Magnetic field effects on the density of states of orthorhombic superconductors

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Abstract

The quasiparticle density of states in a two-dimensional $d$-wave superconductor depends on the orientation of the in-plane external magnetic field $H$. This is because, in the region of the gap nodes, the Doppler shift due to the circulating supercurrents around a vortex core depend on the direction of $H$. For a tetragonal system the induced pattern is four-fold symmetric and, at zero energy, the density of states exhibits minima along the node directions. But $\text{YBa}_2\text{C}_3\text{O}_{6.95}$ is orthorhombic because of the chains and the pattern becomes two-fold symmetric with the position of the minima occurring when $H$ is oriented along the Fermi velocity at a node on the Fermi surface. The effect of impurity scattering in the Born and unitary limit are discussed.

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I. INTRODUCTION

It has become increasingly clear that including the circulating supercurrents outside the vortex core in a $d$-wave superconductor can lead to a qualitative understanding - in the low magnetic field limit, near $H_{c1}$ - of the effect of a magnetic field $\mathbf{H}$ on various properties of a superconductor in the vortex state. The $\sqrt{H}$ dependence of the specific heat predicted by Volovik\cite{Volovik92, Volovik93} and Kopnin and Volovik\cite{Kopnin94, Volovik95} was verified experimentally\cite{Veretin92, Veretin93, Veretin94}. A detailed analysis of the data for $\mathbf{H}$ oriented perpendicular to the CuO$_2$ planes including impurity scattering was given by Kübert and Hirschfeld\cite{Kuebert95} (see also Barash et al.\cite{Barash96}). Transport properties were considered by Kübert and Hirschfeld\cite{Kuebert96} Subsequently the analysis has been extended by Hirschfeld\cite{Hirschfeld97} to include the field $\mathbf{H}$ in the CuO$_2$ plane and he demonstrated a four-fold symmetry in the electronic thermal conductivity. Very recently results have been obtained by Vekhter et al.\cite{Vekhter98, Vekhter99} for the effect of an in-plane magnetic field on the quasiparticle density of states (QDOS) in a tetragonal two dimensional $d$-wave superconductor. The present work extends this previous study to the orthorhombic $d$-wave case and also includes in the calculations the effect of impurity scattering in both, Born’s and resonant scattering limits.

While most high $T_c$ oxides are tetragonal, YBa$_2$Cu$_3$O$_{6.95}$ (YBCO), which is perhaps the most extensively studied of all the oxides, is orthorhombic because its crystal structure includes CuO chains oriented along the $b$-axis, as well as two CuO$_2$ planes per unit cell. Optical measurements reveal that the carrier density in the chains in optimally doped YBCO is of the same order of magnitude as it is in the planes and the ratio of the associated $b$- to $a$-direction plasma frequency is of the order of 2\cite{Optical90}. Similar large in-plane anisotropies are observed in the infrared optical conductivity\cite{Infrared90}, d.c. resistivity\cite{Resistivity90} zero temperature penetration depth\cite{Penetration90} and thermal conductivity\cite{Thermal90}.

Various approaches have been taken to treat band anisotropy including a single tight binding band with different nearest neighbor hopping in $a$- and $b$-direction\cite{Single90, Single91} two band\cite{Two90, Two91} as well as three band\cite{Three90, Three91} models which include the single CuO chain layer as well as two CuO$_2$ plane layers per unit cell with transverse hopping between them. All these models give the same qualitative features and describe reasonably well the $a-b$ band anisotropy.
of YBCO. Additionally, in an orthorhombic structure the superconducting gap will be a mixture\(^3\) of dominant \(d_{x^2-y^2}\) symmetry as well as subdominant \(s_0\) and \(s_{x^2+y^2}\) symmetric functions because they all belong to the same irreducible representation of the \(C_{2v}\) crystal point group.

The simplest approach which contains the physics of the more complex calculations is a single infinite band with distinct effective masses along the \(a\) \((m_a)\) and \(b\) \((m_b)\) directions\(^3\)\(^4\) with a \((d + s)\)-symmetric gap function on the cylindrical Fermi surface\(^4\)\(^5\). For simplicity we will adopt throughout this paper this approach and calculate the effect of an in-plane magnetic field \(H\) on the QDOS assuming a distribution of non overlapping vortex cores and account only for the circulating supercurrents around the vortices. We will also treat the effect of impurities in both, Born’s and resonant scattering limits. Impurities were not considered in the previous calculations in tetragonal symmetry by Vekhter \textit{et al.}\(^6\)\(^7\) which were confined to the pure limit. Thus, our results with impurities in the tetragonal case are the first such results.

II. FORMALISM

We begin with a single free electron band in two dimensions with an ellipsoidal Fermi surface and the single particle energy \(\varepsilon_k\) in the normal state given by the dispersion relation \((\hbar = 1)\)

\[
\varepsilon_k = \frac{k_x^2}{2m_x} + \frac{k_y^2}{2m_y} - \varepsilon_F \tag{1}
\]

where \(k = (k_x, k_y)\) is the momentum vector and \(\varepsilon_F\) the Fermi energy. In Eq. (1) \(m_x\) and \(m_y\) are effective masses with \(m_x > m_y\), \textit{i.e.}\ chains are along the \(k_y\)-axis which increases the electronic transport in that direction. A parameter

\[
\alpha = \frac{m_x - m_y}{m_x + m_y} \tag{2}
\]

is introduced and this is the single parameter which characterizes the band structure anisotropy in our simple model. Consistent with the above assumption for the energy band
dispersion relation is a mixed \((d + s)\)-symmetric gap on the Fermi surface (an ellipse) of the form
\[
\Delta_k = \Delta_0 \left( \cos 2\varphi + s \right), \tag{3}
\]
with \(\Delta_0\) the gap amplitude. In Eq. (3) \(\varphi\) is a polar angle measured from the \(k_x\)-axis in the two dimensional copper oxide Brillouin zone giving the angle of \(k\) (momentum on the Fermi surface) as shown in Fig. 1. The first term in Eq. (3) gives the dominant \(d\)-wave part of the gap which, on its own, would have nodes on the main diagonal at \(\varphi = \pm \pi/4\). The number \(s\) is a measure of the subdominant \(s\)-wave part. Both parts are allowed to exist in an orthorhombic system such as YBCO from group theoretical considerations. The \(s\)-component moves the nodes from \(\varphi = \pm \pi/4\) to \(\varphi = \tan^{-1} \sqrt{(1 + s)/(1 - s)}\) off the main diagonal of the Brillouin zone. For positive values of \(s\) the critical \(\varphi\) defining the node is larger than \(\pi/4\) while the opposite holds for negative values of \(s\).

In order to work with Eqs. (1) and (3) it is convenient to transform to new coordinates \(p = (p_x, p_y)\) in which the Fermi surface is a circle (see Fig. 1). The required transformation is given by
\[
p_i = k_i \sqrt{\frac{m_x + m_y}{2m_i}}, \quad i = x, y \tag{4}
\]
which leads to (Fig. 1)
\[
\tan \phi = \sqrt{\frac{m_y}{m_x}} \tan \varphi, \tag{5}
\]
where \(\phi\) is now the angle of the momentum vector \(p\) in the transformed frame. Clearly, the electron dispersion relation (1) reduces to
\[
\varepsilon_F = \frac{p_{F,x}^2 + p_{F,y}^2}{2\bar{m}} = \frac{p_{F}^2}{2\bar{m}}, \tag{6}
\]
with \(\bar{m} = (m_x + m_y)/2\) the average band mass. Applying the same transformation to the gap (3) gives the order parameter in the \(p\)-frame
\[
\Delta_p = \Delta_0 \left( \frac{\alpha + \cos 2\phi}{1 + \alpha \cos 2\phi} + s \right) \equiv \Delta_0 f(\phi). \tag{7}
\]
We show in Fig. 2 the gap $\Delta_p$ in the $p$-frame for several values of $\alpha$ (the band anisotropy) and $s$ (the gap anisotropy). Frame (a) is for $\alpha = 0$ and $s = 0$ and is the well known pure $d$-wave case for which plus and minus lobes have equal absolute magnitude and the zeros are on the diagonal. In frame (b) $\alpha = 0.4$ and $s = 0$, i.e. the gap in the $k$-frame (laboratory frame) is of pure $d$-wave symmetry but the band structure orthorhombicity leads to a transformed gap with larger positive than negative lobes and the nodes are shifted upwards from $\pm \pi/4$ and similarly for the other symmetry related angles. This trend is even more pronounced in frame (c) where $\alpha = s = 0.4$. In this case $\alpha$ and $s$ add constructively to further increase the positive lobes as compared to the negative ones, and the nodes are shifted to yet larger angles. Finally, frame (d) applies to $\alpha = 0.4$ and $s = -0.4$. For this set of parameters the nodes in the $p$-frame remain on the diagonal but at the same time the negative lobes are dominant over the positive ones. We conclude that a negative value for $s$ can in some sense counteract some of the effects of a positive $\alpha$, but there is no complete cancelation between these two parameters which play quite distinctive roles. The nodes can be made to remain unshifted but the size of the lobes is changed over their $\alpha = s = 0$ values.

In the laboratory frame ($k$, before transformation) the thermodynamic Green’s function takes on the form

$$G(k, \omega_n; r) = \frac{\left(i\omega_n - v_F(k)q_s\right)\tau_0 + \varepsilon_k\tau_3 + \Delta_k\tau_1}{(\omega_n + i v_F(k)q_s)^2 + \varepsilon_k^2 + \Delta_k^2},$$

with $\varepsilon_k$ and $\Delta_k$ given by Eqs. (1) and (3) respectively. In Eq. (8) the $\tau$’s are Pauli $2 \times 2$ matrices and $i\omega_n$ is the $n$’th Matsubara frequency, $\omega_n = (2n + 1)\pi T, n = 0, \pm 1, \pm 2, \ldots$, and $T$ is the temperature. The Doppler shift caused by the presence of circulating supercurrents outside the vortex core (the region which we assume to dominate the physics) is given by $v_F(k)q_s$, where $v_F(k)$ is the electron Fermi velocity on the ellipsoidal Fermi surface in $k$-space (see Fig. 1) and which is given by

$$v_F(k) = \nabla_k\varepsilon_k = \frac{k_{F,x}}{m_x}\hat{x} + \frac{k_{F,y}}{m_y}\hat{y},$$

with $\hat{x}$ and $\hat{y}$ unity vectors in the direction of the $k_x$- and $k_y$-axis. Applying the transformation (4) to get $v_F(k)$ in the $p$-frame leads to
\[ v_F(p) = \frac{1}{\sqrt{m}} \left( \frac{p_{F,x}}{\sqrt{m_x}} \hat{x} + \frac{p_{F,y}}{\sqrt{m_y}} \hat{y} \right). \]  

(10)

The momentum of the superfluid currents outside the vortex core (placed at the position \( \mathbf{r} = 0 \) in the laboratory frame) is assumed to be inversely proportional to the distance \(|\mathbf{r}| = r\) from the core. For a magnetic field \( \mathbf{H} \) in the CuO\(_2\) plane making an angle \( \gamma \) with the \( k_x \)-axis the supercurrents are in a plane perpendicular to \( \mathbf{H} \) and therefore to the \( k_x-k_y \) plane. Assuming circular supercurrents, an approximation discussed in the paper by Vekhter et al.,\(^{12}\) and denoting the vortex winding angle by \( \beta \) one obtains for the \( x \) and \( y \) component of the superfluid momentum \( \mathbf{q}_s \)

\[
\begin{align*}
q_{s,x} &= -|\mathbf{q}_s| \sin \beta \sin \gamma, \\
q_{s,y} &= -|\mathbf{q}_s| \sin \beta \cos \gamma,
\end{align*}
\]  

(11)

so that

\[
v_F(p)\mathbf{q}_s = \frac{p_F}{m_x}|\mathbf{q}_s| \sin \beta \sqrt{1 + \alpha} \left( \sqrt{\frac{1 + \alpha}{1 - \alpha}} \sin \phi \cos \gamma - \cos \phi \sin \gamma \right).
\]  

(12)

If one measures the distance \( r \) in units of the intervortex distance \( R = a^{-1} \sqrt{\frac{\phi_0}{\pi H}} \), where \( \phi_0 \) is the flux quantum and \( a \) a constant of the order of unity, we obtain

\[
v_F(p)\mathbf{q}_s = \frac{E_H}{\rho} \sin \beta \sqrt{1 + \alpha} \left( \sqrt{\frac{1 + \alpha}{1 - \alpha}} \sin \phi \cos \gamma - \cos \phi \sin \gamma \right),
\]  

(13)

with the normalized distance \( \rho = r/R \) and the magnetic energy

\[
E_H = \frac{a}{2} \bar{v}_F \sqrt{\frac{\pi H}{\phi_0}} = \nu \Delta_0,
\]  

(14)

with \( \bar{v}_F \) a suitably defined effective Fermi velocity which can also be made to contain the additional band factor \( \sqrt{1 + \alpha} \) of Eq. (13) and \( \nu \) is a parameter which measures the magnetic energy \( E_H \) in units of the gap. Consequently, we can write

\[
v_F(p)\mathbf{q}_s = \frac{E_H}{\rho} \hbar(\phi, \gamma) \sin \beta,
\]  

(15)

with
\[ h(\phi, \gamma) = \sqrt{\frac{1 + \alpha}{1 - \alpha}} \sin \phi \cos \gamma - \cos \phi \sin \gamma. \] (16)

The QDOS at zero frequency obtained from the Green’s function (8) which includes the circulating supercurrents about the vortex core and which must also be averaged over the vortex unit cell is given by

\[ N(0, \gamma) = \frac{2\pi}{2\pi} \int_0^{2\pi} d\phi \frac{2\pi}{\pi} \int_0^R dr \int_0^{\pi R} \Re \begin{pmatrix} \frac{|v_F(p)q_s|}{\sqrt{(v_F(p)q_s)^2 - \Delta^2}} \\ \sqrt{\Delta^2} f(\phi) \end{pmatrix}. \] (17)

By the square root is meant that branch of the complex function which corresponds to a positive imaginary part. Eq. (17) can be reduced to an one dimensional integral form

\[ N(0, \gamma) = \frac{1}{2\pi} \int_0^{2\pi} d\phi \min \left(1, \frac{\nu^2|h(\phi, \gamma)|^2}{f^2(\phi)}\right). \] (18)

One good approximation to this integral is obtained by noting that the integrand in Eq. (18) is dominated by the nodal region and, thus, we get approximately

\[ N(0, \gamma) \simeq 2 \frac{\nu}{\pi} \sum_{\text{nodes}} \left| h(\phi_n, \gamma) \right|, \] (19)

where the \( \phi_n \) are the nodes of the transformed gap (7) and \( f'(\phi_n) \) is the derivative of this gap function at its nodes. These can be found at

\[ \tan \phi_n = \pm \sqrt{\frac{(1 + \alpha)(1 + s)}{(1 - \alpha)(1 - s)}}, \] (20)

while in the laboratory frame, as we have noted before, the gap has its nodes at \( \tan \varphi_n = \pm \sqrt{(1 + s)/(1 - s)} \). Furthermore, the derivative \( f'(\phi_n) \) at the gap nodes can be worked out to be

\[ f'(\phi_n) = 2(1 + s) \sqrt{(1 - s^2)(1 - \alpha^2)}, \] (21)

and hence an approximation for \( N(0, \gamma) \) follows from Eqs. (18), (21) and the definition of \( h(\phi, \gamma) \) given in Eq. (15) as

\[ N(0, \gamma) = \frac{\nu}{\pi} \sum_{\text{nodes}} \left| \sqrt{\frac{1 + \alpha}{1 - \alpha}} \sin \phi_n \cos \gamma - \cos \phi_n \sin \gamma \right| \] (22)
with distinct contributions from only two of the four nodes.

For one set of two nodes we get

\[
\begin{align*}
\cos \phi_n &= \sqrt{\frac{1}{2} \frac{1 - \alpha(1 - s)}{1 + \alpha s}}, \\
\sin \phi_n &= \sqrt{\frac{1}{2} \frac{1 + \alpha(1 + s)}{1 + \alpha s}},
\end{align*}
\]

while for the other ones \( \phi_n \to \pi - \phi_n \). We therefore arrive at the approximate analytic expression

\[
N(0, \gamma) = \frac{\sqrt{2} \nu}{\pi} \frac{1}{\sqrt{(1 - s^2)(1 - \alpha^2)}} \frac{1}{1 + s} \sqrt{\frac{1 + \alpha}{1 - \alpha}} \\
\times \left\{ (1 + \alpha) \sqrt{\frac{1 + s}{1 + \alpha s}} \cos \gamma - (1 - \alpha) \sqrt{\frac{1 - s}{1 + \alpha s}} \sin \gamma \right\} \\
+ \left\{ (1 + \alpha) \sqrt{\frac{1 + s}{1 + \alpha s}} \cos \gamma + (1 - \alpha) \sqrt{\frac{1 - s}{1 + \alpha s}} \sin \gamma \right\}
\]

\[
= \frac{2\sqrt{2} \nu}{\pi} \frac{1}{\sqrt{(1 - s^2)(1 - \alpha^2)}} \frac{1}{1 + s} \sqrt{\frac{1 + \alpha}{1 - \alpha}} \\
\times \max \left( \left| (1 + \alpha) \sqrt{\frac{1 + s}{1 + \alpha s}} \cos \gamma \right|, \left| (1 - \alpha) \sqrt{\frac{1 - s}{1 + \alpha s}} \sin \gamma \right| \right),
\]

where we have restored factors previously absorbed in the magnetic energy \( E_H \) that appeared explicitly in Eq. (13). In the tetragonal, pure \( d \)-wave case (\( \alpha = s = 0 \)) expression (24) reduces properly to the known result

\[
N(0, \gamma) = \frac{2\sqrt{2} \nu}{\pi} \max (| \sin \gamma |, | \cos \gamma |),
\]

in which case Eq. (24) is known to be an excellent approximation to the one dimensional integral of Eq. (18).

When band anisotropy is included through a finite value of \( \alpha \) or a subdominant \( s \)-wave part, characterized by the parameter \( s \), the analytic expression (24) is not quite as good an approximation as (25) was but it is still acceptable as can be seen in Fig. 3. In this figure we compare with our exact numerical results for \( N(0, \gamma) \) based on the one dimensional integral of Eq. (18). Here only band anisotropy is included with an effective mass anisotropy parameter
\( \alpha = 0.2 \). The dashed line is the exact result \( [13] \), the solid line is based on Eq. \( [24] \). The agreement is good. Note the two-fold symmetry in the pattern obtained, although, since \( s = 0 \), the gap in the laboratory frame has pure \( d \)-wave symmetry with nodes on the main diagonal. It is the band anisotropy that breaks the four-fold symmetry of the tetragonal case. However, it is very important to realize that because of \( \alpha \neq 0 \), i.e. band orthorhombicity, the sharp kinks in the curve for \( N(0, \gamma) \) vs. \( \gamma \) no longer fall at the position of the nodes. This would be the case in a tetragonal system but is not so for the ellipsoidal Fermi surface of Fig. 1. We see from Eq. \( [24] \) that the kink occurs at a critical angle \( \gamma_c \) given by (note that \( s = 0 \)):

\[
\tan \gamma_c = \frac{1 + \alpha}{1 - \alpha},
\]

which is \( \pi/4 \) only for the case \( \alpha = 0 \) (no anisotropy in the electronic band structure). This is an important result because it is often believed that the sharp structure in \( N(0, \gamma) \) as a function of \( \gamma \) - the magnetic field orientation - gives the position of the nodes. This is not true when band anisotropy exists.

The geometry of the situation is shown in Fig. 1 which depicts the laboratory frame while the result \( [24] \) was obtained in the transformed, \( p \)-frame where the Fermi surface is a circle. In this figure \( \mathbf{k}_n \) gives the position of a gap node on the ellipsoidal Fermi surface \( \varepsilon_k = 0 \), in Eq. \( [1] \). The Fermi velocity at that point, \( \mathbf{v}_F(\mathbf{k}_n) \), points in the direction \( \tan^{-1} \left( \frac{1 + \alpha}{1 - \alpha} \tan \varphi \right) \). If the magnetic field \( \mathbf{H} \) is placed in that direction the circulating supercurrents will be in a plane perpendicular to the two dimensional Brillouin zone and oriented along the tangent to the Fermi surface at \( \mathbf{k} = \mathbf{k}_n \) as shown in the figure by the thick shaded line. Thus, there will be no Doppler shift. In the laboratory frame \( \tan \varphi = \sqrt{(1 + s)/(1 - s)} \) from Eq. \( (3) \) and we get immediately the result

\[
\tan \gamma_c = \frac{1 + \alpha}{1 - \alpha} \sqrt{\frac{1 + s}{1 - s}},
\]

for a finite subdominant \( s \)-wave part to the gap. This same result follows from Eq. \( [24] \) when the expression in the absolute value switches sign. For finite values of \( s \), the angle \( \gamma_c \) coincides with the position of the nodes in the \((d + s)\)-symmetric gap in the laboratory
frame only if $\alpha = 0$. We can also see from (27) that a negative value of the subdominant $s$-wave part (i.e. a negative value of $s$) partially compensates for the effect of $\alpha$ but does not cancel it out completely.

In Fig. 5 we show further results for the zero frequency QDOS $N(0, \gamma)$ as a function of magnetic field orientation $\gamma$ for increasingly anisotropic bands. The parameter $\alpha$ is increased from 0.2 in the solid curve to 0.4 (dashed curve), 0.6 (dotted curve), and 0.8 (dashed-dotted curve). It is clear that the amplitude of the predicted oscillations in the QDOS increases considerably with increasing effective mass anisotropy ($\alpha$) and that consequently this anisotropy will be easier to detect as the orthorhombicity of the band structure increases, i.e. as $\alpha$ increases. There is nearly a factor of 6 between the value at minimum and at maximum in the dashed-dotted curve. The pattern of oscillation is also changed as $\alpha$ increases. The intermediate secondary maximum, around $\gamma = 1.5\, \text{rad}$ in the solid curve, is not present any longer in the dashed-dotted curve. Instead there is a minimum.

A fit to data of the form (24) could in principle yield information on the two most important parameters $\alpha$ and $s$ but the position of the sharp structure in the QDOS by itself does not give directly the position of the nodes or the ratio of the subdominant $s$-wave admixture to the dominant $d$-wave component. It is the direction of $H$ giving no Doppler shift which determines the position of the minimum in $N(0, \gamma)$. Before leaving Eq. (24) we note that $N(0, \gamma)$ is proportional to $\nu = E_H/\Delta_0$ and this is the same dependence on the magnetic field as has been found in the tetragonal case. There is no explicit change in this quantity due to anisotropy so that the scaling variable for the QDOS and for the specific heat stays unchanged. This holds for the pure case but will be modified when disorder is considered. In that case scaling breaks down and specific details play a role.

The finite frequency QDOS in a pure orthorhombic superconductor with a $(d + s)$-symmetric gap is also of interest. It follows from the formula

$$
N(\omega, \gamma) = \frac{2\pi}{\rho} \int_0^1 dp \int_0^{2\pi} d\phi \frac{2\pi}{\rho} \Re \left\{ \frac{\tilde{\omega}(\omega) - v_F(p)q_s}{\sqrt{(\tilde{\omega}(\omega) - v_F(p)q_s)^2 - \Delta_{d+s}^2(\omega, \phi)}} \right\},
$$

(28)

which has been written in a form which remains valid even when impurity scattering is included. Here $\rho = r/R$. For the pure case $\tilde{\omega}(\omega) = \omega$ and $\Delta_{d+s}(\omega, \phi) = \Delta_0 f(\phi)$. Results of
the numerical evaluation of Eq. (28) (an approximate analytic formula similar to Eq. (24) can also be derived but is not given here as it has the same form as already presented in the work of Vekhter et al.\textsuperscript{12,13}) gives the results shown in Fig. 6 for four directions of the magnetic field. Here we present numerical results for \( N(\omega, \gamma) \) as a function of \( \omega/\Delta_0 \) for \( \alpha = 0.2 \) and \( \nu = 0.3 \). For the magnetic field in the direction of \( \gamma = 0^\circ \) (antinodal direction in pure \( d \)-wave) the solid curve applies and an \( \omega^2 \) behavior is obtained at small \( \omega \), just as in the tetragonal case.\textsuperscript{14,15} But the linear dependence expected in the nodal direction in the tetragonal case now occurs in some other direction where the Doppler shift at the nodal position is zero, namely at \( \gamma_c \) as defined by Eq. (27) which is where the superfluid momentum \( \mathbf{q}_s \) is perpendicular to the Fermi velocity. For \( \alpha = 0.2, \gamma_c \simeq 56^\circ \) the dashed-dotted curve indeed displays linear dependence.

### III. IMPURITY EFFECTS

We now include in the calculations elastic impurity scattering. In this case the full self consistent Green’s function (8) enters the impurity term and we need to solve two coupled equations, one for the renormalized Matsubara frequency \( \tilde{\omega}(\omega) \) and the other one for the gap \( \tilde{\Delta}_{d+s}(\omega, \phi) \). On the real frequency axis they are:

\[
\begin{align*}
\tilde{\omega}(\rho, \beta, \omega) &= \omega + i\pi t^+ \Omega(\rho, \beta, \omega), \\
\tilde{\Delta}_{d+s}(\rho, \beta, \omega, \phi) &= \Delta_{d+s}(\phi) + i\pi t^+ D(\rho, \beta, \omega),
\end{align*}
\]

with \( \Delta_{d+s}(\phi) = \Delta_p \) of Eq. (7), the pure system gap in the transformed frame. Here \( \rho \) and \( \beta \) are associated with the vortex and \( \phi \) is the polar angle defining the direction of \( \mathbf{p} \). The use of Eqs. (29) confines our analysis to low temperatures where the temperature dependence of the gap function can be neglected. Moreover, these equations are only valid in Born’s approximation, or weak impurity scattering limit. A slightly more complicated set of equations needs to be solved in the unitary limit (strong impurity scattering), namely

\[
\tilde{\omega}(\rho, \beta, \omega) = \omega + i\pi \Gamma^+ \frac{\Omega(\rho, \beta, \omega)}{\Omega^2(\rho, \beta, \omega) + D^2(\rho, \beta, \omega)},
\]

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\[ \tilde{\Delta}_{d+s}(\rho, \beta, \omega, \phi) = \Delta_{d+s}(\phi) + i\pi \Gamma^+ \frac{D(\rho, \beta, \omega)}{\Omega^2(\rho, \beta, \omega) + D^2(\rho, \beta, \omega)}. \]  

(30b)

In the tetragonal case \((\alpha = 0)\), also considered here, the symmetry is described by the C\(_{4v}\) point group and the \((d + is)\)-symmetry of the order parameter is the only possible mixed symmetry allowed under the symmetry operations of this group. In this case Eqs. (29b) and (30b) are to be modified to give

\[ \tilde{\Delta}_s(\rho, \beta, \omega) = \Delta_s + i\pi t^+ D(\rho, \beta, \omega), \]  

(31)

in Born’s limit and

\[ \tilde{\Delta}_s(\rho, \beta, \omega) = \Delta_s + i\pi \Gamma^+ \frac{D(\rho, \beta, \omega)}{\Omega^2(\rho, \beta, \omega) + D^2(\rho, \beta, \omega)}. \]  

(32)

in the resonant scattering limit. \(\Delta_s\) is the s-wave contribution to the order parameter in the clean limit and is equal to zero in pure d-wave symmetry. The renormalized gap function is then written as:

\[ \tilde{\Delta}_{d+is}(\rho, \beta, \omega, \phi) = \Delta_d(\phi) + i\tilde{\Delta}_s(\rho, \beta, \omega). \]  

(33)

Finally, the functions \(D(\rho, \beta, \omega)\) and \(\Omega(\rho, \beta, \omega)\) are defined as

\[ \Omega(\rho, \beta, \omega) = \begin{cases} \frac{\tilde{\omega}(\rho, \beta, \omega) - v_F(p)q_s}{\sqrt{(\tilde{\omega}(\rho, \beta, \omega) - v_F(p)q_s)^2 - \tilde{\Delta}_{d+s}(\rho, \beta, \omega, \phi)^2} } \phi & \text{orthorhombic,} \\
\frac{\tilde{\omega}(\rho, \beta, \omega) - v_F(p)q_s}{\sqrt{(\tilde{\omega}(\rho, \beta, \omega) - v_F(p)q_s)^2 - \Delta_{d+s}(\rho, \beta, \omega, \phi)^2} } \phi & \text{tetragonal,} \end{cases} \]  

(34a)

\[ D(\rho, \beta, \omega) = \begin{cases} \frac{\tilde{\Delta}_{d+s}(\rho, \beta, \omega, \phi)}{\sqrt{(\tilde{\omega}(\rho, \beta, \omega) - v_F(p)q_s)^2 - \Delta_{d+s}(\rho, \beta, \omega, \phi)^2} } \phi & \text{orthorhombic,} \\
\frac{\tilde{\Delta}_s(\rho, \beta, \omega)}{\sqrt{(\tilde{\omega}(\rho, \beta, \omega) - v_F(p)q_s)^2 - \Delta_s^2(\rho, \beta, \omega) - \Delta_d^2(\phi) } \phi & \text{tetragonal,} \end{cases} \]  

(34b)

with \(\langle \cdots \rangle\phi\) the Fermi surface average in the \(p\)-frame. Finally, Eq. (28) still applies for the QDOS and it is only at this later stage that an average over vortex variables is carried out. Eqs. (29) or (30) need to be solved self consistently for different values of \(\rho, \beta,\) and \(\omega\). The two remaining parameters are \(t^+\) or \(\Gamma^+\) which are related to the strength of impurity scattering in the normal state where \(\pi t^+ = \pi \Gamma^+ = 1/2 \tau_{imp}\) and \(\tau_{imp}\) is the impurity scattering
time in the normal state. It should also be noted at this point that the impurity scattering potential in the laboratory frame is now anisotropic. The role of anisotropic impurity scattering in anisotropic superconductors has been studied by Haran and Nagi. According to their results the influence of the impurity concentration on superconductivity varies with the anisotropy of the scattering potential, qualitative changes in, say the temperature dependence of the penetration depth or the energy dependence of the optical conductivity, cannot be expected.

A first result with impurities is given in Fig. 7 for Born scattering with $t^+ = E_H/16$ in a tetragonal system with a pure $d$-wave gap. Here, $\Delta_0 = 24$ meV, $\nu = 0.1$, and what is plotted is the zero frequency value of the QDOS, $N(0, \gamma)$, as a function of the orientation of the in-plane magnetic field $\mathbf{H}$ which makes an angle $\gamma$ with the $\hat{x}$-axis. The solid line includes impurities and is compared with the dotted line for the pure case. We note that the minima are somewhat filled and rounded by the impurities as we might have expected and the maxima are slightly higher and broader. Impurities increase the QDOS in the low energy region. Close examination of the two curves also shows that they both have four-fold symmetry. This is to be expected, but it is pointed out that, even for a tetragonal system, the introduction of impurities introduces a finite $s$-wave component to the gap, which is now of $(d + is)$-symmetry, in Eqs. (31) or (32) because it is the self consistent Green’s function that enters the definition of (34) and this leads to a nonzero value of $D(\rho, \beta, \omega)$. Our final result remains four-fold symmetric, i.e. it retains the full tetragonal symmetry.

The effect of impurity scattering is much larger in the unitary limit. Results are shown in Fig. 8. Again the underlying system has tetragonal symmetry and a pure $d$-wave gap. The impurity scattering parameter is $\Gamma^+ = E_H/16$ with a gap amplitude $\Delta_0 = 24$ meV and $\nu = E_H/\Delta_0 = 0.1$ in Eqs. (30). The solid line represents our results for the value of the QDOS $N(0, \gamma)$ as a function of the magnetic field orientation $\gamma$ in the CuO$_2$ plane. Notice the scale on the vertical axis and that the size of $N(0, \gamma)$ is roughly three times its value for the Born limit (Fig. 7). This changes quite a lot when the frequency is increased. The dashed curve applies to $\omega/\Delta_0 = 0.05$, the dotted one to $\omega/\Delta_0 = 0.1$, and the dashed-dotted
one to $\omega/\Delta_0 = 0.15$. The percent anisotropy in the QDOS is reduced with increasing $\omega$.

Results for the orthorhombic case are shown in Figs. 9 and 10. In these figures $\nu = E_H/\Delta_0 = 0.1$, the band anisotropy $\alpha = 0.41$, and the $s$-wave admixture to the gap is characterized by $s = -0.25$ taken from a previous fit to experimental data in YBCO as discussed by Wu et al.\textsuperscript{32} and Schürrer et al.\textsuperscript{33} Reasonable values for the parameters in our admittedly simplified band structure model, namely $\alpha = (m_x - m_y)/(m_x + m_y)$ and the gap anisotropy, namely $s$, can be set in comparison with penetration depth data on YBCO at optimum doping. The measured ratio of the zero temperature penetration depth depends on the anisotropic effective masses and sets the value of $\alpha = 0.41$ which follows from $\lambda_a/\lambda_b = 1600\,\AA/1030\,\AA$.\textsuperscript{33,35,36,38} Furthermore, in our model the low temperature slopes of the penetration depth are approximated by

$$\frac{d\lambda_{xx}}{dT} \simeq \frac{2\ln(2)}{\Delta_0}(1 - \alpha - s),$$

$$\frac{d\lambda_{yy}}{dT} \simeq \frac{2\ln(2)}{\Delta_0}(1 + \alpha + s).$$

The experiments of Bonn et al.\textsuperscript{38} give $s = -0.25$ as an estimate of the orthorhombicity in the gap. It is these values that we have used to estimate the expected anisotropy in the QDOS for $\mathbf{H}$ in the CuO$_2$ plane. As we have already stressed in the introduction, the band structure in YBCO is much more complex than the model treated here but the simplicity of our model allows us to get insight into the role of orthorhombicity and develop a qualitative picture of its effect. There are no adjustable parameters left.

For the orthorhombic case the pattern in Fig. 9 for $N(0, \gamma)$ vs. $\gamma$ is two-fold symmetric even in the pure case. As before, Born scattering (solid curve with $t^+ = E_H/16$) simply smooths out slightly the minima seen in the pure case curve (dotted line). On the other hand, unitary scattering, solid gray curve for $\Gamma^+ = E_H/16$, pushes the curve up by a factor of about two over the pure limit case and the pattern is also significantly modified and smoother. The small maxima around $\gamma = 1.5\,\text{rad}$ and symmetry related points in the pure curve (dotted) are completely washed out by unitary impurity scattering. The amplitude of the variations in value of $N(0, \gamma)$ is also considerably reduced.

The curves described so far apply to untwinned single crystals. Three more curves are
shown in Fig. 9. The dashed-dotted curve applies to the case of twinned samples and was obtained from the clean limit (dotted curve) by averaging it with a similar curve displaced by 90°. This corresponds to a simple average of equal numbers of twins with \( \hat{x} \)- and \( \hat{y} \)-axis interchanged. It is clear that this average greatly reduces the predicted anisotropy and experiments aimed at discovering this anisotropy are best made on untwinned samples. This is confirmed in preliminary data from Junod’s group who indeed find no significant in-plane anisotropy in the specific heat on twinned single crystals. At first sight the noise in their experiment is below, but of the order of the anisotropy predicted in our calculations. There are many reasons why the actual anisotropy might in fact be even less than the amount shown in our pure twinned curve (dashed-dotted). To mention only one: YBCO is more three dimensional than many of the high \( T_c \) oxides and this implies one more integration in the definition of the QDOS and this can be expected to reduce the anisotropy further. The two other curves in Fig. 9 include impurities and show even less anisotropy than does the pure case. The dashed curve applies to Born scattering with \( t^+ = E_H/16 \) and the dashed gray curve to resonant scattering with \( \Gamma^+ = E_H/16 \).

In Fig. 10 we present finite frequency results for \( N(\omega, \gamma) \) vs. \( \gamma \) (the magnetic field orientation in the CuO\(_2\) plane) for four finite frequency values, namely \( \omega/\Delta_0 = 0.05 \) (dashed-dotted curve), \( \omega/\Delta_0 = 0.1 \) (dashed curve), \( \omega/\Delta_0 = 0.15 \) (dash-double dotted curve), and \( \omega/\Delta_0 = 0.2 \) (dotted curve). The results are to be compared with the solid curve which applies to the case \( \omega = 0 \) and has already been shown in Fig. 8. It is clear that the two pronounced minima in the solid curve become shallower with increasing \( \omega \) and are already quite small for the dotted curve with \( \omega/\Delta_0 = 0.2 \). This complicated pattern should be reflected in the accompanying pattern for the temperature dependence of the specific heat.

More insight into the frequency dependence of the anisotropy can be obtained from the frequency dependence \( N(\omega, \gamma) \) which is shown for several fixed directions \( \gamma \) in Fig. 11 frame (a) and (b). These apply respectively to the tetragonal and orthorhombic case. In frame (a) \( \gamma = 0^\circ \) (antinodal direction) and \( \gamma = 45^\circ \) (nodal direction) are considered. For the pure case the solid curve which applies for \( \gamma = 0^\circ \), shows an \( \omega^2 \) dependence at small \( \omega \) while the dotted
The curve for $\gamma = 45^\circ$ is linear as expected and falls below the value along the antinodal direction. The nodal direction is indeed the direction of the minimum in $N(0, \gamma)$ of Fig. 1. As the frequency $\omega$ is increased the solid and dotted curves rapidly come together and even cross so that the nodal direction has a larger value of $N(\omega, \gamma)$ than the antinodal direction for $\omega$ larger than the crossover frequency. The anisotropy is now very small and will not be observable in specific heat experiments. Dependencies of $N(\omega, \gamma)$ vs. $\omega$ are changed only slightly with the introduction of Born scattering impurities; the dotted curve is for $\gamma = 0^\circ$ and the dashed-dotted one for $\gamma = 45^\circ$, and $t^+ = E_H/16$. On the other hand, the gray curves for resonant scattering with $\Gamma^+ = E_H/16$ are very different and are approximately constant at low $\omega$ with little difference between the two directions. It is obvious that little anisotropy remains in the QDOS. Similar results are given in frame (b) for the orthorhombic case with $\alpha = 0.41$, $s = -0.25$, and $\nu = 0.1$, i.e. the same value of $E_H$ to gap amplitude is used as in frame (a). The most important difference to be noted is that the critical angle, at which an $\omega$ dependence is found in the clean limit, is at the angle $\gamma = 61.3^\circ$ and not at $\gamma = 45^\circ$. Also, the anisotropy is not washed out quite as much in the resonant scattering case when compared to the tetragonal case. Further in this case at sufficiently high frequencies the two curves for $\gamma = 0^\circ$ and $\gamma = 61.3^\circ$ cross and the curve for $\gamma = 0^\circ$ falls below the one for $\gamma = 61.3^\circ$ thus reversing the pattern of maxima and minima shown in Fig. 10 for lower values of $\omega$. We also note that as $\omega$ increases out of zero the QDOS $N(\omega, \gamma)$ decreases for both $\gamma$ values given in frame (a) (tetragonal case) while for the orthorhombic case in frame (b) the reverse is true. This effect is also seen in Figs. 8 and 10. In the tetragonal case the solid line of Fig. 8 for which $\omega = 0$ is above the others for $\omega \neq 0$ while in Fig. 10, the orthorhombic case, it is below.

IV. CONCLUSIONS

We have calculated the effect of the circulating vortex supercurrents on the QDOS of a two dimensional $d$-wave superconductor. For the magnetic field $H$ placed in the CuO$_2$ plane the QDOS varies as a function of the angle $\gamma$ between $H$ and the $\hat{x}$-axis. We have included in
our calculations an $a$-$b$ effective mass anisotropy of about 2 with a view of modeling the band structure of YBCO which is orthorhombic because of the existence of CuO chains, and for which the charge carrier oscillator strength on the chains is approximately of the same order as in the CuO$_2$ planes. In addition, the gap on the Fermi surface was assumed to possess a subdominant s-wave as well as a dominant d-wave character. Consideration of penetration depth data fixes the value of this admixture so that we have no adjustable parameters. Impurities are also included in our calculations in both, Born’s and unitary limits. It is found that the four-fold pattern predicted for the dependence of the zero frequency value of the QDOS in a pure tetragonal system is now changed to a two-fold variation due to the orthorhombicity in the gap or in the band structure. The introduction of impurities leaves the symmetry of the pattern unchanged but can reduce its amplitude. It is also found that the pattern of variation of $N(\omega, \gamma)$ with $\gamma$ is altered as the frequency is increased, although it remains four-fold for tetragonal systems and two-fold for the orthorhombic case.

An important result is that the angle at which minima occur in $N(0, \gamma)$ vs. $\gamma$ does not correspond to the angle at which the zeros occur in the gap as would be the case in a tetragonal system. Instead, the minima occur when the normal state quasiparticle Fermi velocity in the nodal direction is perpendicular to the direction of the vortex supercurrents, i.e. parallel to the direction of the external magnetic field.

Specific heat measurements in clean samples are most favorable for observing the predicted two-fold pattern of anisotropy. To observe it in YBCO detwinned samples are best because an average over equal numbers of twins greatly reduces the predicted anisotropy for detwinned samples. Consideration of more realistic tight binding band structure models are in progress. Our very simple effective mass model, however, has allowed us to understand the important changes orthorhombicity brings to the magnetic field orientation dependence of the QDOS for a two dimensional CuO$_2$ plane with $\mathbf{H}$ in the plane. It has helped us to determine the experimental conditions most favorable to the observation of the predicted anisotropies.
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FIGURES

FIG. 1. The ellipsoidal Fermi surface in \( k \)-space given by \( \varepsilon_k = 0 \) in Eq. (1) (solid line). Here we have used \( \alpha = 0.4 \). Also shown is the vector \( k \) with the direction \( \varphi \) and the corresponding Fermi velocity at \( k \), \( v_F(k) \). Note that it is not parallel to \( k \). The transformed Fermi surface to \( p \)-space is a circle and is shown as a solid, gray line. \( p_F = \sqrt{2m\varepsilon_F} \), with \( \bar{m} = (m_x + m_y)/2 \) and the angle \( \phi \) is identified.

FIG. 2. Order parameters on the transformed Fermi surface (\( p \)-frame) as given by Eq. (7). (a) \( \alpha = s = 0 \) (pure \( d \)-wave gap); (b) \( \alpha = 0.4, s = 0 \); (c) \( \alpha = s = 0.4 \); (d) \( \alpha = 0.4, s = -0.4 \). The straight lines denote the nodal angles.

FIG. 3. The zero frequency value of QDOS, \( N(0, \gamma) \), as a function of magnetic field orientation in the \( \text{CuO}_2 \) plane with \( \gamma \) the angle of \( H \) with respect to the \( k_x \)-axis. The solid line is based on the approximate analytic formula (24) while the dashed line is obtained from numerical evaluation of the exact one dimensional integral (18). Only band anisotropy \( (m_x \pm m_y) \) is included with \( \alpha = 0.2 \) (ellipsoidal Fermi surface) and the gap is pure \( d \)-wave with nodes in the laboratory, \( (k) \)-frame at \( \pm \pi/4 \) and symmetry related points. In the figure \( \nu = E_H/\Delta_0 = 0.3 \).

FIG. 4. The Fermi surface (ellipse) in the laboratory frame. Also shown is the direction of the node \( k_n \) of the gap (\( \varphi_n \)). The direction of the magnetic field \( H \) with the angle \( \gamma \) is taken to be parallel to the Fermi velocity at the node \( v_F(k_n) \) so that the supercurrents defining the vortex flow in a plane (indicated by the thick, solid, gray line) are perpendicular to the \( k_x-k_y \) plane and parallel to the tangent on the Fermi surface at \( v_F(k_n) \).

FIG. 5. The QDOS \( N(0, \gamma) \) at zero frequency as a function of magnetic field orientation in the \( \text{CuO}_2 \) plane (\( \gamma \)) for various values of the band structure anisotropy (\( \alpha \)). As \( \alpha \) increases the amplitude of the oscillations increases: the solid line is for \( \alpha = 0.2 \), the dashed one for \( \alpha = 0.4 \), the dotted one for \( \alpha = 0.6 \), and, finally, the dashed-dotted one for \( \alpha = 0.8 \).
FIG. 6. The frequency dependence ($\omega$) in units of $\Delta_0 (\omega/\Delta_0)$ of the QDOS, $N(\omega, \gamma)$ for the pure case at four different magnetic field orientations, namely $\gamma = 0^\circ$ (solid line), $45^\circ$ (dotted line), $51^\circ$ (dashed line), and $56^\circ$ (dashed-dotted). The $\gamma = 0^\circ$ curve shows $\omega^2$ behavior at low $\omega$ while the $\gamma = 56^\circ$ is linear in $\omega$ as would be the case in zero field for a $d$-wave superconductor.

FIG. 7. The zero frequency value of the QDOS $N(0, \gamma)$ as a function of the magnetic field orientation $\gamma$ for a pure $d$-wave tetragonal ($\alpha = s = 0$) superconductor. The solid line includes some impurities characterized by $t^+ = E_H/16$ and the dashed curve is the clean limit result.

FIG. 8. The dependence of the QDOS, $N(\omega, \gamma)$ on the orientation of the magnetic field in the CuO$_2$ plane ($\gamma$) for four different frequencies $\omega$ in the unitary limit with $\Gamma^+ = E_H/16$. The solid curve is for $\omega = 0$, the dashed one for $\omega/\Delta_0 = 0.05$, dotted for $\omega/\Delta_0 = 0.1$ and dashed-dotted for $\omega/\Delta_0 = 0.15$. $\nu = E_H/\Delta_0 = 0.1$ in a tetragonal system with a pure $d$-wave gap.

FIG. 9. The dependence of the zero frequency QDOS, $N(0, \gamma)$, on the magnetic field orientation $\gamma$ in the CuO$_2$ plane for an orthorhombic system with $\alpha = 0.4$, $s = -0.25$, and $\nu = E_H/\Delta_0 = 0.1$. The dotted curve is for the pure system, the solid one for Born scattering with $t^+ = E_H/16$, and the solid gray curve is for unitary scattering with $\Gamma^+ = E_H/16$. The dashed-dotted curve was obtained from the dotted one by taking the average of it, as is, and its displacement by $90^\circ$; it applies to experiments that average over equal numbers of twins. The dashed curve includes Born scattering and the dashed gray curve unitary scattering. Both are for twinned crystals.

FIG. 10. The dependence of the QDOS, $N(\omega, \gamma)$, on the orientation of the magnetic field $\gamma$ in the CuO$_2$ plane for different frequencies, namely $\omega/\Delta_0 = 0$ (solid line), $\omega/\Delta_0 = 0.05$ (dashed-dotted line), $\omega/\Delta_0 = 0.1$ (dashed line), $\omega/\Delta_0 = 0.15$ (dashed-double dotted line), and $\omega/\Delta_0 = 0.2$ (dotted line). Orthorhombic $d$-wave with $\alpha = 0.4$, $s = -0.25$, $\nu = 0.1$, and $\Gamma^+ = E_H/16$. 23
FIG. 11. The frequency dependence ($\omega$) in units of the gap amplitude $\Delta_0$ of the QDOS, $N(\omega, \gamma)$, for various values of the magnetic field orientation $\gamma$ and impurity content. The solid and dashed lines are for the pure case. The dashed and dashed-dotted ones are for $t^+ = E_H/16$ and the solid gray and dashed gray ones for $\Gamma^+ = E_H/16$. In each pair of curves the first is for $\gamma = 0^\circ$ while the second is in the direction where two node regions have no Doppler shift due to the magnetic field. In (a) which applies to the tetragonal case this is for $\gamma = 45^\circ$ which is the nodal direction but in (b) which applies to the orthorhombic case the critical direction is for $\gamma = 61.3^\circ$. This is different from the nodal direction in the laboratory frame.
$N(0, \gamma)$, arb. units

$\gamma$, rad

- **Eq. (24)**
- **Eq. (18)**
$N(0, \gamma)$, arb. units

\[ \alpha = 0.2 \]

\[ \alpha = 0.4 \]

\[ \alpha = 0.6 \]

\[ \alpha = 0.8 \]

$\gamma, \text{ rad}$
\[ N(\omega, t^+, \gamma), \text{arb. units} \]

- \[ \gamma = 0^\circ \]
- \[ \gamma = 45^\circ \]
- \[ \gamma = 50.77^\circ \]
- \[ \gamma = 56.15^\circ \]
$N(0, \gamma)$, arb. units

$\gamma$, rad

- - - clean limit
- - - $t^+ = E_H/16$
\[\frac{\omega}{\Delta_0} = 0\]
\[\frac{\omega}{\Delta_0} = 0.05\]
\[\frac{\omega}{\Delta_0} = 0.1\]
\[\frac{\omega}{\Delta_0} = 0.15\]

\[N(\omega, \gamma), \text{ arb. units}\]
CLEAN LIMIT,

\[ \text{twinned} \quad + \quad E \quad = \quad \frac{E_H}{16}, \text{twinned} \quad \sim \quad N(0, \gamma), \text{arb. units} \]
\[ N(\omega, \gamma), \text{ arb. units} \]

\[ \frac{\omega}{\Delta_0} = 0 \quad \quad \frac{\omega}{\Delta_0} = 0.05 \quad \quad \frac{\omega}{\Delta_0} = 0.1 \]

\[ \frac{\omega}{\Delta_0} = 0.15 \quad \quad \frac{\omega}{\Delta_0} = 0.2 \]
\begin{align*}
\text{(a)} \quad \gamma = 0^\circ, \quad \Gamma^+ = E_H/16, \quad \gamma = 0^\circ, \\
\gamma = 45^\circ, \quad \Gamma^+ = E_H/16, \quad \gamma = 45^\circ.
\end{align*}