Quasi-Particle density of states of disordered d-wave superconductors

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We present a numerical study of the quasi-particle density of states (DoS) of two-dimensional d-wave superconductors in the presence of smooth disorder. We find power law scaling of the DoS with an exponent depending on the strength of the disorder and the superconducting order parameter in quantitative agreement with the theory of Nersesyan et al. (Phys. Rev. Lett. 72, 2628 (1994)). For strong disorder a transition to a constant DoS occurs. Our results are in contrast to the case of short-ranged disorder.

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In recent years, motivated by its relevance to the physics of the cuprates, d-wave superconductivity has become a subject of intensive research. The key feature distinguishing d-wave superconductors from their s-wave relatives is the existence of four zero energy 'nodes' on the Fermi surface, in the vicinity of which low energy quasi-particle excitations exist. This fermion system—four species of relativistic quasi-particles, subject to weak static disorder—has vital influence on low energy transport and thermodynamic properties and, therefore, must be a central element of any comprehensive theory of the d-wave superconductor.

Irritatingly, it has proven excruciatingly difficult to reach consensus on even basic characteristics of these states. The extent of disagreement is most clearly displayed in the debate on the energy dependent mean quasi-particle density of states (DoS), \( \rho(E) \): On the one hand, application of self-consistent approximation schemes \[1,2\] or non-perturbative approaches specific to certain realizations of the disorder \[3,4\], has led to the prediction of a finite or even diverging quasi-particle DoS at zero energy. In contrast, field theory approaches to the problem \[8,9,11\] categorically predict \( \rho(E) = 0 \), as in the non-disordered Dirac system. Yet, even these theories within themselves come to varying conclusions as to the energy dependence of the DoS for \( E \neq 0 \).

Recently it has become clear that much of this controversy roots in the fact that, unlike with more conventional disordered fermion systems, the standard paradigm of 'insensitivity of global observables to microscopic details of the disorder' is apparently violated in the d-wave system. Broadly speaking, two different categories of disorder have to be distinguished: (i) hard scattering off s-wave impurities, mixing the formerly isolated four low energy quasi-particle sectors, and (ii) soft scattering which predominantly leads to randomisation within these sectors. Which of these categories is more relevant to the physics of the cuprates is not straightforward to decide (see, however, our comments below), and both have been investigated theoretically. As for (i), there is now overwhelming evidence that, apart from the case of asymptotically strong impurities (impurities at the 'unitary limit') \[8,9,11\], the DoS vanishes as \( E \to 0 \). Away from zero energy a variety of different DoS profiles, depending on the realization of the disorder distribution, exist.

The subject of this Letter is a numerical study of the complementary case, (ii). What makes this regime special, and why is it necessary to discriminate between (i) and (ii) at all? The distinguishing feature of the soft scattering regime is that the four low energy sectors are decoupled. The absence of inter-node coupling has profound and qualitative influence on the low energy properties of the system. Indeed \[12\], it is the nodal coupling criterion, and not so much the specifics of a short range correlated disorder distribution \[1\], that holds responsible for much of the discrepancy between the field theory approaches to the problem.

Before turning to our numerical analysis of the quasi-particle spectrum for soft scattering, let us briefly summarize some key features of the system: Each node accommodates a system of Dirac fermions subject to a random vector potential which describes the stochastic low momentum transfer scattering. For low energies and finite size systems – the 'zero-dimensional' limit – the properties of the system become fully universal and can be described in terms of a suitably constructed random matrix theory (RMT) \[13\] (a). Due to the non-standard symmetries of random gauge Dirac fermions (symmetries of class AIII in the terminology of Ref. \[14\]) this theory differs profoundly from standard Wigner-Dyson RMT. The opposite extreme, thermodynamically extended systems is widely accessible to analytical approaches, too \[14,15\]. Specifically, for the d-wave problem Nersesyan, Tsvelik and Wenger (NTW) \[8\] have shown that the DoS scales as (b)

\[
\rho(E) \sim |E|^\alpha, \quad \alpha = \frac{1 - g}{1 + g}, \quad g = \frac{W^2}{16\pi\Delta t}, \quad (1)
\]

where \( W \) is the strength of the disorder, and \( t \) and \( \Delta \) are the tight binding coupling strength and order parameter of the superconductor, respectively. It has been argued...
that at $g = 1$, i.e. at the zero of the exponent in (1), a transition to a qualitatively different phase takes place. On the strong disorder side of this transition, $g > 1$, the DoS is expected to be energy independent, $\rho(E) = \text{const.}$ (c). Further, (d), any amount of hard scattering coupling the low energy nodes represents a marginally relevant perturbation driving the system towards the coupled regimes (i) mentioned above.

For completeness we mention that all these features find their common origin in the fact that the low energy physics of isolated nodes is described by a Wess-Zumino-Witten (WZW) model on a group manifold that depends on the treatment of the disorder (replica [12] or super-symmetry [12]). In NTW’s analysis of this connection it has erroneously been assumed that the WZW action globally describes the low-energy quasi-particle system, independent of the form factor of the scattering. In fact, however, the WZW model is readily destabilized by inter-node scattering which is one way of explaining the aforementioned qualitative differences between cases (i) and (ii). For a detailed account of the WZW-formulation, and its destruction, we refer to Ref. [12].

Below we will put the phenomenology (a-d) to a numerical test. Before turning to a more detailed description of our analysis, let us summarize the main results. We find that the large scale structure of the energy dependence of the DoS can be characterized in terms of three different regimes: For low energies $E$ above the chemical potential $\mu$ the DoS is symmetric $\rho(E) = \rho(-E)$ the DoS profile is dominated by finite size effects. At $E = 0$ the DoS vanishes in a way which (for strong enough disorder) is described by RMT. The extent of the low energy regime shrinks with increasing system size. For larger energies, it is succeeded by a regime of power law scaling. Varying the two basic parameters $\Delta/t$ and $W/t$ characterizing the model, we find agreement with eq. (1). For disorder strength in excess of $g = 1$, the DoS assumes a constant value, in accord with the prediction of Ref. [17]. The scaling regime ends at energies of the order of $\Delta$ where a non-universal high energy regime, not considered in this Letter, begins. Upon lowering the correlation length of the disorder, the scaling behaviour observed in the center portions of the band is rapidly destructed.

We consider the lattice quasi-particle Hamiltonian

$$H = \sum_{ij,\sigma} (t_{ij} - \mu \delta_{ij}) c_{i\sigma}^\dagger c_{j\sigma} + \sum_{ij} \Delta_{ij} \epsilon_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.},$$

(2)

with the matrix elements $t_{ij}$, chemical potential $\mu$, and order parameter $\Delta_{ij}$. The sums run over points of a two-dimensional square lattice with spacing $a$ and the operators $c_{i\sigma}^\dagger$ create a spin-1/2 particle of spin $\sigma$ at site $i$. In the following, we take only into account on-site potentials and nearest-neighbor hopping, $t_{ij} = \epsilon_i \delta_{ij} + t a \delta_{i,j \pm e_x}$, where $e_k$ is the unit vector in $k$-direction. For convenience we set $\mu = 0$ (the half-filled band.) The order parameter $\Delta_{ij} = \langle \delta_{ij} x_{\sigma} e_x - \delta_{ij} y_{\sigma} e_y \rangle$ has $d_{x^2-y^2}$-symmetry.

In the following we will only consider disorder in the on-site potentials $\epsilon_i$ and not determine the order parameter self-consistently. (As pointed out in [11], a self-consistent determination of the order parameter may be necessary to quantitatively compare with experimental data.) Finite correlations in the disorder potential are introduced through

$$\rho(E) = \frac{W}{\sqrt{\Sigma}} \sum_j f_j \exp\left(-\frac{|r_j - r_i|^2}{\xi^2}\right),$$

(3)

$\Sigma = \sum_j \exp(-2|x_j|/\xi^2)$, where the $f_j$ are independent random variables, uniformly distributed in the interval $[-1/2, 1/2]$, and $W$ is a measure of the strength of the disorder. Taking $\xi = 2a$ the coupling of the four Dirac nodes is much weaker than the coupling of states in the vicinity of a single node (by a factor of $\exp(-2\xi^2)$).

In the following, we take the lattice constant $a$ and the hopping amplitude $t$ as the measures of length and energy, respectively. The linear dimensions of the system vary between 15 and 45 and the spectrum is averaged over 64 points in the first Brillouin zone. We diagonalize the Hamiltonian (2) for 16 to 56 disorder realizations and calculate the DoS $\rho(E) = L^{-2} \sum_i \delta_i (E - E_i)$, where $\delta_i (E)$ is a normalized Gaussian of width $\Gamma$. A finite $\Gamma$ smoothes the DoS, but also washes out narrow features.

Fig. 1 shows the DoS for various values of disorder. The three regimes mentioned earlier are the low-energy region where the bump develops, the intermediate regime up to the approximate crossing point near $E = 1$, and the high-energy regime beyond. We will first discuss the most interesting intermediate regime before turning our attention to low energies. In order to compare our data to the results of NTW, we fit the data to power laws $\rho(E) \propto$
FIG. 2. Double logarithmic plot of the density of states of Fig. 1. Disorder ranges from $W = 1$ to 10. Dots (●) represent data and lines power law fits to the respective intervals. Inset: Density of states for $W = 2$ and $L = 15$ (dotted), 25 (short-dashed), 35 (long-dashed), and 45 (solid). Note that the numerical uncertainties are considerably smaller than the amplitude of the fluctuations.

FIG. 3. Exponents $\alpha$ extracted from the fitted curves in Fig. 2 as a function of disorder $W$ for $\Delta = 1$. The solid curve is the result of NTW, eq. (1).

$E^\alpha$ in a interval $[E_{\text{min}}, E_{\text{max}}]$. $E_{\text{min}}$ is chosen such as to exclude the first maximum. From the inset in Fig. 2 it is clear that this feature as well as the fluctuations are finite-size effects that appear to vanish in the large system limit. The upper limit $E_{\text{max}}$ is a high energy cutoff of the order of $\Delta$ beyond which the NTW theory no longer applies. At the systems sizes considered in this work, the ratio $E_{\text{max}}/E_{\text{min}}$ is about 5. This is a rather narrow range to establish a power law. Nevertheless, we feel that our procedure is justified in the present case, as it is not just a single power law with a single exponent that we are dealing with. Instead, eq. (1) predicts that there is a whole family of power laws with the exponents depending in a unique way on the parameters $W$ and $\Delta$. It is the agreement of this whole functional dependence that gives us confidence in the validity of our analysis even when the establishment of every single power law might be questionable. Figure 3 shows the exponents $\alpha$ extracted from the fitted curves in Fig. 2 together with the result of eq. (1) of [8]. A good agreement is apparent up to a disorder strength of $W \approx 7$ where the NTW exponent changes sign. Numerically, we do not find a divergent DoS at stronger disorder but rather a finite value ($\alpha = 0$) as predicted by Gurarie [17].

To further test eq. (1) we fix the disorder strength $W = 3$ and vary the order parameter $\Delta$. Figure 4 shows the DoS for $\Delta$ between 0.1 and 1.0 as a function of $E/\Delta$. This rescaling takes care of the fact that the mean level spacing of the clean system is proportional to $\Delta$. The anisotropy dependence of the fitted exponents is shown in Fig. 5. Again, reasonably good agreement with eq. (1) is found for $\Delta > 0.2$ while a constant and not a diverging DoS is found at $\Delta = 0.1$.

The inset of Fig. 1 shows that the DoS does indeed vanish at $E = 0$. At weak disorder ($W \leq 4$) we see a remnant of the clean spectrum. Here the disorder is too weak to couple neighboring states in momentum space. At $W \approx 5$ this coupling exceeds the level separation and the universal RMT behaviour for systems of class AIII, with a DoS 'microgap' linear in energy, develops [19].

To conclude the central part of our analysis, we have presented a numerical study of the quasi-particle spectrum in $d$-wave superconductors with soft scattering. In the regime of moderate disorder strength, we obtain scaling of the DoS that agrees quantitatively with the analytical results of NTW. For strong disorder, the analysis confirms the recent prediction [17] of an energetically constant background DoS. In a way our analysis is complementary to recent studies of hard scattering systems [11] and we are left with the question which of these alternatives is more relevant to the physics of 'real' cuprates. It is probably difficult to give a universally applicable answer to this question. On the face of it, disorder in high $T_c$ superconductors is due to small metallic donors, e.g. Zn-impurities, in favour of the hard variant, (i). (Concrete evidence for the presence of hard scattering in
Zn-doped systems is provided by the experimental observation of so-called mid-gap resonances [i.e. resonances due to bound states forming in the immediate vicinity of a strong local impurity]. On the other hand, the very existence of a $d$-wave phase, stabilized through a mechanism unknown at present, would not be compatible with too strong an amount of—pairbreaking—hard scattering, i.e. the renormalized effective potential seen by the quasi-particle states may well carry characteristics of type (ii) and be predominantly soft (see Refs. [2] for a more elaborate discussion of this point.) Equally important, the net features of the quasi-particle system are not only determined by the fixed microscopic structure of the disorder background but also depend on temperature and observation energy. E.g. consider a system with a certain residual amount of hard scattering superimposed on a predominantly soft background. For quasi-particle energies in excess of the the inter-node scattering rate, the coupling between the nodes is inessential and the characteristics of the soft system will prevail. Lowering the energies, a crossover towards the hard system takes place.

Although the picture above suggests, that 'real life' systems will typically display complex crossover behaviour, recent progress in purely theoretical understanding of disorder in $d$-wave superconductors has been tremendous. It seems to be clear now, that much of the controversy that developed around the profile of the quasi-particle DoS is related to non-congruent modellings of the disorder. Indeed, the majority of theoretical approaches to the problem sits comfortably with one of the disorder realizations investigated numerically in this work or in complementary papers [1-3]. (There is one prominent exception to that rule, viz. Refs. [1] where a finite DoS for continuously distributed disorder was predicted. To our understanding the discrepancy is explained by the peculiar lattice implementation underlying these papers (see Ref. [2] for a more elaborate discussion of this point) which implies that no superconductor is modelled.) Broadly speaking, there seem to be three categories of disorder that have to be distinguished: binary alloy type scatterer at the unitary limit, large momentum transfer scatterers of non-unitary type and soft disorder. In spite of the relative—as compared to normal metals—complexity of this classification, the categories within themselves still display a large amount of universality.

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