \left[\frac{\pi}{2} \cot\left(\frac{\pi\alpha}{2}\right) + \frac{1}{2-\alpha}\left(\frac{\xi}{D}\right)^{2-\alpha}\right]. \tag{5}$$

In deriving (5) we have used

$$\int_0^\infty \mathrm{d}x \, x^{\alpha-1} P \frac{1}{1-x^2} = \frac{\pi}{2} \cot\left(\frac{\pi\alpha}{2}\right).$$

When $\alpha \to 1$, one recovers, for $(\xi/D) < 1$, the same behaviour as in (3).

Similarly, (4) becomes

$$-\int_{-D}^{D} \mathrm{d}\xi' \tanh\left(\frac{\xi'}{2T}\right) \frac{|\xi'|^{\alpha-1}}{\xi - \xi'} \begin{cases} \approx 2\xi^{\alpha-1}\left[\dfrac{\pi}{2}\tan\left(\dfrac{\pi\alpha}{2}\right) - \dfrac{1}{1-\alpha}\xi^{1-\alpha}\right] & (T \to 0) \quad (6a) \\ \approx 2(T)^{\alpha-1}\dfrac{1}{1-\alpha}\left[1 - \left(\dfrac{D}{T}\right)^{\alpha-1}\right] & (\xi \to 0). \quad (6b) \end{cases}$$

Again, by letting $\alpha \to 1$ in (6), the logarithmic singularity (4) is obtained. It was for just this reason that, in (6*b*), the otherwise arbitrary constant was chosen to be one.

As expected, the effective coupling $J_{\rm eff}$, corrected to second order, increases when $j < 0$ (antiferromagnetic case) and decreases when $j > 0$.

In the limit $T \to 0$, the total transition probability is obtained from (5) and (6*a*) in the form

$$\frac{1}{2}\left\langle \sum_{\lambda\lambda'} |t_{\lambda\lambda'}|^2 \right\rangle \equiv \frac{1}{\tau(\xi)} \approx \frac{3c}{2} j^2 S(S+1) \sum_{i=1}^{N} \left| \phi_4(\xi, i) - j \left(\pi \tan\left(\frac{\pi\alpha}{2}\right)\right) \xi^{\alpha-1} \phi_6(\xi, i) \right| \tag{7}$$

$$\phi_{2p}(\xi, i) \equiv |\psi_\xi(\boldsymbol{R}_i)|^{2p}.$$

In the antiferromagnetic case we have

$$\begin{aligned} \frac{1}{\tau(\xi)} &\approx \tfrac{3}{2} c S(S+1) j^2 \left| I_4(\xi) + |j| I_6(\xi) \pi \tan\left(\frac{\pi\alpha}{2}\right) \xi^{\alpha-1} \right| \\ I_{2p}(\xi) &= \sum_{i=1}^{N} \phi_{2p}(\xi, i). \end{aligned} \tag{7'}$$

In equation (7) we kept the leading orders in the coupling and replaced the sum over the impurities with the sum over the whole lattice multiplied by the concentration c. This emphasizes the fact that the relevant amplitude is given by the momenta $I_{2p}(\xi)$, associated with the global behaviour of the wavefunction, rather than by the amplitude of the wavefunction at a particular lattice site. The scaling of the momenta with N is sensitive to the degree of localization ($I_4(\xi)$ is usually called the inverse participation ratio). For instance, if the scattering states were plane waves, we would have $I_6/I_4 \approx 1/N$, so that the natural perturbation parameter would be j/N. In our context this parameter is dependent on the exponent $\beta = \beta(\xi)$, ($\psi_\xi(\boldsymbol{r}) \approx 1/(|\boldsymbol{r}|^{\beta(\xi)})$). We are mainly interested in the case $0 < \beta < d/2$ (d being the dimension of the system), which corresponds to states that, although critical, are non-integrable and can be considered as extended. This is the most favourable situation in that, already, from single-impurity scattering one can have a significant amplitude, but for power-decaying functions a localization length can be hardly defined so that when $d/2 < \beta$ the global contribution is strictly different from zero; its actual order of magnitude cannot be determined in the present general treatment.

It is easily seen that the algebraic decay of the wavefunctions implies, for the momenta, the following behaviour

$$I_4(\xi) \approx \frac{c_4(\xi)}{N^{[d-4\beta(\xi)]/d}} \qquad I_6(\xi) \approx \frac{c_6(\xi)}{N^{[2d-6\beta(\xi)]/d}}$$

where $c_4(\xi)$ and $c_6(\xi)$ are strictly positive; as a result the natural perturbation parameter is now $j/N^{[d-2\beta(\xi)]/d}$. The ξ dependence of the momenta $I_{2p}(\xi)$ is very irregular (see, e.g., [8] where $I_4(\xi)$ is exhibited for the OT and a related generalized norm is computed for the PT).

It is not possible to obtain from (7′) the conductivity σ in a closed form; it is nonetheless possible to determine a lower and an upper bound for σ. Indeed, denoting the extrema of $\beta(\xi)$ in the interval $|\xi| \leqslant D$ by $\beta_{\rm min}$ and $\beta_{\rm max}$, we have

$$\frac{K_{2p}}{N^{[(p-1)d-2p\beta_{\rm min}]/d}} \leqslant I_{2p} \leqslant \frac{K'_{2p}}{N^{[(p-1)d-2p\beta_{\rm max}]/d}} \tag{8}$$

where K_{2p}, K'_{2p} are some positive constants. By means of (8) one concludes that

$$\frac{1}{\tau_1} \leqslant \frac{1}{\tau(\xi)} \leqslant \frac{1}{\tau_2}$$

$$\frac{1}{\tau_1} = \tfrac{3}{2} c S(S+1) j^2 K_4 (1 + j_1' \xi^{\alpha-1}) \frac{1}{N^{[1-4\beta_{\min}]/d}} \tag{9}$$

$$j_1' = O\left(\frac{1}{N^{[1-2\beta_{\min}]/d}}\right)$$

where for $1/\tau_2$ one must replace K_4 with K_4', $\beta_{\min}$ with $\beta_{\max}$ and j_1' with j_2'.

In terms of τ_1 and τ_2, for a given particle velocity at the Fermi energy, one can obtain the bounds σ_1 and σ_2 from the well known formula

$$\sigma = \frac{e^2}{12\pi^3} \int \tau(\xi) v^2(\xi) \left(-\frac{\mathrm{d}f}{\mathrm{d}\xi}\right) \nu(\xi)\, \mathrm{d}\xi \tag{10}$$

so that the low-T behaviour becomes

$$\sigma_2 \leqslant \sigma \leqslant \sigma_1$$

whence

$$\rho_1 \left(1 + j_1' \left(\frac{D}{T}\right)^{1-\alpha}\right) \leqslant \rho \leqslant \rho_2 \left(1 + j_2' \left(\frac{D}{T}\right)^{1-\alpha}\right). \tag{11}$$

Provided one also includes the second term in the right-hand side of (6*a*), it is easily verified that when $\alpha \to 1$ the usual logarithmic behaviour is recovered.

3. Conclusions

In this paper we studied the Kondo effect for electrons hopping on quasiperiodic tilings. On the basis of known results (referring to the 1D case and to the 2D case) we assumed wavefunctions with algebraic decay and singular continuous spectra.

We have shown that under these conditions the resistivity exhibits a power-law behaviour at low temperatures with an exponent dependent on the singularity of the density of states at the Fermi energy; the degree of localization of the wavefunctions has an influence on the amplitudes involved, but not on the exponent. A sensitive dependence is expected on the region where the Fermi energy is located, as long as, in principle, a whole spectrum of exponents can appear (in particular one cannot exclude also smooth portions with standard Kondo behaviour). The effect refers to defect-free tilings; phasonic disorder tends to destroy the singular behaviour of the density of states, thus extending the smooth portions of the spectrum.

It is known that the Fermi energy of quasicrystals lies in a pseudogap of the order of 1 eV associated with the interaction of the Fermi surface with the Jones zone. The scale of the pseudogap refers to the coarse-grained behaviour of the density of states; in fact the presently obtained defect-free quasicrystals exhibit a finer structure on smaller scales [11] (the characteristic energy scale can be of the order of 10^{-1}–10^{-2} eV) together with a strong departure from the free-electron model [4]. We suggest that the critical states arising in 1D and 2D tilings are physically relevant also in 3D defect-free quasicrystals. To our knowledge, the presently available magnetic icosahedral phases have an excessive amount of disorder to resolve a singular behaviour in the energy spectrum [12]. If $\nu(\xi)$ is predominantly smooth with isolated peaks, our effect can be obtained provided that the Fermi energy is tuned close to the singularity. The quality of the detection is clearly improved by reducing the error in tuning and by using samples with high Kondo temperature T_K. An error in tuning of the order of 10^{-4} eV, e.g., defines a range of detection from T_K down to 1 K. A high density of peaks in $\nu(\xi)$ is a more interesting situation: if $k_B T_K \approx 10^{-2}$ eV, an average spacing between peaks and valleys of the order of $\approx 10^{-3}$ eV makes the effect almost generic (occurring with a probability of order unity without tuning). A comprehensive physical description, which should include the competition with other effects such as direct electron–electron scattering and phonon hopping, goes clearly beyond the aim of our treatment.

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