Density of states in unconventional superconductors: Impurity-scattering effects

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(Received 31 January 1994)

The density of states in unconventional superconductors, $N_s(E)$, is very sensitive to impurity scattering, especially at low energies. We investigate the behavior of $N_s(E)$, using both numerical calculations and analytic approximations; we discuss the Born limit, the unitarity limit, and the crossover between these two cases. We consider a two-dimensional electron gas with a d-wave order parameter of the form $\Delta(\hat{\mathbf{k}})=\Delta(\hat{\mathbf{k}}_x^2-\hat{\mathbf{k}}_y^2)$. The low-energy structure in $N_s(E)$ should be quite general, applying to all gaps with the same general behavior.

I. INTRODUCTION

Scattering by ordinary, nonmagnetic impurities leads to important changes in the properties of unconventional superconductors; for example, the density of states[1-3] $N_s(E)$, the transition temperature[1-4] T_c, and the penetration depth λ (Refs. 5–8) are all strongly affected. These phenomena have been subjected to detailed scrutiny in the context of high-T_c and heavy Fermion superconductors.

Underlying many of these effects is one fundamental fact, namely, that impurity scattering causes a significant change in the low-energy density of states, when the order parameter $\Delta(\hat{\mathbf{k}})$ is unconventional. By unconventional, we mean that $\Delta(\hat{\mathbf{k}})$ has less rotational symmetry than the normal-state lattice; symmetry considerations often force such an order parameter to vanish at certain points or lines on the Fermi surface.[1]

Our purpose in this paper is to describe the behavior of $N_s(E)$ at low energy. In doing this, we are led to consider the low-energy behavior of the impurity self-energy $a_3(\varepsilon)$. To increase our understanding we develop simple analytic approximations for $a_3(\varepsilon)$ and for $N_s(E)$, for both the Born and unitarity limits, and compare these to exact numerical results. We also show how $N_s(E=0)$ evolves as we go continuously from the Born to the unitarity limit, keeping the scattering time τ fixed. Our main analytic results are Eq. (18) for $N_s(E)$ in the unitary limit, and Eq. (29) for $N_s(E)$ in the Born limit. The physical origin of unitarity limit scattering is unclear at present, although such scattering has been invoked as a possible explanation of experimental data.[7]

We use weak-coupling theory, in the framework of the quasiclassical equations.[9] Two types of effect are not included in our work: (1) localization effects, as recently discussed by Lee[10] and (2) strong-coupling effects.[4,5,11] Our work should directly apply to many situations, and provide physical insight in cases in which the abovementioned complications arise.

II. BASIC THEORY

For specificity, we consider a scenario relevant to high-T_c materials. We treat a two-dimensional Fermi liquid, with a circular Fermi surface, and an order parameter of the following form:[5,7,8]

$$\Delta(\hat{\mathbf{k}})=\Delta(\hat{\mathbf{k}}_x^2-\hat{\mathbf{k}}_y^2)=\Delta\cos(2\phi) . \tag{1}$$

Here ϕ is the polar angle in the xy plane. This gap vanishes linearly at four points on the Fermi surface, and has zero angular average. We expect that the low-energy behavior of $N_s(E)$ depends mainly on these factors, so that our results are quite generic.

Gaps of the form (1) have emerged as candidates for the order parameter in the high-T_c materials, so it is important to establish the expected properties of superconductors with such gaps. Microscopic theories, based on various model assumptions, have indicated that such an order parameter is a strong possibility.[12,13] In addition, various pieces of experimental evidence have provided support for such an unconventional parameter.[14,15]

The density of states is given in terms of the $\hat{\tau}_3$ component of the quasiclassical propagator $\hat{g}(\varepsilon,\phi)$:[9]

$$N_s(E)=\frac{N(0)}{\pi}\mathrm{Im}\int_0^{2\pi}\frac{d\phi}{2\pi}g_3(i\varepsilon\to E-i\eta,\phi) \tag{2}$$

$$=\frac{N(0)}{\pi}\mathrm{Im}\langle g_3(i\varepsilon\to E-i\eta,\phi)\rangle . \tag{3}$$

Here ε is a Matsubara frequency, and the angular average over ϕ is denoted by $\langle\ \rangle$. The propagator is given in terms of the impurity self-energy $a_3(\varepsilon)$ by the following equations:[6]

$$g_3(\varepsilon,\phi)=\frac{-i\pi(\varepsilon+ia_3)}{[(\varepsilon+ia_3)^2+\Delta^2\cos^2 2\phi]^{1/2}} . \tag{4}$$

The self-energy is given by[6]

$$a_3(\varepsilon)=\frac{cN(0)v^2\langle g_3\rangle}{1-(N(0)v\langle g_3\rangle)^2} . \tag{5}$$

Here, c is the density of impurities, and v is the strength of the impurity potential, taken to be s wave.

The angular integral needed for both (5) and (3) can be done; this yields

$$\langle g_3\rangle=\frac{-2i\tilde{\varepsilon}}{[\tilde{\varepsilon}^2+\Delta^2]^{1/2}}K\left[\frac{\Delta^2}{\tilde{\varepsilon}^2+\Delta^2}\right] . \tag{6}$$

Here, $K(x)$ is the elliptic integral,[16] and the function $\tilde{\varepsilon}(\varepsilon)$ is defined by

$$\tilde{\varepsilon}=\varepsilon+ia_3(\varepsilon) . \tag{7}$$

For the low-energy ($E \ll \Delta$) phenomena at issue in this paper, the important point is that at small values of $\tilde{\varepsilon}$ ($\tilde{\varepsilon} \ll \Delta$), the elliptic integral has a logarithmic singularity:[16]

$$K\left[\frac{\Delta^2}{\tilde{\varepsilon}^2+\Delta^2}\right] \approx \frac{1}{2}\ln\left[\frac{16\Delta^2}{\tilde{\varepsilon}^2}\right] . \tag{8}$$

This singular behavior is due to the fact that the gap vanishes at the four points $\phi=\pi/4$, $3\pi/4$, $5\pi/4$, $7\pi/4$. The contribution to the angular integral in (2) from the vicinity of these points gives the logarithmic term.

We must also solve for the magnitude Δ, using the gap equation[8]

$$\frac{1}{g}=\frac{2N(0)T}{\Delta^2}\sum_{\varepsilon}{}'\sqrt{\tilde{\varepsilon}^2+\Delta^2} \times\left\{E\left[\frac{\Delta^2}{\tilde{\varepsilon}^2+\Delta^2}\right] -\frac{\varepsilon^2}{\tilde{\varepsilon}^2+\Delta^2}K\left[\frac{\Delta^2}{\tilde{\varepsilon}^2+\Delta^2}\right]\right\} . \tag{9}$$

The prime indicates that the sum needs an upper cutoff, while $E(x)$ is the other elliptic function.[16] The coupling constant is denoted by g.

So, we must solve Eqs. (9) and (5) self-consistently for a_3 and Δ, and then use these to compute $N_s(E)$ via (3).

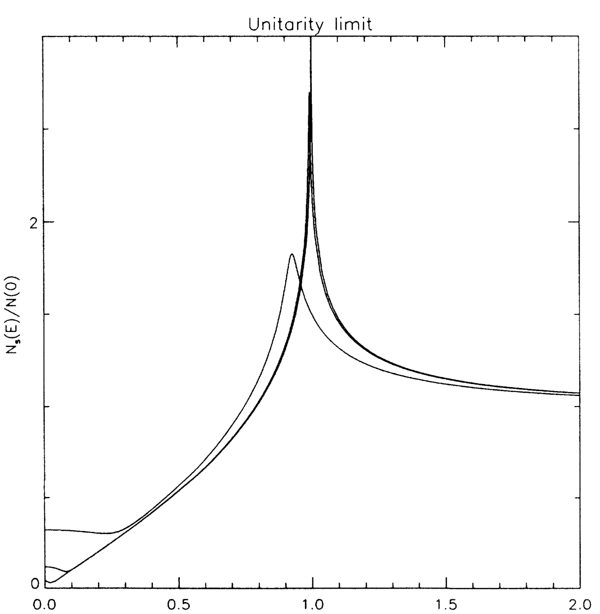

FIG. 1. Plot of $N_s(E)$ versus E, in the unitarity limit, for several values of τ. The curve with the largest $N_s(E=0)$ has $1/2\tau T_{c0}=10^{-1}$; succeeding curves have $1/2\tau T_{c0}=10^{-2}$ and 10^{-3}. The energy gap in the absence of impurities is denoted by Δ_0.

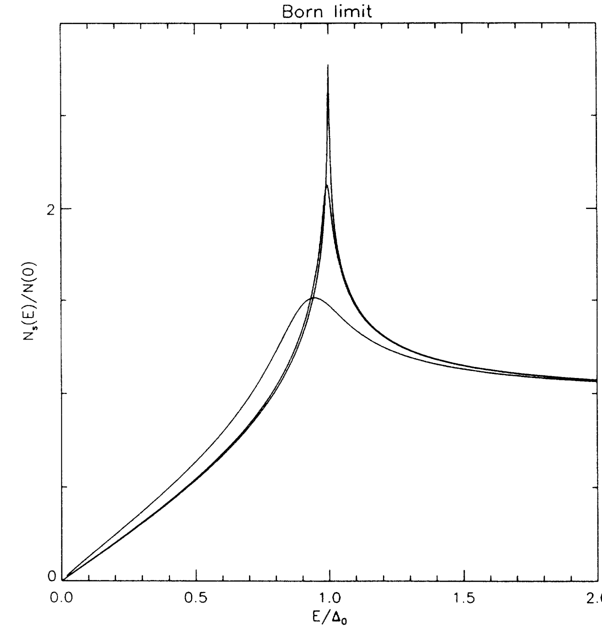

FIG. 2. Plot of $N_s(E)$ versus E, in the Born limit, for several values of τ. The curve with the steepest structure at $E=\Delta_0$ has $1/2\tau T_{c0}=10^{-3}$; succeeding curves have $1/2\tau T_{c0}=10^{-2}$ and 10^{-1}. The energy gap in the absence of impurities is denoted by Δ_0.

The impurity effects depend upon the two parameters c and v. It is often convenient to calculate in terms of two other parameters, given by

$$\sigma=\frac{(N(0)\pi v)^2}{1+(N(0)\pi v)^2} , \tag{10}$$

$$\frac{1}{2\tau}=\frac{cN(0)\pi v^2}{1+(N(0)\pi v)^2} . \tag{11}$$

Here, $1/\tau$ is the normal-state scattering rate. The parameter σ measures how strong the scattering potential of a single impurity is; the Born limit is defined by $\sigma \ll 1$, while the unitarity limit is given by $\sigma \rightarrow 1$. In Fig. 1 we show plots of $N_s(E)$ in the unitarity limit, for several values of τ. Figure 2 shows similar plots for the Born limit.

III. STUDY OF $N_s(E=0)$

An important theme that has emerged in the study of impurity scattering in unconventional superconductors is that many properties, with τ held fixed, depend strongly on the value of σ. The unitarity and Born answers can be quite different, even if the normal-state scattering time is the same.[3,5–8] The density of states at zero energy,[1–3] $N_s(E=0)$, is an important example of this phenomenon.

To illustrate this point, in Figs. 3 and 4 we show computed values of $N_s(E=0)$, as a function of σ, at a fixed value of τ. We have put Δ at its $T=0$ value; we also note that at the value of τ chosen ($1/2\tau T_{c0}=10^{-3}$), Δ is not significantly changed by the impurity scattering.

Figure 3 plots $N_s(E=0)$ on a logarithmic scale, which

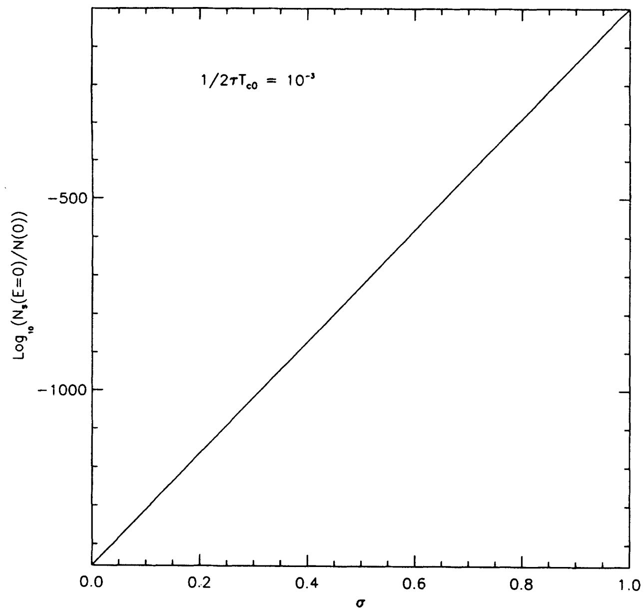

FIG. 3. Plot of $N_s(E=0)$ versus σ, with τ held fixed at $1/2\tau T_{c0}=10^{-3}$. Note that a logarithmic scale is used for $N_s(E=0)$. The parameter σ is defined in Eq. (10); $\sigma=0$ in the Born limit, while $\sigma=1$ in the unitarity limit.

allows us to show its tremendous variation (1500 orders of magnitude) as σ goes from zero to one. We can see that $N_s(E=0)$ is essentially exponential in σ over the entire range. Figure 4 allows us a good look at the structure near $\sigma=1$, where $N_s(E=0)$ becomes an appreciable fraction of $N(0)$.

These results suggest that an experiment which is sensitive to $N_s(E)$ near $E=0$ could be quite interesting.

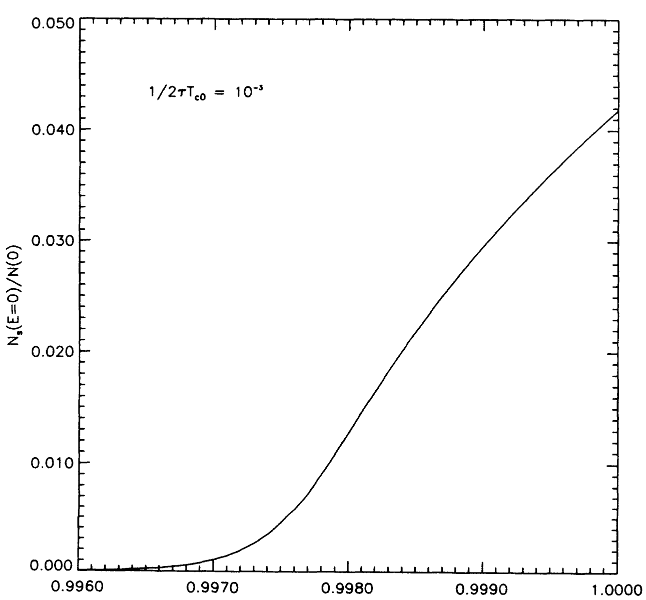

FIG. 4. Expanded version of Fig. 3, showing more detail at the $\sigma=1$ (unitarity limit) end of the graph. Note that a linear scale is now used for $N_s(E=0)$.

Varying an external variable such as the pressure would presumably lead to changes in the parameters such as v and $N(0)$, which could be reflected in drastic changes in $N_s(E)$.

IV. UNITARITY LIMIT

In this section we concentrate on the unitarity limit ($v\rightarrow\infty,\sigma\rightarrow1$). We show how to derive simple analytic expressions for $a_3(\varepsilon)$ and $N_s(E)$ which are valid at low energies. The impurity scattering is taken to be weak enough so that at small values of ε, $\tilde{\varepsilon}\ll\Delta$. To start, we note that as $v\rightarrow\infty$, Eq. (5) becomes

$$ia_3(\varepsilon)=\frac{c(\tilde{\varepsilon}^2+\Delta^2)^{1/2}}{2N(0)\tilde{\varepsilon}K[\Delta^2/(\tilde{\varepsilon}^2+\Delta^2)]} . \tag{12}$$

This equation is exact in the unitarity limit. We now make approximations suitable for $\tilde{\varepsilon}\ll\Delta$, to get

$$ia_3(\varepsilon)=\frac{c\Delta}{N(0)\tilde{\varepsilon}\ln(16\Delta^2/\tilde{\varepsilon}^2)} . \tag{13}$$

We can then derive a quadratic equation for $\tilde{\varepsilon}$, the solution of which yields

$$\tilde{\varepsilon}=\frac{\varepsilon}{2}+\sqrt{\varepsilon^2/4+c\Delta/N(0)\ln(16\Delta^2/\tilde{\varepsilon}^2)} . \tag{14}$$

Equation (14) is still not an explicit solution for $\tilde{\varepsilon}(\varepsilon)$, since $\tilde{\varepsilon}$ itself appears in the square root. To make progress we define γ as follows:

$$\gamma=ia_3(0)=\tilde{\varepsilon}(0) . \tag{15}$$

Note that γ is given by the solution of the following equation:[7,8]

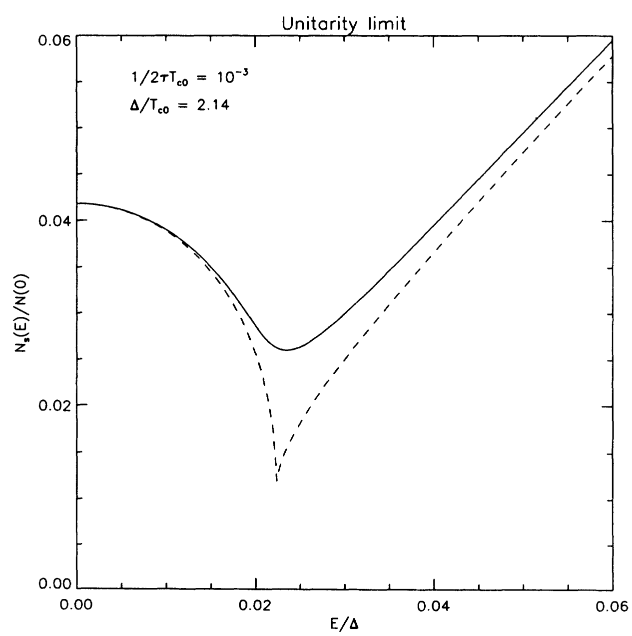

FIG. 5. Plot of $N_s(E)$ versus E for the unitarity limit, showing behavior at small E. Solid line is the exact result, while the dashed line shows the approximate formula, Eq. (18). We chose τ such that $1/2\tau T_{c0}=10^{-3}$.

$$\gamma^2=\frac{c\Delta}{2N(0)\ln(4\Delta/\gamma)} . \tag{16}$$

Then, as a first approximation to (14) we take as our solution[8]

$$\tilde{\varepsilon}=\frac{\varepsilon}{2}+\sqrt{\varepsilon^2/4+\gamma^2} . \tag{17}$$

We can use (17) to compute $N_s(E)$, by substituting it into (3) and (4). This gives the following:

$$N_s(E)=\begin{cases}\frac{N(0)}{\pi}\left[\sqrt{4\gamma^2/\Delta^2-E^2/\Delta^2}\ln\frac{4\Delta}{\gamma}+\frac{E}{\Delta}\left[\frac{\pi}{2}-\arccos(E/2\gamma)\right]\right], & E<2\gamma \\ \frac{N(0)}{2}[E/\Delta+\sqrt{E^2/\Delta^2-4\gamma^2/\Delta^2}], & E>2\gamma .\end{cases} \tag{18}$$

Figure 5 shows a comparison of the analytic formula (18) with the exact computed answer. As can be seen, the formula becomes exact at low enough energies, and does not do a bad job at energies somewhat greater than 2γ. The answer at $E=0$ is given by

$$N_s(E=0)=\frac{2N(0)}{\pi\Delta}\gamma\ln\frac{\Delta}{\gamma} , \tag{19}$$

which also correlates well with Fig. 4.

V. BORN LIMIT

In this section we discuss the Born limit ($\sigma\to 0$, τ constant); as in the previous section, we assume that τ is long enough so that at low energy we have $\tilde{\varepsilon}\ll\Delta$. Our equation for $a_3(\varepsilon)$ in the Born limit is given by

$$ia_3(\varepsilon)=\frac{\tilde{\varepsilon}}{\pi\tau[\tilde{\varepsilon}^2+\Delta^2]^{1/2}}K\left[\frac{\Delta^2}{\tilde{\varepsilon}^2+\Delta^2}\right] . \tag{20}$$

For small $\tilde{\varepsilon}$ ($\tilde{\varepsilon}\ll\Delta$) we approximate this as

$$ia_3(\varepsilon)=\frac{\tilde{\varepsilon}}{2\pi\tau\Delta}\ln\left[\frac{16\Delta^2}{\tilde{\varepsilon}^2}\right] . \tag{21}$$

Our implicit equation for $\tilde{\varepsilon}$ is then

$$\tilde{\varepsilon}(\varepsilon)=\varepsilon+\frac{\tilde{\varepsilon}}{2\pi\tau\Delta}\ln\left[\frac{16\Delta^2}{\tilde{\varepsilon}^2}\right] . \tag{22}$$

If we define the Born limit value of $\tilde{\varepsilon}(0)$ as β,

$$\beta\equiv\tilde{\varepsilon}(0)=ia_3(0) , \tag{23}$$

then Eq. (22) yields

$$\beta=4\Delta e^{-\pi\tau\Delta} . \tag{24}$$

We can see that when impurity scattering is not too strong, β will be an extremely small energy scale. For example, if $1/\tau\Delta=10^{-1}$, then $\beta/\Delta=4\times e^{-10\pi}=9\times 10^{-14}$. When β/Δ is very small, so is $N_s(E=0)$:[1,2]

$$N_s(E=0)=\frac{2N(0)\beta}{\pi\Delta}\ln\left[\frac{\Delta}{\beta}\right] . \tag{25}$$

It is difficult to formulate a simple analytic approximation which captures the behavior of $N_s(E)$ at very low energies and yet is accurate at the physically more important higher energies, of order $E\approx 10^{-2}\Delta$. So we present a derivation of a relatively simple formula for $N_s(E)$ which is accurate over a wide range of energy, but which misses the structure of $N_s(E)$ at small values of E. To start our derivation, we rewrite (22) as follows:

$$\tilde{\varepsilon}=\frac{\varepsilon}{1+(1/2\pi\tau\Delta)\ln(\tilde{\varepsilon}^2/16\Delta^2)} . \tag{26}$$

Now, if we simply replace $\tilde{\varepsilon}$ by $\tilde{\varepsilon}=\beta+(\pi\tau\Delta)\varepsilon$ on the right-hand side, this would give a formula for $\tilde{\varepsilon}(\varepsilon)$ which works for $\varepsilon\lesssim\beta$, but which fails at higher energy. So we follow a different path. As long as $1/\pi\tau\Delta$ is small, and as long as ε is large enough so that $\ln(\tilde{\varepsilon}/4\Delta)$ is not too large, then the second term in the denominator of (26) is a small perturbation. Under these conditions, we can obtain a very accurate answer by iterating (26) once, and then substituting for $\tilde{\varepsilon}$. Rather than simply replacing $\tilde{\varepsilon}$ by ε, it is more accurate to make the following substitution:

$$\tilde{\varepsilon}\to 4\Delta\left[\frac{\varepsilon}{4\Delta}\right]^{\pi\tau\Delta/(1+\pi\tau\Delta)} .$$

It can be seen from (22) that when $\tilde{\varepsilon}-\varepsilon$ is small, this substitution is quite good. Thus our approximate formula for $\tilde{\varepsilon}(\varepsilon)$ is

$$\tilde{\varepsilon}(\varepsilon)=\frac{\varepsilon}{1+[1/(1+\pi\tau\Delta)](1/2)\ln(\varepsilon^2/16\Delta^2)} . \tag{27}$$

We then note that Eqs. (3) and (5), in the Born limit, imply that the density of states is given in terms of $\tilde{\varepsilon}$ by the following equation:

$$N_s(E)=-2\tau N(0)\,\mathrm{Re}[\tilde{\varepsilon}(i\varepsilon\to E-i\eta)] . \tag{28}$$

Using the approximation (27) in the general formula (28) yields

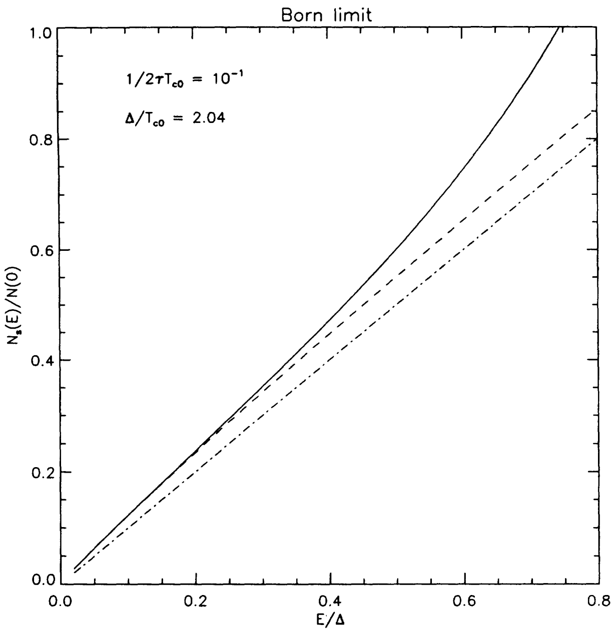

FIG. 6. Plot of $N_s(E)$ versus E for the Born limit. Solid line is the exact result, the dashed line represents the approximate formula Eq. (29), while the dashed-dot line plots E/Δ. We chose $1/2\tau T_{c0}=10^{-1}$.

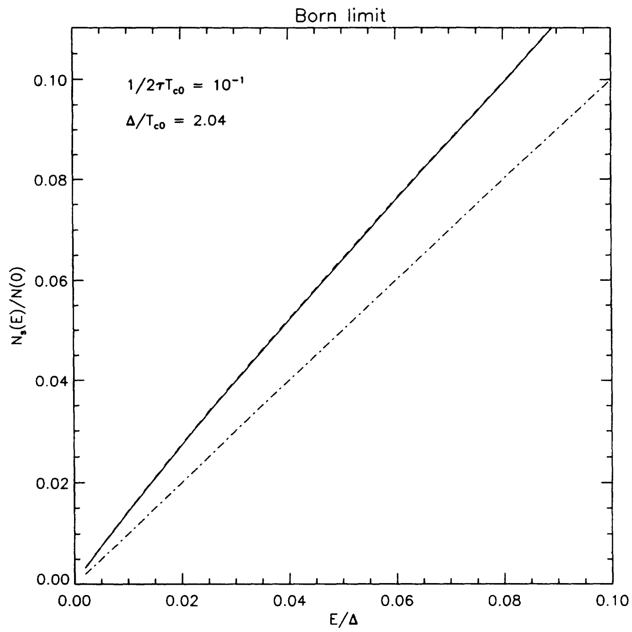

FIG. 7. Expanded version of Fig. 6, showing behavior at lower values of E. Note that the solid line (exact result) and the dashed line [Eq. (29)] are in complete agreement.

$$N_s(E)=\frac{\pi\tau}{1+\pi\tau\Delta}\,\frac{N(0)E}{\{1+[1/(1+\pi\tau\Delta)]\ln(E/4\Delta)\}^2+\{[1/(1+\pi\tau\Delta)](\pi/2)\}^2}\ . \tag{29}$$

As long as $1/\tau\Delta$ is not too large, Eq. (29) is very accurate over a wide range of energies. Figures (6) and (7) show a comparison between the exact $N_s(E)$ and the above approximation; even for quite strong impurity scattering ($1/2\tau T_{c0}=10^{-1}$), the approximate formula does very well for $E/\Delta \lesssim 0.2$. In the same figures we also plot E/Δ, which is the low-energy, pure limit answer for $N_s(E)/N(0)$.

ACKNOWLEDGMENTS

We thank Tom Lemberger for stimulating discussions. This work was supported by the DOE Grant No. DE-FG02-90ER45427 through the Midwest Superconductivity Consortium.

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