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Low-energy quasiparticle excitations in dirty *d*-wave superconductors and the Bogoliubov–de Gennes kicked rotator

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We investigate the quasiparticle density of states in disordered *d*-wave superconductors. By constructing a quantum map describing the quasiparticle dynamics in such a medium, we explore deviations of the density of states from its universal form ($\propto E$), and show that additional low-energy quasiparticle states exist provided (i) the range of the impurity potential is much larger than the Fermi wavelength (allowing one to use recently developed semiclassical methods), (ii) classical trajectories exist along which the pair potential changes sign, and (iii) the diffractive scattering length is longer than the superconducting coherence length. In the classically chaotic regime, universal random matrix theory behavior is restored by quantum dynamical diffraction which shifts the low-energy states away from zero energy, and the quasiparticle density of states exhibits a linear pseudogap below an energy threshold $E^* \ll \Delta_0$, much smaller than the superconducting gap.

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In recent years, considerable attention has been focused on the low-energy properties of the quasiparticle spectrum of disordered cuprate superconductors.[1,2] Because many of the cuprate superconductors are randomly chemically doped insulators and disorder is a pair breaker for *d*-wave superconductors, the role of nonmagnetic impurities is particularly important for an understanding of the *d*-wave superconducting state, its quasiparticle spectral and transport properties. Of special interest is the low-energy behavior of the single-particle Density of States (DOS) $\rho(E)$.

In an early work,[3] the self consistent *T*-matrix approximation was shown to break down for two-dimensional (2D) *d*-wave superconductors. This led to a series of papers using nonperturbative methods, which predicted (at first sight) contradictory results: vanishing,[3–6] constant,[7,8] and diverging[9,10] DOS as $E \to 0$. On the numerical side, several investigations also predicted both vanishing,[11,12] and diverging[13,14] DOS at zero energy. It was soon argued, based on numerical analysis, that the reason behind these contradicting predictions is the fact that the microscopic details of disorder (i.e., details beyond the transport mean free path ℓ, such as the density of scatterers or the correlation length ζ of the impurity potential) as well as the symmetries of the clean Hamiltonian matter both qualitatively and quantitatively[13,15] (see also Ref. 16). An important feature shared by the numerics of Refs. 11–15 is that the disorder is introduced via isolated *pointlike* scatterers. Long-wavelength disorder, which may arise due to chemical doping away from CuO_2 planes, or can be induced via ion radiation techniques[17] or via a scanning tunnel microscope tip,[18] is thus ignored. Effects of long-wavelength disorder are expected to become dominant when the CuO_2 planes have almost no atomic disorder,[19] they are the main focus of this paper.

It has recently been realized, in the context of mesoscopic physics and weak localization, that ζ and ℓ, together with the Fermi wavelength λ_F, define two classes of complex quantum systems: quantum disordered systems where $\lambda_F \ell/\zeta^2 > 1$ and quantum chaotic systems for which $\lambda_F \ell/\zeta^2 < 1$.[20] The latter class is characterized by the emergence of a *diffractive scattering* time scale, $\tau_E = \nu^{-1} \ln[\zeta/\lambda_F]$, defined as the time it takes for the classically chaotic dynamics (with Lyapunov exponent ν) to stretch a wave packet of minimal initial extension λ_F to a length ζ. In contrast to quantum disordered systems, quantum chaotic systems exhibit nonuniversal properties due to their short-time classical (i.e., deterministic) dynamics. In particular, significant deviations from Random matrix theory (RMT) emerge, as was recently found by Adagideli *et al.*[10] in the context of impurities in *d*-wave superconductors. These authors used a semiclassical approach to calculate the low-energy DOS for a collection of *extended* scatterers (a quantum chaotic system) and found an asymptotic behavior $\rho(E) \sim 1/E|\ln E^2|^3$ as $E \to 0$. They nevertheless argued that the RMT predictions of a linear pseudogap would be restored at lower energy $E < E^*$, i.e., that the singularity in the DOS would be cut off at an energy E^* related to τ_E, by diffractive (nonclassical) scattering occurring at larger times $\tau > \tau_E$. The purpose of the present paper is to investigate the modifications that the DOS undergoes as the correlation length of the impurity potential increases and τ_E becomes relevant. We will focus our attention on (i) providing for numerical checks of the theory of Adagideli *et al.* in the case of long-wavelength disorder,[10] (ii) finding out whether for some E^* the DOS is suppressed for $E < E^*$, in agreement with RMT predictions,[4–6] and (iii) investigate the transition region between extended and pointlike disorder.

We start by introducing a quantum map model for quasiparticle states in disordered *d*-wave superconductors. The main motivation behind this model is to investigate discrepancies (in low-energy DOS) between pointlike versus extended disorder as well as the transition region, i.e., the regime in which the impurity size is intermediate. To the best of our knowledge no disorder model which includes extended impurities as well as pointlike in *d*-wave superconductors has been studied numerically so far. This map has two additional advantages: First, as both the density and cor-

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relation length of impurities can be tuned independently, it is possible to interpolate between the two extreme regimes of strong disorder: unitary disorder (i.e., disorder due to dilute, pointlike scatterers,[6,9,15,16], viz., quantum disorder) and quasiclassical disorder[10] (i.e., disorder due to extended scatterers, viz. quantum chaotic). Second, from a numerical point of view, it allows for the investigation of very large system sizes, i.e., lattice sizes of up to 256×256, which are necessary for both variations of the disorder correlation length and the numerical extraction of the parametric behavior of the DOS. Our reasons why a dynamical model is relevant are (i) In absence of superconductivity, many properties of quasiparticles in disordered media (such as Anderson localization) are correctly described by 1D maps.[21] In fact it has been shown by Altland and Zirnbauer that one of those maps, the 1D kicked rotator, and quasi-one-dimensional metallic wires are described by the same effective field theory.[22] Recent numerical investigations in $D=2$ suggest that this is also true in higher dimensions.[23] (ii) In the presence of superconductivity, Andreev maps based on the kicked rotator have recently been shown to adequately describe quantum dots in contact with a superconductor.[24]

We first briefly discuss generic properties of quantum maps for uncoupled quasiparticles. The dynamics corresponds to a succession of free propagations, interrupted by sudden *kicks* of period τ_0, i.e., instantaneous perturbations. Quantum maps are conveniently represented by a unitary, *Floquet* operator F, giving the time-evolution after p kicks as $u(p)=F^p u(0)$, for an initial wave function $u(0)$. The matrix F has eigenvalues $\exp(-i\varepsilon_m)$, which define quasienergies $\varepsilon_m\in(-\pi,\pi)$ (energies and quasienergies are expressed in units of $\hbar/\tau_0$). While the energy is not conserved, the periodicity of the kick still preserves quasienergies, much in the same way as a periodic potential breaks translational symmetry, but still preserves quasimomentum. Time evolution of hole excitations (being the time-reversed of electronic excitations) is given by $v(p)=(F^*)^p v(0)$. Specializing to the D-dimensional kicked rotator, we write the Floquet operator as[25]

$$F=\exp\left(-i\frac{KI}{\hbar\tau_0}\Pi_{j=1}^{D}\cos r_j\right)\exp\left(i\frac{\hbar\tau_0}{2I}\vec{\nabla}^2\right). \tag{1}$$

It describes the free motion of a particle with dimensionless coordinates $\{r_j\}$ (e.g., expressed in units of a lattice constant), which is interrupted at periodic time intervals τ_0 by a kick of strength $K\cdot\Pi_{j=1}^{D}\cos r_j$. I is the moment of inertia of the particle, and K is the kicking strength. For $D=1$ and 2, increasing K makes the classical dynamics evolve from integrable ($K=0$) to fully chaotic [$K\gtrsim7$, with Lyapunov exponent $\lambda\approx\ln(K/2)$]. For $0<K<7$ stable and unstable motion coexist (a so-called mixed phase space).[25] Increasing K is thus tantamount to increasing the amount of disorder, the fully chaotic regime corresponding to a finite density of impurities.

Electron and hole excitations inside a superconductor are however coupled by a nonvanishing pair-potential. Accordingly we extend the kicked rotator of Eq. (1) to a Bogoliubov–de Gennes form. We discuss this construction for the case $D=2$. First, we replace the free quasiparticle motion by a coupled electron and hole dynamics,

$$\mathcal{F}_0=\exp(-i\mathcal{H}\tau_0/\hbar), \tag{2a}$$

$$\mathcal{H}=H\sigma_z+\Delta\sigma_x. \tag{2b}$$

Here, $H=-(\hbar^2\vec{\nabla}^2/2I)-E_F$, with E_F the Fermi energy, $\sigma_{x,z}$ are Pauli matrices acting in particle-hole space, and Δ is the superconducting pair potential. Second, the coupled quasiparticle motion is followed by a kick

$$\mathcal{F}_K=\exp(-i\mathcal{H}_K/\hbar), \tag{3a}$$

$$\mathcal{H}_K=\frac{KI}{\tau_0}\cos x\cos y\,\sigma_z. \tag{3b}$$

Exponentiating the Pauli matrices, we end up with the Bogoliubov–de Gennes–Floquet (BdGF) operator

$$\mathcal{F}=\mathcal{F}_K\mathcal{F}_0, \tag{4a}$$

$$\mathcal{F}_0=\cos\sqrt{(H^2+\Delta^2)(\tau_0/\hbar)^2}\,\mathcal{I}+\frac{i\sin\sqrt{(H^2+\Delta^2)(\tau_0/\hbar)^2}}{\sqrt{H^2+\Delta^2}}[H\sigma_z+\Delta\sigma_x], \tag{4b}$$

$$\mathcal{F}_K=\cos\left[\frac{KI}{\hbar\tau_0}\cos x\cos y\right]\mathcal{I}+i\sin\left[\frac{KI}{\hbar\tau_0}\cos x\cos y\right]\sigma_z, \tag{4c}$$

with $\mathcal{I}$, the identity matrix in particle-hole space. For $\Delta=0$, Eq. (4) describes uncoupled electron and hole excitations in a disordered $2D$ metal. Once this metal becomes superconducting, Δ couples these excitations during their free propagation, while it is neglected during the instantaneous kick. As in the case of a BdG eigenproblem, the $2M$ quasienergies [with average spacing $\delta\equiv\langle\varepsilon_{m+1}-\varepsilon_m\rangle=\pi/M$] of the BdGF equation $\mathcal{F}\phi_m=\exp(-i\varepsilon_m)\phi_m$, come in pairs with opposite sign $\varepsilon_m=-\varepsilon_{2M-m+1}$, similarly to the spectral properties of a BdG Hamiltonian. These considerations establish the correspondence between the map of Eq. (4) and quasiparticles in a dirty superconductor.

We next quantize the phase space on a four-torus $\{x,y;p_x,p_y\}$, with dimensionless momentum $p_{x,y}=-i\hbar_{\text{eff}}\partial/\partial(x,y)\in(0,2\pi)$.[25] The effective Planck constant $\hbar_{\text{eff}}\equiv\hbar\tau_0/I_0$ takes on values $\hbar_{\text{eff}}=2\pi/M$, with integer $M=L_x\cdot L_y$, in term of the real-space linear system sizes $L_{x,y}$ (also expressed in units of a lattice spacing), and the impurities have a spatial extension $\zeta=O(L_x,L_y)$. The BdGF operator is then a $2M\times2M$ unitary matrix, and we consider the two cases of d-wave $[\Delta(p_x,p_y)=\Delta_0(p_x^2-p_y^2)/(p_x^2+p_y^2)]$ and extended s-wave $[\Delta(p_x,p_y)=\Delta_0|p_x^2-p_y^2|/(p_x^2+p_y^2)]$ pair potentials, for which $\mathcal{F}_0$ is diagonal in momentum representation. Noting that $\mathcal{F}_K$ is diagonal in real-space representation, we rewrite $\mathcal{F}$ as

$$\mathcal{F}_{\vec{p}\vec{p}'}=([\mathcal{U}\mathcal{F}_K\mathcal{U}^\dagger]\mathcal{F}_0)_{\vec{p}\vec{p}'}, \tag{5}$$

where $\mathcal{U}=U\mathcal{I}$, and U is the unitary matrix of the $2D$ Fourier transform between real-space and momentum coordinates,

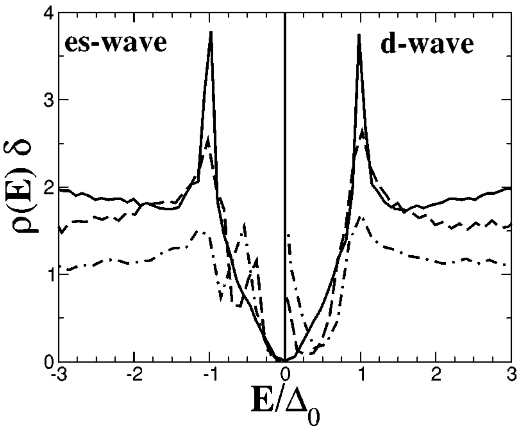

FIG. 1. Density of states for the *d*-wave (right) and extended *s*-wave (left) Bogoliubov–de Gennes kicked rotator defined by Eqs. (2)–(4), and parameters $L_x \times L_y = 128 \times 128$, $\Delta_0 = 0.4$, $E_F = 2\pi^2/5$, and $K=0$ (solid lines), 2 (dashed lines), and 8 (dotted-dashed lines).

$U_{\vec{p}\vec{p}'} = M^{-1/2}\exp[(2\pi i/M)\vec{p}\cdot\vec{p}']$. We numerically extract the quasienergy DOS from the eigenvalues $\sin\varepsilon_m$ of the Hermitean matrix $(1/2i)(\mathcal{F}-\mathcal{F}^\dagger)$, which we diagonalize using the Lanczos algorithm.[26]

In Fig. 1 we show the quasienergy DOS for *d*-wave and extended *s*-wave pair potentials away from half filling ($E_F = 2\pi^2/5 < \pi^2/2$), as the kicking strength increases. In the clean case ($K=0$) the two DOS are the same. The gap singularity at $E/\Delta_0 = 1$ gets washed out as K increases in both cases, however, a peak emerges in the *d*-wave DOS around $E=0$, while $\rho(E)=0$ in the extended *s*-wave case. This is in agreement with Refs. 10, 27, i.e., the existence of low-energy states requires a change in the sign of the pair potential. In the extended *s*-wave case, the low-energy peak is shifted by an energy corresponding to the gap averaged over all momenta mixed by the impurity potential.

We focus on the *d*-wave symmetry from now on. A closer look at the DOS in the fully chaotic regime with $K=8$, is provided in Fig. 2. It indicates that the characteristic semiclassical singularity exhibited by the DOS as $E\to 0$ is cut off at an energy $E^* \ll \Delta_0$, where a sharp drop occurs and $\rho(E)\to 0$. RMT predicts such a drop to occur over an energy scale given by the Thouless energy,[2] which in our case is however significantly larger than Δ_0.[28] We thus attribute this drop to the emergence of diffractive scattering at times larger than τ_E[20] as follows. According to Ref. 10, the DOS corresponding to low-energy semiclassical states can be estimated from a mapping onto a tight-binding chain with random hoppings, for which the eigenfunctions are localized with an energy-dependent localization length $\xi(E)$.[29] At low energies, ξ exceeds the diffractive scattering length $v_F\tau_E$ (v_F is the Fermi velocity) in which case hoppings between otherwise uncoupled tight-binding chains (corresponding to different classical trajectories) have to be taken into account. The emergence of these processes signals the breakdown of semiclassics and the restoration of RMT. One thus expects the vanishing of the DOS below a threshold energy given by the condition $\xi(E^*) \approx v_F\tau_E$. Since $\xi(E)$ is bounded by the superconducting coherence length, $\xi(E) \gtrsim \hbar v_F/\Delta_0$,[10] the observation of the semiclassical peak in the DOS requires a long enough diffractive scattering length $v_F\tau_E > \hbar v_F/\Delta_0$. While preliminary results corroborate this argument, a detailed investigation of E^* will be presented elsewhere.[30]

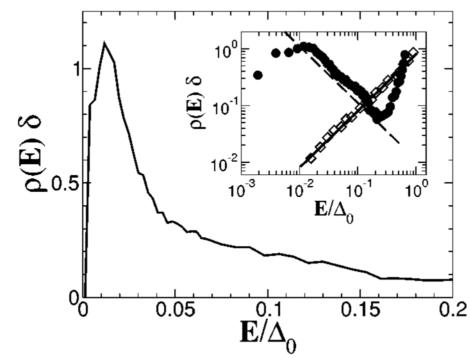

FIG. 2. Main plot: Low-energy DOS for the *d*-wave Bogoliubov–de Gennes kicked rotator of Eqs. (2)–(4), $L_x \times L_y = 256\times 256$, $\Delta_0 = 0.4$, $E_F = 2\pi^2/5$, and $K=8$. Inset: Asymptotic of the density of states at low excitation energy for the same set of parameters, for long-wavelength disorder (quantum chaotic; black circles) and diffractive disorder as defined in Eq. (6) with $N_H = 27$ (quantum disorder; empty diamonds). The solid and dashed lines indicate a $\propto E$ and $\propto E^{-1}$ behavior, respectively.

In the inset to Fig. 2 we show the asymptotic behavior of the DOS on a log-log scale. Once abstraction is made of the drop in the DOS below E^*, the semiclassical data exhibit a singular behavior slightly below $\propto E^{-1}$ (black circles) which is in qualitative agreement with the prediction $\rho(E) \propto E^{-1}|\ln E|^{-3}$ of Ref. 10.

Having established the validity of semiclassical predictions in the quantum chaotic regime, we next decrease the range of the disorder and enter the quantum disordered regime. We accomplish this via the inclusion of higher harmonics to the kicking potential, and replace Eq. (3) by

$$\mathcal{H}_K = \frac{KI}{N_H^2 \tau_0} \sum_{l,m=1}^{N_H} \cos[lx]\cos[my]\sigma_z . \tag{6}$$

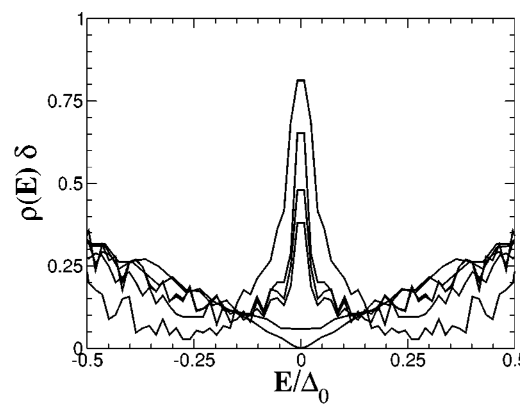

FIG. 3. Low-energy DOS for the *d*-wave Bogoliubov–de Gennes kicked rotator with decreasing disorder range as defined in Eqs. (2), (4), and (6), with $L_x \times L_y = 256\times 256$, $\Delta_0 = 0.4$, $E_F = 2\pi^2/5$, $K=8$, and $N_H = 1, 3, 5, 7, 17$, and 27 (from top to bottom).

The typical impurity size decreases as $\zeta \propto N_H^{-1}$. Figure 3 shows the disappearance of the low-energy peak in the DOS as N_H increases. For the set of parameter considered, once $N_H \simeq 27$ is reached, the DOS vanishes at $E=0$. Note that the resolution used in Fig. 3 does not allow to see the opening of the RMT gap below E^*. A more precise look at the DOS for $N_H=27$ is provided on the inset to Fig. 2 (empty diamonds). The data clearly indicate the expected RMT linear suppression of the DOS.

Our results thus clarify the competition between RMT[2] and semiclassics.[10] The next step is to investigate the effect that the semiclassical low-energy states have on the transport properties and to explore the parametric dependence of E^*. Work along those lines is in progress.[30]

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