Microscopic interpretation of the Dynes formula for the tunneling density of states

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Excellent fits of the tunneling density of states in disordered superconductors can be often achieved making use of the phenomenological Dynes formula. However, no consistent derivation of this formula has been available so far. The Dynes formula can be interpreted by the simplest causal frequency-dependent gap function $\Delta(\omega)$ with a vanishing gap at the Fermi level. Here we show, within the coherent potential approximation, that precisely such a gap function describes superconductors with a Lorentzian distribution of pair-breaking fields and arbitrary potential disorder. We predict spectral and thermodynamic properties of such superconductors.

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I. INTRODUCTION

The tunneling density of states $N(\omega)$ is a basic characteristic of the single-particle properties of superconductors. The knowledge of $N(\omega)$ has played a major role in identification of the pairing mechanism in conventional superconductors, and with a similar aim $N(\omega)$ is often also studied in modern superconductors [1]. On the other hand, $N(\omega)$ is also used as a diagnostic tool enabling us to discover the existence of pair-breaking processes in superconductors and to quantify their extent [2]. Such studies are important from the basic physics point of view, for instance in the context of the still not completely understood superconductor-insulator transitions [3,4], but also from the point of view of applied physics, since in many electronic applications of superconductors such pair-breaking processes are to be avoided [5].

The presence of pair-breaking processes shows up in the tunneling experiment as a finite density of states within the ideal superconducting gap $\bar{\Delta}$. Long ago, a simple phenomenological formula has been proposed for superconductors with such processes [6],

$$N(\omega) = N_0 \mathrm{Re}\left[\frac{\omega + i\Gamma}{\sqrt{(\omega + i\Gamma)^2 - \bar{\Delta}^2}}\right], \tag{1}$$

which is now known as the Dynes formula. The parameter Γ in this formula quantifies the effect of the pair-breaking processes, and N_0 is the normal-state density of states at the Fermi level.

In order to demonstrate the quality of fits which can be achieved making use of Eq. (1), in Fig. 1 we reproduce the recently measured low-temperature tunneling data on a series of MoC films with varying thickness [4], together with their fits to the Dynes formula. Similarly perfect agreement between experimental data for disordered superconductors and the Dynes formula has in fact been observed quite frequently, see, e.g., Refs. [7,8], indicating that Eq. (1) should be caused by a generic mechanism.

The only mechanism leading to the Dynes formula which has been suggested so far postulates that its appearance in tunneling experiments is caused by inelasticity of the tunneling process [9]. However, this mechanism can not explain the systematic changes of $N(\omega)$ observed in Fig. 1, which must have a truly intrinsic origin. The aim of this paper therefore is to propose a generic and intrinsic microscopic interpretation of the Dynes formula.

II. GAP FUNCTION

Let us start by noting that, within the Eliashberg theory, $N(\omega)$ is completely determined, once the gap function $\Delta(\omega)$ is known:

$$N(\omega) = N_0 \mathrm{Re}\left[\frac{\omega}{\sqrt{\omega^2 - \Delta^2(\omega)}}\right]. \tag{2}$$

According to Eq. (1), $N(\omega)$ is finite at the Fermi level and this requires that $\Delta(\omega)$ vanishes as $\omega \to 0$. The gap function $\Delta(\omega)$ should also be causal, i.e., analytic in the upper half plane, and it should approach $\bar{\Delta}$ in the high-energy limit. It is known [10] that the simplest function with these properties,

$$\Delta(\omega) = \frac{\omega\bar{\Delta}}{\omega + i\Gamma}, \tag{3}$$

does lead to the Dynes formula, when inserted into Eq. (2). Therefore our task in the rest of this paper is to find a microscopic explanation of Eq. (3).

It is worth pointing out that Mikhailovsky *et al.* [10] did find a mechanism leading to Eq. (3). In fact, by a careful analysis of the Eliashberg equations they have shown that Eq. (3) applies even in a clean system, since the electron-phonon scattering has also a pair-breaking component at finite temperatures T. However, the mechanism of Mikhailovsky *et al.* predicts that Γ scales with T according to $\Gamma \propto T^3$, and therefore it is not of direct relevance to the experiments of Refs. [4,7,8] and the like, where the parameter Γ is only weakly T dependent and does not vanish in the low-temperature limit.

The explanation of Eq. (3) should be therefore sought in the presence of elastic pair-breaking processes, such as scattering on magnetic impurities [11] and/or fluctuating order parameter [12]. However, the latter possibility seems to be ruled out by the spatial homogeneity of the tunneling spectra observed in Ref. [4]. Moreover, a fluctuating order parameter is expected to produce appreciable change of $N(\omega)$ only for $|\omega| \approx \bar{\Delta}$ [12]. Therefore in this paper we will concentrate only on the effect of magnetic impurities.

It should be pointed out that, when the magnetic impurities are treated in the Born approximation [11], the functional form Eq. (3) does arise, but only in the limit $\Gamma \gg \bar{\Delta}$, which is not

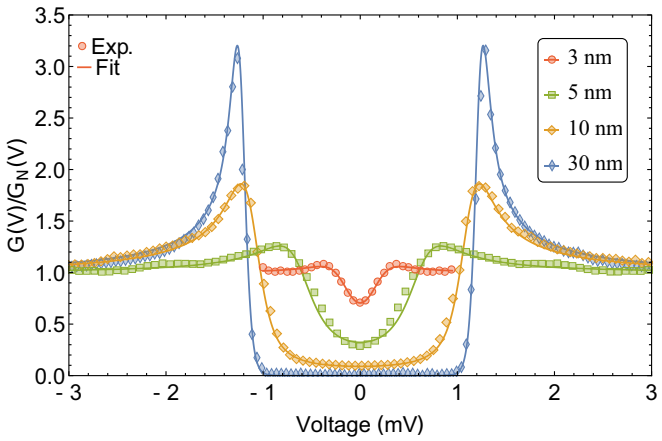

FIG. 1. Normalized tunneling conductance of thin MoC films with varying thickness at T ≈ 500 mK, from Ref. [4], with fits to the thermally smeared Dynes formula. For further details see Appendix F.

of direct relevance to the data in Fig. 1. Subsequent theoretical work which went beyond the Born approximation concentrated on the limit of dilute magnetic impurities. Within the T-matrix approximation, which should be essentially exact in the dilute impurity limit, Shiba has found magnetic impurity-induced bound states inside the energy gap in the absence of additional potential disorder [13], and the precise energy of such bound states was found to depend on the coupling strength to the impurities. Furthermore, finite concentration of magnetic impurities was shown to lead to the formation of impurity bands centered at the bound-state energies, see Fig. 2. Provided the magnetic impurities are dilute, later it was shown that the presence of additional strong potential disorder does not change these results [14], and very recently it has been argued that even going beyond mean-field theory leads to only marginal changes of Shiba's results [15].

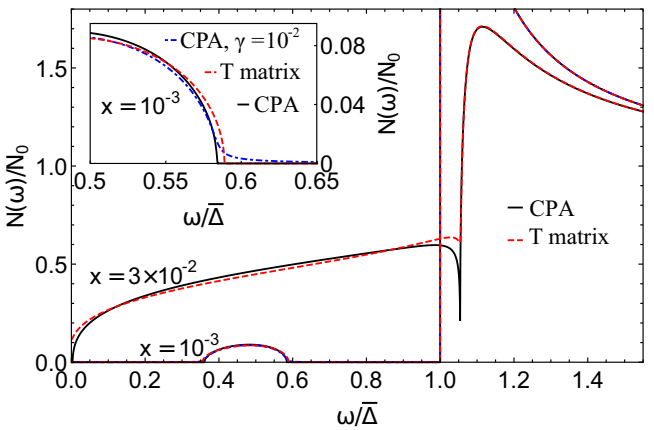

FIG. 2. $N(\omega)$ for a superconductor with dilute pair-breaking impurities with $\lambda_0 = 0.6$ and $\pi N_0 \bar{\Delta} = 0.05$. Results for two impurity concentrations are shown, $x = 0.001$ and $x = 0.03$. The inset shows that, within CPA, the hard spectral edge of the impurity band softens if we replace the delta functions in Eq. (6) by Lorentzians with widths γV_0.

It seems to be clear then that, in order to reproduce Eq. (1) in the physically relevant case $\Gamma \lesssim \bar{\Delta}$, one has to allow for spatially varying coupling strengths to impurities, but in such a way which leads to a spatially uniform gap function. This forces us to allow for a dense distribution of impurities, and therefore we have to abandon the previously used techniques [13–15]. In this paper we have chosen to make use of the coherent potential approximation (CPA), which is well known to provide a successful description of single-particle properties in disordered systems [16–18].

III. CPA EQUATIONS

Within CPA we look for an averaged Nambu-Gorkov Green's function $\hat{G}_M$ defined by $\hat{G}_M^{-1} = \hat{G}_0^{-1} - \hat{\Sigma}$, where $\hat{G}_0^{-1}(\mathbf{k},\omega_n) = i\omega_n\tau_0 - \varepsilon_{\mathbf{k}}\tau_3$ is the bare Green's function and $\hat{\Sigma}_n = -i\Gamma_n\tau_0 + \Phi_n\tau_1 + \chi_n\tau_3$ is a local translationally invariant self-energy generated by disorder and pairing interactions. We work in imaginary time formalism, the index n denotes the Matsubara frequency, and τ_i are the Pauli matrices.

For the impurity potential we take

$$\hat{V} = \bar{\Delta}\tau_1 + U\tau_3 + V\tau_0.$$

The first term is the spatially homogeneous pairing interaction; the second term is a fluctuating potential which is usually large in samples described by Eq. (1), and the last term is a much weaker classical pair-breaking field, polarized along a fixed direction in spin space [19]. We assume that the fields U and V are distributed according to independent and spatially uncorrelated even functions $P_s(U)$ and $P_m(V)$.

In CPA the self-energy $\hat{\Sigma}$ is chosen so that, on average, electrons described by $\hat{G}_M$ do not scatter on the random potential $\hat{V}$. As shown in Appendix A, this leads to the following self-consistent equation for the self-energy,

$$\langle(\hat{V} - \hat{\Sigma})[\mathbf{1} - \hat{G}_{\rm loc}(\hat{V} - \hat{\Sigma})]^{-1}\rangle_{U,V} = 0, \tag{4}$$

where the angular brackets denote averaging with respect to U,V and $\hat{G}_{\rm loc} = (\hat{G}_M)_{ii}$ is the diagonal component (in coordinate space) of $\hat{G}_M$.

For a particle-hole symmetric system, the defining Eq. (4) of CPA is compatible with $\chi_n = 0$, see Appendix B. In what follows we use dimensionless pair-conserving and pair-breaking fields $\mu = \pi N_0 U$ and $\lambda = \pi N_0 V$, respectively. For convenience, we also make use of the dimensionless quantities $\gamma_n = \pi N_0 \Gamma_n, \Lambda_n = \lambda + i\gamma_n$, and $\delta_n = \pi N_0(\bar{\Delta} - \Phi_n)$, as well as of the auxiliary variables

$$z_n = x_n + iy_n = \frac{\Phi_n + i(\omega_n + \Gamma_n)}{\sqrt{(\omega_n + \Gamma_n)^2 + \Phi_n^2}},$$

which satisfy the identity $|z_n|^2 = 1$. In terms of these variables, Eq. (4) can be rewritten as a single complex equation, see Appendix B,

$$\left\langle \frac{z_n + \delta_n - \Lambda_n}{(z_n + \delta_n - \Lambda_n)(z_n^* + \delta_n + \Lambda_n) + \mu^2} \right\rangle_{\mu,\lambda} = z_n. \tag{5}$$

By solving Eq. (5), we can find the normal and anomalous self-energies Γ_n and Φ_n, or, alternatively, the wave-function renormalization $Z_n = 1 + \Gamma_n/\omega_n$ and the gap function $\Delta_n = \Phi_n/Z_n$.

Dilute gas of identical magnetic impurities

In order to proceed, we need to specify the probability distributions $P_s(U)$ and $P_m(V)$. We will start by considering the well studied example with vanishing potential disorder and

$$P_m(V) = (1-x)\delta(V) + \frac{x}{2}[\delta(V-V_0) + \delta(V+V_0)], \quad (6)$$

which describes a set of magnetic impurities with magnetic field $\pm V_0$ and concentration x. Making use of this distribution in Eq. (5) and assuming that $x \ll 1$, to first order in the impurity concentration we find

$$Z_n = 1 + \frac{\Gamma_0(1+\lambda_0^2)\sqrt{\omega_n^2+\Delta_n^2}}{(1+\lambda_0^2)^2\omega_n^2 + (1-\lambda_0^2)^2\Delta_n^2},$$

$$\bar{\Delta} = \left[1 + 2\Gamma_0 \frac{\sqrt{\omega_n^2+\Delta_n^2}}{(1+\lambda_0^2)^2\omega_n^2 + (1-\lambda_0^2)^2\Delta_n^2}\right]\Delta_n,$$

where $\Gamma_0 = x\pi N_0 V_0^2$ and $\lambda_0 = \pi N_0 V_0$. These are the well-known self-consistent equations of the T-matrix approximation [13], which shows that CPA becomes exact in the low-density limit.

In Fig. 2 we compare $N(\omega)$ for a superconductor with a dilute gas of pair-breaking impurities, calculated within the T-matrix approximation and the full CPA. Both approximations result in a qualitatively similar density of states. As expected, the agreement between the two approximations improves as the impurity concentration x decreases. Somewhat surprisingly, CPA predicts systematically narrower impurity bands.

IV. THE DYNES SUPERCONDUCTORS

Now we turn to the main result of this paper. In order to take into account the spatial distribution of coupling strengths to magnetic impurities, instead of Eq. (6) we consider the so-called Lloyd model [20],

$$P_m(V) = \frac{1}{\pi}\frac{\Gamma}{V^2+\Gamma^2},$$

with a continuous spread of impurity strengths ranging up to $\sim\Gamma$. We emphasize that we don't need to make any further assumptions about $P_s(U)$.

Let us for definiteness consider $\omega_n > 0$ and assume that $y_n > \gamma_n > 0$. Inserting $P_m(V)$ into Eq. (5), we notice that averaging with respect to λ can be readily performed in the complex plane of λ, leading to

$$\left\langle \frac{\zeta_n}{|\zeta_n|^2+\mu^2} \right\rangle_\mu = z_n, \quad (7)$$

where we have introduced $\zeta_n = (x_n+\delta_n) + i(y_n+\lambda_0-\gamma_n)$ with $\lambda_0 = \pi N_0\Gamma$.

Comparing the phases of both sides of Eq. (7) leads to

$$\Delta_n = \frac{\omega_n\bar{\Delta}}{\omega_n+\Gamma}.$$

After analytic continuation to the real axis this result reduces to Eq. (3) meaning that, within CPA, the Lorentzian distribution $P_m(V)$ of pair-breaking fields generates precisely that frequency-dependent gap function $\Delta(\omega)$ which reproduces the Dynes tunneling density of states Eq. (1). Moreover, the Dynes parameter Γ is given directly by the width of the Lorentzian $P_m(V)$. Note that in the absence of pair breaking, i.e., for $\Gamma = 0$, CPA predicts $\Delta(\omega) = \bar{\Delta}$, which is consistent with the Anderson theorem.

Comparing the amplitudes of both sides of Eq. (7) we find that $|\zeta_n| = F$ is independent of frequency and the constant F is fixed by $\int d\mu P_s(\mu)F/(\mu^2+F^2) = 1$. The self-energy Γ_n can be determined from $|\zeta_n| = F$. After analytic continuation to the real axis the wave-function renormalization $Z(\omega) = 1 + i\Gamma(\omega)/\omega$ reads

$$Z(\omega) = \left(1 + \frac{i\Gamma_s}{\Omega}\right)\left(1 + \frac{i\Gamma}{\omega}\right), \quad (8)$$

where $\Gamma_s = (1-F)/\pi N_0$ is the pair-conserving scattering rate and $\Omega = [(\omega+i\Gamma)^2 - \bar{\Delta}^2]^{1/2}$. The function $Z(\omega)$ is seen to be a product of two factors. The first factor, due to pair-conserving scattering, reproduces the Born approximation [21], albeit with a generalized Γ_s. The second factor, due to pair-breaking processes, has the same form as found previously for inelastic processes at finite temperatures [10]. Strongly disordered samples which we are interested in are described by $\Gamma \lesssim \bar{\Delta} \ll \Gamma_s$.

The criterion for applicability of our results, $y_n > \gamma_n$, is satisfied for $F > g = \pi N_0(\Gamma^2+\bar{\Delta}^2)^{1/2}$. If for $P_s(U)$ we take, as an order-of-magnitude estimate, a box distribution of width $2U_0$, we find $F = \pi N_0 U_0/\tan(\pi N_0 U_0)$. On the other hand, for samples with $\Gamma \lesssim \bar{\Delta}$ we have $g \ll 1$. From here it follows that $F > g$ holds provided that $U_0 \lesssim 1/(2N_0)$, i.e., up to large potential disorder. In Appendix C we argue that the existence of a critical value of U_0 is an artifact of the CPA approximation.

We emphasize that our microscopics goes beyond the phenomenology of Eq. (1) by predicting *both* of the Eliashberg functions, $\Delta(\omega)$ and $Z(\omega)$. The resulting retarded electron Green's function reads

$$\hat{G}_M(\mathbf{k},\omega) = \frac{(1+i\Gamma_s/\Omega)[(\omega+i\Gamma)\tau_0 + \bar{\Delta}\tau_1] + \varepsilon_{\mathbf{k}}\tau_3}{(\Omega+i\Gamma_s)^2 - \varepsilon_{\mathbf{k}}^2}. \quad (9)$$

Note that Eq. (9) is the simplest consistent generalization of the BCS Green's function which takes into account both the pair-conserving and the pair-breaking scattering processes with rates Γ_s and Γ, respectively. Superconductors described by Eq. (9) will be called Dynes superconductors in what follows.

A. Thermodynamics

Next we consider the thermodynamic properties of the Dynes superconductors. To this end, we realize that the off-diagonal part $\bar{\Delta}$ of the potential $\hat{V}$ has to come from a phonon-induced anomalous self-energy. As shown in detail in Appendix D, within the BCS approximation with dimensionless coupling constant $\lambda \ll 1$ and cutoff frequency Ω, the self-consistent equation for the Dynes superconductors reads as

$$\bar{\Delta} = \lambda\pi T \sum_{\omega_n=-\Omega}^{\Omega} \frac{\bar{\Delta}}{\sqrt{(|\omega_n|+\Gamma)^2 + \bar{\Delta}^2}}. \quad (10)$$

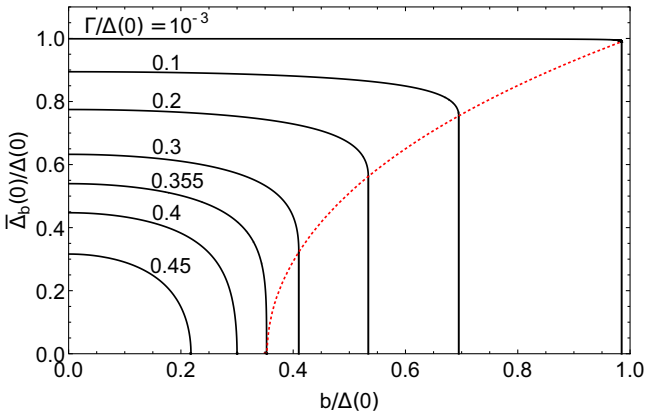

FIG. 3. The order parameter at $T = 0$ in a magnetic field b, $\bar{\Delta}_b(0)$, as a function of b for several Γ. First-order transitions for small Γ are shown by the dotted line.

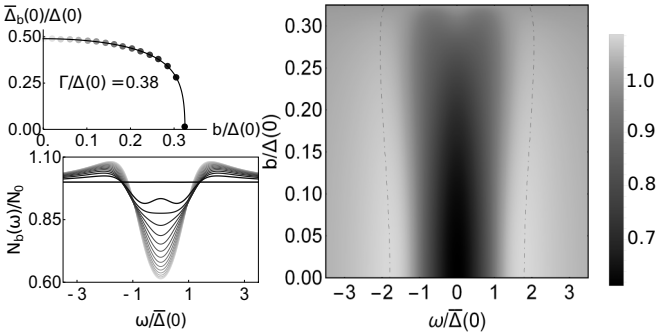

FIG. 4. Right panel: map of $N_b(\omega)$ at $T = 0$ in the (ω, b) plane for a Dynes superconductor with $\Gamma/\Delta(0) = 0.38$. The dash-dotted curve marks the positions of the maxima of $N_b(\omega)$ at fixed b. The lower left panel shows $N_b(\omega)$ for several values of b. The self-consistent values of $\bar{\Delta}_b(0)$ for the same b values are plotted in the upper left panel.

Making use of Eq. (10), we can calculate the temperature dependence $\bar{\Delta} = \bar{\Delta}(T)$ as a function of the parameter Γ. We find that the critical temperature of a dirty Dynes superconductor $\bar{T}_c$ is governed by the same equation as in the Abrikosov-Gorkov theory, $\psi(\frac{1}{2} + \frac{\alpha}{x}) - \psi(\frac{1}{2}) = \ln(\frac{1}{x})$, where $\psi(x)$ is the digamma function, $\alpha = \Gamma/(2\pi T_c), x = \bar{T}_c/T_c$, and T_c is the critical temperature of the clean system. This is because, as already mentioned, close to the critical temperature, Eq. (3) applies to superconductors with pair breaking even in the Born approximation.

Below T_c it is convenient to normalize $\bar{\Delta}(T)$ in terms of $\Delta(0)$, the zero-temperature gap of the clean system. At $T = 0$ we find $\bar{\Delta}(0) = \sqrt{\Delta(0)[\Delta(0) - 2\Gamma]}$, therefore the critical disorder strength for complete disappearance of superconductivity is $\Gamma_c = \Delta(0)/2$. The $\bar{\Delta} = \bar{\Delta}(T)$ curves for varying Γ are essentially BCS-like, as shown in detail in Appendix D. The ratio $\bar{\Delta}(0)/\bar{T}_c$ increases by a factor $\mathcal{R}$ with respect to the clean-system value $\Delta(0)/T_c$, and $\mathcal{R}$ slightly grows with Γ. For $\Gamma \to \Gamma_c$ we find $\mathcal{R}(\Gamma_c) \approx 1.45$, which is however much less than $\mathcal{R}(\Gamma_c) \approx 2.52$ within the Abrikosov-Gorkov theory.

B. Effect of external magnetic field

Finally we study the density of states of a Dynes superconductor in an external magnetic field B. We assume that the superconductor is sufficiently dirty, so that the suppression of $\bar{\Delta}$ by B can be roughly estimated by keeping only the Zeeman coupling, as explained in Appendix E. In this approximation the effect of B is fully described by simply changing the bare electron Green's function to $\hat{G}_0^{-1}(\mathbf{k}, \omega_n) = (i\omega_n - b)\tau_0 - \varepsilon_{\mathbf{k}}\tau_3$ with $b = \mu_B B$. One can check that the CPA expressions remain valid, if we make the substitution $\omega_n \to \omega_n + ib$. In particular, Eq. (10) is replaced by the following self-consistent equation,

$$\bar{\Delta} = 2\lambda\pi T \sum_{\omega_n > 0}^{\Omega} \mathrm{Re}\left[\frac{\bar{\Delta}}{\sqrt{(\omega_n + \Gamma + ib)^2 + \bar{\Delta}^2}}\right]. \qquad (11)$$

As was to be expected, the theory with only Zeeman coupling, Eq. (11), predicts a first-order transition at small Γ, but, as shown in Fig. 3, the transition becomes continuous for $\Gamma > \Gamma_c \approx 0.355\Delta(0)$, as one would expect in the full theory with orbital effects included.

In Appendix E we argue furthermore that, sufficiently far away from the vortex cores, the density of states in a finite magnetic field $N_b(\omega)$ can be described by considering only the Zeeman coupling, and this leads to $N_b(\omega) = \sum_{\pm} N(\omega \pm b)/2$. In Fig. 4 we plot the evolution of $N_b(\omega)$ with b for a Dynes superconductor with $\Gamma/\Delta(0) = 0.38$. Due to the Zeeman coupling, the peak-to-peak distance of the density of states exhibits only small changes with b, up to the critical field b_c. This means that gap filling rather than gap closing with increasing b can be observed in dirty Dynes superconductors. Note, however, that the order parameter $\bar{\Delta}_b(0)$ does behave in a standard way and vanishes at b_c, see the left panel of Fig. 4. Very recently, similar behavior of $N(\omega)$ in magnetic fields has been observed experimentally [22].

V. CONCLUSIONS

We have identified a class of gapless superconductors, the Dynes superconductors, which are distinguished by a sufficiently broad distribution of pair-breaking fields. The Dynes superconductors are described by two scattering rates, Γ_s and Γ, for pair-conserving and pair-breaking processes, respectively. The Green function of a canonical Dynes superconductor is given by Eq. (9). We have shown that this functional form follows from the CPA equations with a Lorentzian distribution of pair-breaking fields and arbitrary potential disorder. The Dynes superconductors are always gapless from T_c all the way down to the lowest temperatures, and their thermodynamic properties differ from predictions of the Abrikosov-Gorkov theory.

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APPENDIX A: COHERENT POTENTIAL APPROXIMATION

For convenience we present a short sketch of the derivation of Eq. (4) from the main text. Let $\hat{G}$ be the full Green's function of the disordered system (i.e., a matrix whose indices describe the lattice sites and the Nambu components) and let $\hat{G}_0$ be the bare Green's function of the clean system. Then $\hat{G}$ satisfies the matrix equation

$$\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{V} \hat{G}, \tag{A1}$$

which corresponds to repeated scattering of the bare electrons (described by $\hat{G}_0$) by the random potential $\hat{V}$. Equivalently, Eq. (A1) can be written in terms of the T matrix $\hat{T}_0$ in the form $\hat{G} = \hat{G}_0 + \hat{G}_0 \hat{T}_0 \hat{G}_0$. Comparing these two expressions for $\hat{G}$, one finds easily that

$$\hat{T}_0 = \hat{V}(\mathbf{1} - \hat{G}_0 \hat{V})^{-1}. \tag{A2}$$

In CPA we look for an optimal averaged Nambu-Gorkov Green's function $\hat{G}_M$ describing the disordered medium. Let us express this effective Green's function in terms of the self-energy by the Dyson equation

$$\hat{G}_M^{-1} = \hat{G}_0^{-1} - \hat{\Sigma}. \tag{A3}$$

From similar considerations which led to Eq. (A1) it follows that the full Green's function of the disordered system $\hat{G}$ satisfies the matrix equation

$$\hat{G} = \hat{G}_M + \hat{G}_M(\hat{V} - \hat{\Sigma})\hat{G}, \tag{A4}$$

which shows that electrons described by the effective Green's function $\hat{G}_M$ interact with a reduced potential $\hat{V} - \hat{\Sigma}$.

In order to fix the optimal self-energy $\hat{\Sigma}$, let us rewrite Eq. (A4) for the full Green's function $\hat{G}$ in terms of the T matrix of the effective medium $\hat{T}$ by $\hat{G} = \hat{G}_M + \hat{G}_M \hat{T} \hat{G}_M$. A calculation completely analogous to that leading to Eq. (A2) leads then to an expression for the T matrix of the effective medium:

$$\hat{T} = (\hat{V} - \hat{\Sigma})[\mathbf{1} - \hat{G}_M(\hat{V} - \hat{\Sigma})]^{-1}. \tag{A5}$$

Note that Eq. (A5) differs from Eq. (A2) by simply replacing $\hat{V}$ by $\hat{V} - \hat{\Sigma}$ and $\hat{G}_0$ by $\hat{G}_M$, i.e., $\hat{T}$ describes residual scattering on disorder, not taken into account in the effective medium description. Two points are to be noted: (i) $\hat{T}$ for a given sample depends on the choice of the random potential, and (ii) $\hat{T}$ is a matrix in the coordinate space.

Now it is natural to choose the effective medium so that, after averaging over disorder, the residual scattering is minimized, $\langle \hat{T} \rangle = 0$. Within CPA one requires that only the site-diagonal components of the T matrix vanish. This leads to the self-consistent equation [17]

$$\langle (\hat{V} - \hat{\Sigma})[\mathbf{1} - \hat{G}_{\rm loc}(\hat{V} - \hat{\Sigma})]^{-1} \rangle = 0,$$

where $\hat{G}_{\rm loc} = (\hat{G}_M)_{ii}$ is the diagonal component (in coordinate space) of $\hat{G}_M$. This is Eq. (4) from the main text.

APPENDIX B: DERIVATION OF EQ. (5)

Let us take for the self-energy the ansatz $\hat{\Sigma}_n = -i\Gamma_n \tau_0 + \Phi_n \tau_1 + \chi_n \tau_3$ from the main text, and making use of Eq. (A3) let us calculate the averaged Green's function $\hat{G}_M(\mathbf{k},\omega_n)$. We find

$$\hat{G}_M(\mathbf{k},\omega_n) = -\frac{i(\omega_n + \Gamma_n)\tau_0 + \Phi_n \tau_1 + (\varepsilon_{\mathbf{k}} + \chi_n)\tau_3}{(\omega_n + \Gamma_n)^2 + \Phi_n^2 + (\varepsilon_{\mathbf{k}} + \chi_n)^2}. \tag{B1}$$

The local Green's function $\hat{G}_{\rm loc}(\omega_n)$ can be found by Fourier transforming the function $\hat{G}_M(\mathbf{k},\omega_n)$ from momentum ($\mathbf{k}$) to real ($\mathbf{r}$) space and by taking $\mathbf{r} = 0$. Replacing the momentum summation by energy integration and assuming a constant density of states N_0 in the vicinity of the Fermi level, a standard calculation leads to

$$\hat{G}_{\rm loc}(\omega_n) = -\pi N_0 \frac{i(\omega_n + \Gamma_n)\tau_0 + \phi_n \tau_1}{\sqrt{(\omega_n + \Gamma_n)^2 + \phi_n^2}}. \tag{B2}$$

Note that, as usual, the component of $\hat{G}_{\rm loc}$ proportional to the Pauli matrix τ_3 vanishes. This is a consequence of the assumed particle-hole symmetry of the problem.

Evaluating the matrix inverse entering Eq. (4) is straightforward, since $\hat{G}_{\rm loc}, \hat{V}$, and $\hat{\Sigma}$ are matrices 2×2. Making use of the explicit form of the potential $\hat{V} = \bar{\Delta}\tau_1 + U\tau_3 + V\tau_0$ from the main text we find

$$[\tau_0 - \hat{G}_{\rm loc}(\hat{V} - \hat{\Sigma})]^{-1} = \frac{a_n \tau_0 + i b_n \tau_1 + i c_n \tau_2 + i d_n \tau_3}{a_n^2 + b_n^2 + c_n^2 + d_n^2}, \tag{B3}$$

where we have introduced auxiliary variables

$$a_n = 1 + \pi N_0 \frac{i(\omega_n + \Gamma_n)(V + i\Gamma_n) + \phi_n(\bar{\Delta} - \phi_n)}{\sqrt{(\omega_n + \Gamma_n)^2 + \phi_n^2}},$$

$$b_n = \pi N_0 \frac{i\phi_n(V + i\Gamma_n) - (\omega_n + \Gamma_n)(\bar{\Delta} - \phi_n)}{\sqrt{(\omega_n + \Gamma_n)^2 + \phi_n^2}},$$

$$c_n = \pi N_0 \frac{\phi_n(U - \chi_n)}{\sqrt{(\omega_n + \Gamma_n)^2 + \phi_n^2}},$$

$$d_n = \pi N_0 \frac{(\omega_n + \Gamma_n)(\chi_n - U)}{\sqrt{(\omega_n + \Gamma_n)^2 + \phi_n^2}}.$$

Inserting the result Eq. (B3) into Eq. (4), we obtain four equations, which follow from requiring that the coefficients in front of the Pauli matrices τ_i with $i = 0, \ldots, 3$ vanish:

$$\left\langle \frac{(V + i\Gamma_n)a_n + i(\bar{\Delta} - \phi_n)b_n + i(U - \chi_n)d_n}{a_n^2 + b_n^2 + c_n^2 + d_n^2} \right\rangle = 0, \tag{B4}$$

$$\left\langle \frac{i(V + i\Gamma_n)b_n + (\bar{\Delta} - \phi_n)a_n + (U - \chi_n)c_n}{a_n^2 + b_n^2 + c_n^2 + d_n^2} \right\rangle = 0, \tag{B5}$$

$$\left\langle \frac{i(V + i\Gamma_n)c_n + (\bar{\Delta} - \phi_n)d_n - (U - \chi_n)b_n}{a_n^2 + b_n^2 + c_n^2 + d_n^2} \right\rangle = 0, \tag{B6}$$

$$\left\langle \frac{i(V + i\Gamma_n)d_n - (\bar{\Delta} - \phi_n)c_n + (U - \chi_n)a_n}{a_n^2 + b_n^2 + c_n^2 + d_n^2} \right\rangle = 0. \tag{B7}$$

If one makes use of the explicit form of the auxiliary variables a_n, b_n, c_n, and d_n, the last two equations (B6) and (B7) can be easily solved. In fact, Eq. (B6) is trivially satisfied, and Eq. (B7) can be written as

$$\left\langle \frac{U - \chi_n}{a_n^2 + b_n^2 + [\pi N_0(U - \chi_n)]^2} \right\rangle = 0.$$

Note that the variables a_n and b_n do not include the scalar potential U. But since the distribution function $P(U)$ is supposed to be even, one checks easily that Eq. (B7) is solved by requiring $\chi_n = 0$.

Finally, if we take the sum and the difference of Eqs. (B4) and (B5) and if we make use of the result $\chi_n = 0$, we obtain another set of two equations. They can be written down in a simple form by using the dimensionless variables μ, Λ_n,δ_n, and z_n defined in the main text:

$$\left\langle \frac{(\delta_n+\Lambda_n)(1+z_n^*(\delta_n-\Lambda_n))+z_n^*\mu^2}{(1+z_n^*(\delta_n-\Lambda_n))(1+z_n(\delta_n+\Lambda_n))+\mu^2} \right\rangle = 0,$$

$$\left\langle \frac{(\delta_n-\Lambda_n)(1+z_n(\delta_n+\Lambda_n))+z_n\mu^2}{(1+z_n^*(\delta_n-\Lambda_n))(1+z_n(\delta_n+\Lambda_n))+\mu^2} \right\rangle = 0.$$

Assuming that ϕ_n and Γ_n are purely real, we can easily see that they reduce to just one equation after complex conjugation and substitution $V \to -V$ in one of them. After some trivial algebra we are therefore left with just one complex integral CPA equation in the form of Eq. (5) from the main text.

APPENDIX C: CPA IN THE NORMAL STATE

In the normal state our model for disorder implies that electrons with spin σ experience a random potential $W = U + \sigma V$ with distribution functions

$$P_\sigma(W) = \int dU \int dV\, P_s(U) P_m(V) \delta(U + \sigma V - W). \quad \text{(C1)}$$

Note that since $P_m(V)$ is even, we have $P_\uparrow(W) = P_\downarrow(W) \equiv P(W)$. In the upper half-plane $\omega_n > 0$, Eq. (4) from the main text is solved for this distribution function by a frequency-independent self-energy $\Sigma_n = -i\Gamma_N$, where $\Gamma_N = (1 - F_N)/(\pi N_0)$ and the constant F_N is given by

$$1 = \left\langle \frac{F_N}{F_N^2 + (\pi N_0 W)^2} \right\rangle_W. \quad \text{(C2)}$$

Note that Eq. (C2) does not have a solution for sufficiently broad distributions $P(W)$. This is an artifact of the CPA, as can be shown readily, if we take for $P_s(U)$ and $P_m(V)$ Lorentzians with widths Γ_s and Γ, respectively. In fact, in that case also $P(W)$ is a Lorentzian with width $\Gamma + \Gamma_s$ and Eq. (C2) implies that $1 - F_N = \pi N_0(\Gamma + \Gamma_s)$, or, in other words, the normal-state self-energy is given by the width of $P(W)$, $\Gamma_N = \Gamma + \Gamma_s$. However, since Eq. (C2) clearly requires that $F_N > 0$, the CPA solution is valid only for $\pi N_0 \Gamma_N < 1$.

On the other hand, as shown by Lloyd [20], the normal-state model with a Lorentzian distribution $P(W)$ is exactly solvable for all values of Γ_N, thus the criterion $\pi N_0 \Gamma_N < 1$ can not have any physical meaning and it must be an artifact of the CPA. It should be pointed out, however, that in its region of validity, the CPA does reproduce the exact self-energy of the Lloyd model [20].

APPENDIX D: THERMODYNAMICS OF THE DYNES SUPERCONDUCTORS

Let us assume that the pairing in the Dynes superconductors is driven by a local phonon-mediated electron-electron interaction $U_{\rm ph}$ which is present up to a finite frequency cutoff Ω. Then, at the mean-field level, the off-diagonal part of the potential $\hat{V}$ is determined by the self-consistent equation

$$\bar{\Delta} = U_{\rm ph} \langle \psi_\uparrow(\mathbf{r}) \psi_\downarrow(\mathbf{r}) \rangle, \quad \text{(D1)}$$

where $\psi_\sigma(\mathbf{r})$ are the annihilation operators for electrons at site $\mathbf{r}$. After Fourier transformation to momentum space with annihilation operators $c_{\mathbf{k}\sigma}$, this equation can be written as

$$\bar{\Delta} = \frac{U_{\rm ph}}{N} \sum_{\mathbf{k}} \langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle = -\frac{U_{\rm ph}}{N} \sum_{\mathbf{k}} \hat{G}_M^{12}(\mathbf{k}, \tau = 0^+), \quad \text{(D2)}$$

where N is the number of lattice sites and $\hat{G}_M^{12}$ is the off-diagonal component of the averaged Green's function. Performing the temporal Fourier transformation of the Green's function and making use of the explicit form of $\hat{G}_M$, Eq. (B1), together with the result $\chi_n = 0$, Eq. (D2) can be written as

$$\bar{\Delta} = U_{\rm ph} \frac{T}{N} \sum_{\mathbf{k},\omega_m} \frac{Z_m \Delta_m}{Z_m^2(\omega_m^2 + \Delta_m^2) + \varepsilon_{\mathbf{k}}^2}. \quad \text{(D3)}$$

Let us note that the momentum summation in Eq. (D3) can be replaced by energy integration, which in turn can be performed explicitly. Imposing furthermore the frequency cutoff Ω, this leads to the result

$$\bar{\Delta} = \lambda \pi T \sum_{\omega_m=-\Omega}^{\Omega} \frac{\Delta_m}{\sqrt{\omega_m^2 + \Delta_m^2}}, \quad \text{(D4)}$$

where $\lambda = N_0 U_{\rm ph}$ is a dimensionless coupling constant. Note that the wave-function renormalization Z_m drops out from the right-hand side. If in Eq. (D4) we make use of the frequency dependence of the gap function of a Dynes superconductor, valid for both signs of ω_n,

$$\Delta_m = \frac{|\omega_m|}{|\omega_m| + \Gamma} \bar{\Delta},$$

we finally end up with the self-consistent Eq. (10) from the main text. It is worth pointing out that Eq. (10) from the main text does not contain the pair-conserving scattering rate Γ_s, and this is consistent with the Anderson theorem.

In Fig. 5 we show the temperature dependence of the ideal gaps $\bar{\Delta}(T)$ of Dynes superconductors for various pair-breaking parameters Γ, which are seen to be essentially BCS-like for all admissible values of Γ.

APPENDIX E: EFFECT OF FINITE EXTERNAL MAGNETIC FIELD

External magnetic field interacts with electrons via two different mechanisms: via the Zeeman coupling and by minimal coupling between the electron's momentum and the vector potential, which for brevity will be called orbital coupling. In order to compare the relative importance of the Zeeman and orbital couplings, we will estimate the critical fields, i.e., those fields which lead to a complete destruction of superconductivity, for both mechanisms taken separately. Let us start by considering the orbital coupling. In a dirty type-II superconductor such as MoC, the upper critical field H_{c2} can be estimated as $\mu_0 H_{c2} \sim \Phi_0/(\xi_0 \ell)$, where Φ_0 is the flux quantum, $\xi_0 \sim \hbar v_F/\Delta$ is the coherence length, and ℓ is the mean free path. On the other hand, due to the Zeeman coupling, the

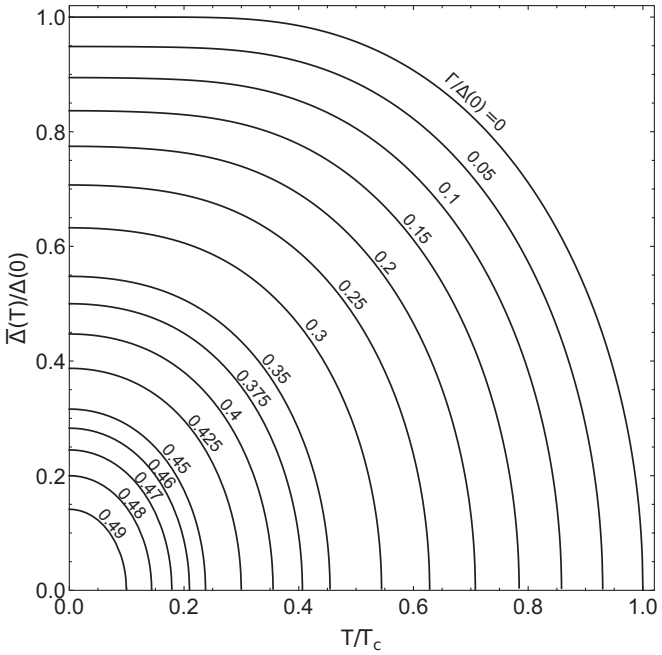

FIG. 5. Numerically determined ideal gaps $\bar{\Delta}(T)$ of Dynes superconductors for various pair-breaking parameters Γ for fixed $\lambda \ll 1$ and Ω. The gaps are measured in units of $\Delta(0)$, which is the gap of the clean system at $T = 0$. Temperature is displayed in units of T_c, which is the critical temperature of the clean system.

Cooper pairing will be destroyed by the Pauli depairing field H_P, which can be estimated as $\mu_0 H_P \sim \Delta/\mu_B$, where μ_B is the Bohr magneton [23]. Comparing the two estimates we find $H_P/H_{c2} \sim k_F \ell$, which shows that in materials which are close to the metal-insulator transition, the Zeeman and orbital couplings are of the same order of magnitude. This suggests that the suppression of $\bar{\Delta}$ with magnetic field in such samples should be described qualitatively correctly by keeping only the Zeeman coupling, of course only at sufficiently large Γ, where the transition is continuous. This approximation has been used in the main text in Figs. 3 and 4.

However, since the Zeeman and orbital couplings are of comparable magnitude, it is legitimate to ask whether it is sufficient to keep only the Zeeman coupling in calculating the effect of the magnetic field on the density of states $N_b(\omega)$. To answer this question, let us remember that, in a wide field range, type-II superconductors exhibit the vortex state. If the density of states is to be measured sufficiently far away from the vortex cores, as is assumed in this work, then the orbital effect of the magnetic field can be taken into account by the Doppler shift, which is proportional to the local momentum of the supercurrent flow $\mathbf{q}$ in the point where the density of states is being measured [24]. This changes the bare electron Green's function in the presence of magnetic field to

$$\hat{G}_0^{-1}(\mathbf{k},\omega_n) = (i\omega_n - b - \delta_{\mathbf{k}})\tau_0 - \varepsilon_{\mathbf{k}}\tau_3,$$

where b is the Zeeman energy and $\delta_{\mathbf{k}} = \mathbf{v}_{\mathbf{k}} \cdot \mathbf{q}$ is the Doppler shift. Note that both pair-breaking fields b and $\delta_{\mathbf{k}}$ enter the Green's function in the same way, the only difference being that $\delta_{\mathbf{k}}$ depends on the direction of $\mathbf{k}$, while b is direction independent.

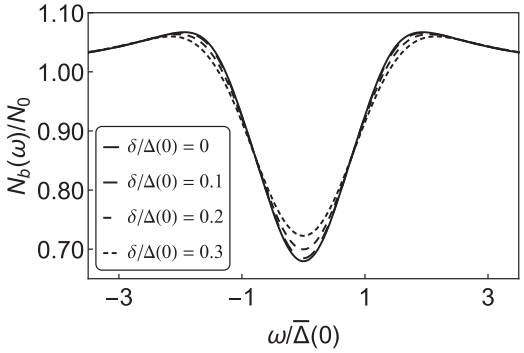

FIG. 6. Density of states $N_b(\omega)$ of a Dynes superconductor with $\Gamma/\Delta(0) = 0.38$ and Zeeman coupling $b/\Delta(0) = 0.16$, when the gap is reduced to $\bar{\Delta}_b(0)/\Delta(0) = 0.46$ (see Fig. 4 of the main text). Note that the effect of the orbital coupling δ is very mild up to large values $\delta \sim 2b$. Moreover, the peak-to-peak distance of $N_b(\omega)$ exhibits further increase due to orbital effects.

In the presence of the Doppler shift, the density of states of a 3D superconductor changes to

$$N_b(\omega) = \frac{1}{4}\sum_{\pm}\int_0^{\pi} d\theta \sin\theta N(\omega \pm b - v_F q\cos\theta), \quad \text{(E1)}$$

which shows that the Doppler shift and the Zeeman coupling modify the density of states in a similar fashion.

Finally, we need to fix the magnitude of $\delta = v_F q$. Obviously, δ is position dependent, but it is easy to see that on the boundaries of the flux-lattice cells, δ has to vanish by symmetry. This means that the results presented in Fig. 4 of the main text are directly applicable at such boundaries [25]. Moreover, Fig. 6 shows that the orbital effects on $N_b(\omega)$ are small with respect to the effect of the Zeeman coupling up to large values of δ, which shows that keeping only the Zeeman coupling in estimating $N_b(\omega)$ should be a good approximation in a quite broad range of positions away from the vortex centers.

APPENDIX F: REMARKS ON THE EXPERIMENT OF SZABÓ *et al.*

The differential tunneling conductance at a finite voltage V between a featureless normal metal and a superconductor with density of states $N(\omega)$ is at finite temperatures given by

$$G(V) \propto \int d\omega N(\omega + eV)\left(-\frac{\partial f}{\partial \omega}\right), \quad \text{(F1)}$$

where $f(\omega)$ is the Fermi-Dirac distribution. Note that in the zero-temperature limit $-\partial f/\partial\omega$ reduces to a delta-function and $G(V)$ becomes directly proportional to $N(eV)$. The fits shown in Fig. 1 of the main text were done making use of Eq. (F1) with $f(\omega)$ taken at the finite experimental temperature, and the density of states $N(\omega)$ was described by the Dynes formula. Fitting parameters $\bar{\Delta}$ and Γ which have been used in those fits are shown in Table I.

Note that with decreasing film thickness d, the pair-breaking parameter Γ increases (the slight nonmonotonicity of the $\Gamma(d)$ dependence will be discussed later), while the ideal superconducting gap $\bar{\Delta}$ decreases. Let us first discuss the

TABLE I. Fitting parameters $\bar{\Delta}$ and Γ which have been used in Fig. 1 of the main text for films with varying thickness d.

d(nm)	3	5	10	30
$\bar{\Delta}$(meV)	0.19	0.63	1.12	1.22
Γ(meV)	0.16	0.21	0.1	10^{-3}

d dependence of Γ. If our interpretation of the Dynes formula in terms of the Lorentzian distribution of pair-breaking fields is applicable to the data of Szabó *et al.* [4], then the width of the distribution $P_m(V)$ has to increase with decreasing d. This will obviously happen if the effective concentration of the pair breakers grows with decreasing d. One possible scenario of how this could happen is to assume that the pair breakers are located in the vicinity of the interface between the film and the substrate.

Next we discuss the thickness dependence of $\bar{\Delta}$. Since Γ in the thickest sample is negligible and since $T \ll \bar{\Delta}$, we will assume that the $T = 0$ gap of a system without pair breakers, $\Delta(0)$, is equal to the value of $\bar{\Delta}$ for $d = 30$ nm, in other words $\Delta(0) = 1.22$ meV. Switching on a finite pair-breaking Γ should lead then to a decrease of $\bar{\Delta}(0)$ described by $\bar{\Delta}(0) = \sqrt{\Delta(0)[\Delta(0) - 2\Gamma]}$, see main text. This prediction is shown in Fig. 7, together with the experimental data taken from Table I. Here we have assumed that the $T = 0$ values $\bar{\Delta}(0)$ can be approximated by the measured values of $\bar{\Delta}$. This should be a good approximation, except perhaps for the thinnest sample, whose T_c is roughly only two times larger than the experimental temperature.

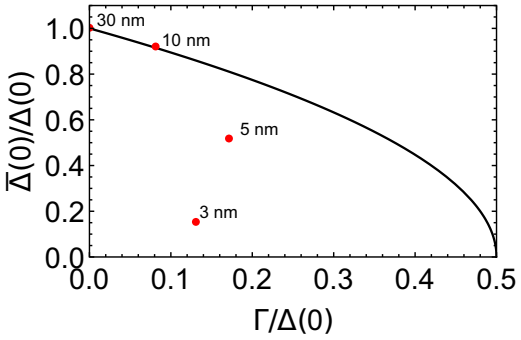

FIG. 7. Theoretical prediction for the evolution of the ideal superconducting gap $\bar{\Delta}(0)$ with the pair-breaking parameter Γ of a Dynes superconductor. Experimental data are shown as red dots.

Figure 7 shows that the initial decrease of $\bar{\Delta}(0)$ with increasing Γ is captured well by our theory. However, the agreement between theory and experiment breaks down for the two thinnest films. This signals that different physical phenomena, not included in our theory, start to play role in such very thin films. We have learned recently that there are indications that in those films, which are close to the Ioffe-Regel limit, the normal-state density of states might exhibit the Altshuler-Aronov singularity [26]. If this were true, then the normal-state conductance $G_N(V)$ would not be constant and, in the most naive approach, different $G(V)/G_N(V)$ curves would have to be fitted by the Dynes formula. It is plausible that also the nonmonotonic behavior of $\Gamma(d)$ might be caused by the same physics.

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