Pressure induced superconductor quantum critical point in multi-band systems

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In multi-band superconductors as inter-metallic systems and heavy fermions, external pressure can reduce the critical temperature and eventually destroy superconductivity driving these systems to the normal state. In many cases this transition is continuous and is associated with a superconducting quantum critical point (SQCP). In this work we study a two-band superconductor in the presence of hybridization $V$. This one-body mixing term is due to the overlap of the different wave-functions. It can be tuned by external pressure and turns out as an important control parameter to study the phase diagram and the nature of the phase transitions. We use a BCS approximation and include both inter and intra-band attractive interactions. For negligible inter-band interactions, as hybridization (pressure) increases we find a SQCP separating a superconductor from a normal state at a critical value of the hybridization $V_c$. We obtain the behavior of the electronic specific heat close to the SQCP and the shape of the critical line as $V$ approaches $V_c$.

I. INTRODUCTION

The study of asymmetric superconductivity, i.e., of superconductivity in systems where different types of quasiparticles coexist at a common Fermi surface has raised a lot of interest in the last years. This in part is due to the relevance of this problem for many different areas in physics. It arises in cold atomic systems with superfluid phases\textsuperscript{1}, in color superconductivity in the core of neutron stars\textsuperscript{2,3,4} and in condensed matter physics\textsuperscript{5}. Furthermore it is closely related to inhomogeneous superconductivity, as FFLO phase\textsuperscript{6}, since this is a possible ground state for asymmetric systems. In condensed matter, as inter-metallic materials, due to electrons from different orbitals at the Fermi surface, there is a natural mismatch of their Fermi wave-vectors. This arises because of the different effective masses of these quasi-particles or because they occur in distinct numbers per atom.

Then, in multi-band systems, even in the absence of external magnetic fields, one has to consider the possibility of inhomogeneous superconductivity or other types of exotic ground states as gapless superconducting phases\textsuperscript{7,8} or phase separation\textsuperscript{9}.

In this paper we focus on the problem of driving a multi-band superconductor to the normal state by applying external pressure. When this occurs continuously, this transition is associated with a SQCP. The theories which have been proposed for the SQCP rely in general on the presence of disorder or magnetic impurities\textsuperscript{10}. However, there is no reason to expect that this should play a role in clean systems driven to a normal state by external pressure. In the model we discuss here, mixing transfers electrons that participate in Cooper pairing to a normal band eventually destroying superconductivity. Since there is no dissipation in the normal band, superconductivity disappears due to a loss of coherence in the system. Our model considers two hybridized bands in the presence of inter and intra-band attractive interactions. These interactions are competing and determine the nature of the zero temperature phase transitions to the normal state as hybridization (pressure) increases. We show that only when intra-band interactions are dominant this transition is continuous. Otherwise it is first order and accompanied by phase separation as usual in this case.

The problem of superconductivity in systems with overlapping bands has been treated originally by Suhl, Matthias and Walker\textsuperscript{11}. The relevance of the different interactions\textsuperscript{12} has been discussed in terms of an energy associated with the Fermi surface mismatch, $\Delta(\delta_{k_F}) = v_F \delta_{k_F}$ and the critical temperature, $k_B T_c$. Only when the former is much smaller then the latter inter-band interactions become important. In our approach the mismatch $\delta_{k_F}$ depends on hybridization and can be controlled by pressure.

II. MODEL AND FORMALISM

We consider a model with two types of quasi-particles, $a$ and $b$, with an attractive inter-band interaction\textsuperscript{13} $\tilde{g}$, an attractive intra-band interaction $\tilde{U}$ and a hybridization term $V$ that mixes different quasi-particles states\textsuperscript{14}. This one-body mixing term $V$ is related to the overlap of the wave functions and can be tuned by external parameters, like pressure, allowing to explore the phase diagram and quantum phase transitions of the model. The Hamiltonian is given by

\begin{equation}
H = \sum_{k,\sigma} \epsilon_k^a a^\dagger_{k\sigma} a_{k\sigma} + \sum_{k,\sigma} \epsilon_k^b b^\dagger_{k\sigma} b_{k\sigma} + \tilde{g} \sum_{k,k',\sigma} a^\dagger_{k\sigma} b^\dagger_{-k'\sigma} b_{-k'\sigma} a_{k\sigma} + \tilde{U} \sum_{k,k',\sigma} b^\dagger_{k\sigma} b^\dagger_{-k'\sigma} b_{-k'\sigma} b_{k\sigma} + \sum_{k,\sigma} V_k \left( a^\dagger_{k\sigma} b_{k\sigma} + b^\dagger_{k\sigma} a_{k\sigma} \right) \tag{1}
\end{equation}

where $a^\dagger_{k\sigma}$ and $b^\dagger_{k\sigma}$ are creation operators for the light $a$ and the heavy $b$ quasi-particles, respectively. The index $l = a, b$. The dispersion relations $\epsilon_k^a = \frac{\hbar^2 k^2}{2m_a} - \mu$ and the ratio between effective masses is taken as $\alpha = \alpha_{ab} = \frac{\epsilon_{k_F}^b}{\epsilon_{k_F}^a}$.
atoms in an optical lattice with two atomic states \( \text{eff} \)ective Rabi frequency which is directly proportional to
transition metals fermions crystalline potential. In the quark problem, it is the
\( \Delta = \epsilon_{k} \), such that,

\[ V_{i} = \frac{\epsilon_{k}^{a} \epsilon_{k}^{b}}{\mu_{a}} - \left( \frac{4}{3} \right)^{1/2} \Delta_{ab} \]

As mentioned before, the poles of these propagators give the excitations of the system. Also from the discontinuity of the Greens functions on the real axis we can obtain the anomalous correlation functions characterizing the superconducting state. In general the appearance of exotic superconducting phases is related to the existence of soft modes in the spectrum of excitations. In the present case, for the energy of the excitations to vanish, it is required that \( \left[ \epsilon_{k}^{a} \epsilon_{k}^{b} - (V_{i}^{2} - \Delta_{ab}^{2}) \right]^{2} + \Delta_{ab}^{2} \epsilon_{k}^{a} = 0 \). This can occur by tuning the hybridization parameter, such that, \( V_{i} = \Delta_{ab} \) in which case gapless excitations appear at \( k = k_{F} \) where \( \epsilon_{k}^{a} = 0 \). Without this fine tuning there are no gapless modes. However, in case the intra-band interaction vanishes there is a zero energy mode for the wave-vector \( k \), such that, \( \epsilon_{k}^{a} \epsilon_{k}^{b} - (V_{i}^{2} - \Delta_{ab}^{2}) = 0 \). We will see the effects of this behavior in the next section.

If, for symmetry reasons, we neglect the term linear in \( \alpha \epsilon_{k} \), then we see the effects of this behavior in the next section.

\[ \langle \langle b_{k \sigma}; b_{-k - \sigma} \rangle \rangle = \Delta \left[ \omega^{2} - \epsilon_{k}^{2} \right] + 2 \frac{\Delta_{ab} \omega}{\omega^{2} + C_{2} \omega^{2} + C_{1} \omega + C_{0}} \]

with

\[ N(\omega) = \Delta_{ab}^{2} V_{i}^{2} - (\omega - \epsilon_{k}^{a}) (\omega - \epsilon_{k}^{b}) + \frac{\Delta_{ab}}{\Delta_{ab}} (\omega + \epsilon_{k}^{a}) \]

and

\[ C_{2} = - \left[ \epsilon_{k}^{a} + \epsilon_{k}^{b} + \Delta_{ab}^{2} + 2 \left( \Delta_{ab}^{2} + V_{i}^{2} \right) \right] \]

\[ C_{1} = 4 \Delta_{ab} \Delta \]

\[ C_{0} = \left[ \epsilon_{k}^{a} \epsilon_{k}^{b} - (V_{i}^{2} - \Delta_{ab}^{2}) \right]^{2} + \Delta_{ab}^{2} \epsilon_{k}^{a} \]

The order parameters that characterize the different superconducting phases described by the above Hamiltonian are, \( \Delta_{ab} = - g \sum_{k \sigma} \langle b_{-k - \sigma} a_{k \sigma} \rangle \) and \( \Delta = - U \sum_{k} \langle b_{-k - \sigma} b_{k \sigma} \rangle \). These are related to inter-band and intra-band superconductivity, respectively. The anomalous correlation functions can be obtained from the Greens functions which also yield the spectrum of excitations in the superconducting phases. We use the equation of motion method to calculate standard and anomalous Greens functions. Excitonic types of correlations that just renormalize the hybridization are neglected. The relevant anomalous Greens functions are, \( \langle \langle \Delta_{ab}; b_{-k - \sigma} \rangle \rangle \) and \( \langle \langle b_{k \sigma}; b_{-k - \sigma} \rangle \rangle \). When we write the equations of motion for them, new Greens functions are generated. Some of these are of higher order, as they contain a larger number of creation and annihilation operators than just the two of the initials Greens functions. For these, we apply a BCS type of decoupling to reduce them to the order of the originals propagators. Finally, writing the equations of motion for the new Greens functions, we obtain a closed system of equations that can be solved. The anomalous propagators from which the order parameters are self-consistently obtained are given by

\[ \frac{\Delta_{ab}^{2} V_{i}^{2}}{\omega^{2} + C_{2} \omega^{2} + C_{1} \omega + C_{0}} \]

with

\[ N(\omega) = \Delta_{ab}^{2} V_{i}^{2} - (\omega - \epsilon_{k}^{a}) (\omega - \epsilon_{k}^{b}) + \frac{\Delta_{ab}}{\Delta_{ab}} (\omega + \epsilon_{k}^{a}) \]
where in $B_k$ and $\omega_j(k)$, we substituted $\epsilon_k^a = \epsilon$ and $\epsilon_k^b = \alpha + (\alpha \epsilon - b)$.

$$\frac{1}{U \rho_b} = \sum_{j=1}^{\omega_D} \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{dy}{2\sqrt{B(\epsilon)}} \left[ \frac{\alpha^2 \omega_j^a(\epsilon) - (\epsilon + b - \alpha)^2}{2\alpha^2 \omega_j^b(\epsilon)} + \frac{\beta \omega_j^a(\epsilon)}{2} \right].$$

In this equation, we substituted $\epsilon_k^a = \epsilon$ and $\epsilon_k^b = (\epsilon + b - \alpha)/\alpha$ in $B_k$ and $\omega_j(k)$. The quantities $\rho_a$ and $\rho_b$ are the density of states at the Fermi level of the $a$ and $b$ bands and $\omega_D$ is an energy cut-off. The right hand side of Eqs.8 and 10 define the gap functions $f(\Delta_{ab}, \Delta)$ and $f_b(\Delta_{ab}, \Delta)$, respectively. In the next section we discuss the behavior of the dispersion relations, of the gap functions and obtain the free energy of the system. From these quantities we obtain the phase diagrams for finite and zero temperatures.

III. RESULTS AND DISCUSSIONS

A. Zero temperature phase diagrams for pure inter or intra-band interactions

For completeness we discuss briefly the behavior of the system at zero temperature. For purely inter-band interactions the transitions are discontinuous and there is no SQCP in the system (see Figs. 1 and 2). From the ground state energy we can identify three characteristic values of the hybridization. Starting from the superconducting ground state, as hybridization increases at a value $V = V_1$ appears a minimum in the ground state energy at the origin ($\Delta = 0$) that coexists with an absolute minimum at finite $\Delta_{ab}$ associated with the superconducting state. Further increasing $V$ there is a first order phase transition to the normal state at $V = V_2$, for which the energies of the normal and superconducting states are degenerate. For still larger $V$, the superconducting state remains as a metastable state until $V = V_3$, where it stops being a minimum of the energy. The values $V = V_1, V = V_2$ and $V = V_3$ for a fixed set of parameters ($\omega_D, \rho_n, \theta$) yield zero temperature phase diagrams shown in Ref.5. It is interesting to point out that in the inter-band case sufficiently large values of $V$ can give rise to soft modes in the dispersion relations which are associated with the presence of Fermi surfaces in the superconducting state.

For purely intra-bands interactions, as in the general case, the dispersion relations of the excitations in the superconductor do not vanish for any $k$ or $V$, since the equation $\left[ \epsilon_k^a \epsilon_k^b - V^2 \right]_a + \Delta^2 \epsilon_k^a_0 = 0$ does not present any non-trivial solution. For $T = 0$, differently from the inter-band case, as $V$ increases the value of $\Delta$ the minimum of the ground state energy vanishes continuously as the system enters in the normal phase. There are no metastable states in this case. We also observe from the gap equation that a minimum value of the interaction $g_b(V)$ is required to sustain superconductivity. At this value of the interaction there is a continuous second order phase transition and this mixing dependent critical interaction $g_b(V_c)$ (or interaction dependent critical hybridization) characterizes a superconducting quantum critical point. In practice this SQCP can be reached applying pressure to the system which is a common procedure, for example, in the study of HF materials.

B. General case at $T \neq 0$

In this section we consider both intra and inter-band interactions and discuss the phase diagrams in the presence of controlled mixing and finite temperatures. For simplicity, and to show clearly the effect of each term we assume strong inter or intra-band terms and in each case the other interaction is added perturbatively or neglected.

For dominant inter-bands interactions, such that, $\Delta \rightarrow 0$, we see in figures 1 and 2 that the phase transitions that were initially discontinuous, of first order, become continuous as temperature increases.

FIG. 1: (Color online) 3D Graph of the asymmetrical gap function $f(\Delta_{ab}, \Delta = 0)$ versus the inter-band superconducting order parameter $\Delta_{ab}$ and temperature. See text for parameters used in the graph.

Figure 1 shows the inter-band gap function as a function of the order parameter $\Delta_{ab}$ and temperature. Notice that close to where the transition changes from first to second order, there is a reentrant behavior which can also be seen in figure 3. In figures 1 and 2 we took $\Delta = 0$, $V = 0.1$, $\alpha = 1/7$ and $b = 0.30$. Similar values for the parameters were used in the other figures.

We now treat the case of dominant intra-band interactions, the inter-band term being considered perturbatively ($\Delta_{ab} \rightarrow 0$) with minor effects. In practice for inter-metallic compounds this is the case of greater interest. Therefore, we will analyze how the usual intra-band superconductivity changes under the influence of temper-
ature and pressure (hybridization). We obtain the variation of the electronic term of the specific heat in the normal phase as hybridization changes and the system goes through the SQCP.

Figure 2 shows the phase diagram where the critical temperature is plotted as a function of hybridization. The critical line is a line of second order phase transitions. For these values of parameters we observe that hybridization initially increases the critical temperature before destroying superconductivity. Since the transitions are continuous there is a SQCP at a critical value of the hybridization $V_c$. For values of $V$ close to $V_c$, the critical line vanishes at the SQCP as $T_c \propto |V - V_c|^\psi$ with a mean-field shift exponent $\psi = 1/2$ as shown in the inset of Fig. 2.

In the next section we calculate the linear term of the electronic specific heat in the normal phase as the system approaches the SQCP.

C. Specific Heat

The free energy of the system can be obtained in terms of the elementary excitations. It is given by,

$$ F = \frac{\Delta_{ab}^2}{g} + \frac{\Delta^2}{U} + \sum_k f(\omega^0_1(k), \omega^0_2(k)) \tag{11} $$

$$ - \frac{T}{2} \sum_k \left[ \sum_{n=1}^2 \ln \left( 2 \left( 1 + \cosh \left( \frac{\omega_n}{k_BT} \right) \right) \right) \right] $$

where $\omega^0_1$ and $\omega^0_2$ are the dispersion relations for $\Delta = \Delta_{ab} = 0$, such that, the function $f(\omega^0_1, \omega^0_2)$ yields the normal contribution to the free energy.

Notice that instead of obtaining the gap functions from the Greens functions they can be found by minimization of the free energy with respect to the order parameters. For illustration we consider the purely inter-band case. We get,

$$ \frac{\partial F}{\partial \Delta_{ab}} = \frac{2\Delta_{ab}}{g} + \sum_k \sum_{n=1}^2 \left\{ \frac{T}{2} \left[ \frac{1}{T} \frac{\partial \omega_n}{\partial \Delta_{ab}} \sinh \left( \frac{\omega_n}{k_BT} \right) \right] \right\} \tag{12} $$

However, $\sinh (x)/(1 + \cosh (x)) = \tanh (x/2)$ and making $\partial F/\partial \Delta_{ab} = 0$, we find

$$ \frac{2\Delta_{ab}}{g} = \frac{1}{2} \sum_k \sum_{n=1}^2 \frac{\partial \omega_n}{\partial \Delta_{ab}} \tanh \left( \frac{\omega_n}{2k_BT} \right) \tag{13} $$

Since,

$$ \frac{\partial \omega_{1,2}}{\partial \Delta_{ab}} = \frac{1}{2\omega_{1,2}} \left( \frac{\partial A_k}{\partial \Delta_{ab}} \pm \frac{1}{2\sqrt{B_k}} \frac{\partial B_k}{\partial \Delta_{ab}} \right) \tag{14} $$

and,

$$ \frac{\partial A_k}{\partial \Delta_{ab}} = 2\Delta_{ab} \quad \text{(15)} $$

also

$$ \frac{\partial B_k}{\partial \Delta_{ab}} = 2\Delta_{ab} \left[ (\varepsilon^a_k - \varepsilon^b_k)^2 + 4V^2 \right] \tag{16} $$

we get,

$$ \frac{\partial \omega_n}{\partial \Delta_{ab}} = 4\Delta_{ab} \left( \omega_n^2 - E^2 \right) \tag{17} $$

where

$$ E^2 = \varepsilon^a_k \omega^b_k + \Delta_{ab}^2 - V^2 \tag{18} $$
Then,
\[ \omega_{1,2}^2 - E^2 = \frac{1}{2} \left[ \left( \varepsilon_k^n - \varepsilon_k^b \right)^2 + 4V^2 \right] \pm \sqrt{B_k} \]  
(19)

Finally, we get,
\[ \frac{1}{g} = \sum_k \sum_{n=1}^2 \frac{(-1)^{n+1}}{2\sqrt{B_k}} \left[ \left( \frac{\omega_n^2 - E^2}{2\omega_n} \right) \tanh \left( \frac{\omega_n}{2k_BT} \right) \right] \]  
(20)

which is the gap equation obtained previously directly from the Greens function. The specific heat is given by,
\[ C_V(V,T) = -T \left( \frac{\partial^2 F}{\partial T^2} \right). \]  
(21)

Using the equation for the free energy, we find,
\[ C_V(V,T) = \frac{1}{4k_B} \sum_k \sum_{n=1}^2 \frac{\omega_n^2}{T^2} \text{sech} \left( \frac{\omega_n}{2T} \right) \]  
(22)
or,
\[ C_V = \frac{\pi}{k_B} \sum_{n=1}^2 \frac{1}{T^2} \int_0^{\omega_n} \omega_n^2(k) \text{sech} \left( \frac{\omega_n}{2k_BT} \right) k^2 d^3k. \]  
(23)

This is shown in figure 4 at the critical value of the hybridization.

![Figure 4](image)

**FIG. 4:** (Color online) Electronic specific heat as a function of temperature along the critical trajectory ($V = V_c$). The parameters used are given in the text.

The linearly temperature dependent term of the electronic specific heat on the normal phase at very low temperatures and in particular along the critical trajectory is given by,
\[ C_v = \frac{\pi^2}{3} k_B T \sum_{i=1,2} \rho_i(\mu_0) = \gamma T \]  
(24)

where $\rho_i(\mu_0)$ is the density of states of the hybrid bands at the Fermi level. This is given by,
\[ \rho_i(\omega) = \frac{V}{2\pi^2} \frac{4\pi k^2}{\omega} \frac{d\omega}{dk} \]  
(25)

where
\[ \frac{\partial \omega_{1,2}}{\partial k} = 2k \left\{ \alpha^+ \pm \sqrt{\frac{\alpha^-(\alpha^2-k^2-b^2)}{2(k^2-b^2)}} \right\} \]  
(26)

with
\[ \alpha^+ = 1 + \frac{\alpha}{2} \]  
\[ b^- = 1 - \frac{b}{2}. \]  
(27)

We wish to calculate $\rho_i(\omega)$ at the Fermi surface, i.e., for $k = k_{F_1,2}$, such that, $\omega_1(k_{F_1}) = 0$ and $\omega_2(k_{F_2}) = 0$. We finally get,
\[ \rho_{1,2}(\omega = \mu_0 = 0) = \frac{V}{2\pi^2} \frac{k_{F_1,2}}{\alpha^+ \pm \frac{\alpha(\alpha-k_{F_1,2}^2-b)}{\sqrt{\left(\alpha-k_{F_1,2}^2-b^2\right)^2 + V^2}}} \]  
(28)

The values of $k_{F_{1,2}}$ can be easily obtained and we get the results for the coefficient $\gamma(V)$ of the linear term of the specific heat as a function of hybridization shown in Figure 5. We have used the same set of parameters which yield the phase diagram shown in Figure 5. From these figures we notice that the maximum $T_c$ occurs in a region of the phase diagram where $\gamma$ is increasing with $V$. At the critical value of the hybridization the coefficient of the linear term is passing through a broad maximum. The values of $\gamma$ can be measured all along in the normal phase, above $T_c$, as hybridization is increasing with external pressure and passes through the superconducting quantum critical point at $V_c$. A behavior of $\gamma$ as a function of pressure as that shown in Figure 5 would be a strong indication that the present mechanism is responsible for destroying superconductivity. Since $\gamma$ is proportional to the total density of states at the Fermi level Figure 5 is helpful to understand the initial increase of $T_c$ with hybridization as shown in Figure 5. In the BCS approximation used here this is related to the density of states at the Fermi level and this, as shown by the behavior of $\gamma$, increases initially as $V$ increases.

The results of this paper are obtained using a mean field approximation which does not include fluctuations. The mean-field character of the theory is reflected, for example, in the shape of the critical line that vanishes as $T_c \propto \sqrt{|V-V_c|}$ close to the SQCP as shown in Figure 5. The specific heat calculated above was obtained in the normal phase and is due solely to the contributions of unpaired quasi-particles in the hybridized bands. There are no effects of fluctuations since they are not taken into account.

Due to the nature of the approximations we used, we can expect that the superconducting temperatures reflects the variations in the density of states and consequently in $\gamma$ as hybridization is changed. As pointed out before the increase in $T_c$ for small $V$ is entirely consistent with the behavior of $\gamma$ shown in Figure 5. What
Superconductor-normal transition is continuous as \( V \) increases, being as \( \delta k \) increases the mismatch dependent term of the electronic contribution to the specific heat in the normal phase as a function of hybridization and first order transitions. In the present case the ties which however always occur discontinuously through known Fermi wave-vectors of the hybrid bands. As it is well known, this can give rise to superconducting instabilities which however always occur discontinuously through first order transitions. In the present case the \( T = 0 \) superconductor-normal transition is continuous being associated with a SQCP. Since there is no dissipation in the electronic bands but a lack of coherence in one of them we may attribute to this the destruction of the superconducting phase.

It is clear that in inter-metallic systems hybridization occurs even at zero pressure. The point we wish to emphasize is that this depends on applied pressure and for this reason it can be used as a control parameter. A final remark is that as a matter of fact the control parameter is \( V/\mu_a = \sqrt{\mu_a/\mu_f} = \sqrt{b} \), one of the hybrid bands is above the Fermi level and \( \gamma \) has a discontinuity.

is remarkable however is that superconductivity is destroyed while still both bands contribute to the density of states at the Fermi level. It can be easily shown that

\[
k_F^2 - k_F^2 = 2 \sqrt{\left(\frac{\alpha}{\beta}\right)^2 + \frac{\gamma}{\alpha}},
\]

such that, hybridization increases the mismatch \( \delta k_F = |k_F^2 - k_F^2| \) between the Fermi wave-vectors of the hybrid bands. As it is well known, this can give rise to superconducting instabilities which however always occur discontinuously through first order transitions. In the present case the \( T = 0 \) superconductor-normal transition is continuous being associated with a SQCP. Since there is no dissipation in the electronic bands but a lack of coherence in one of them we may attribute to this the destruction of the superconducting phase.

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\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig5.png}
\caption{(Color online) Coefficient of the linear temperature dependent term of the electronic contribution to the specific heat in the normal phase as a function of hybridization and at \( V = V_c \) for the same parameters as in figure 3. It is also shown the value \( V_{\max} \) for which \( T_c \) is a maximum in figure 3. For \( V = V^* = \frac{\nu_a}{\mu_a} = \sqrt{\mu_a/\mu_f} = \sqrt{b} \), one of the hybrid bands is above the Fermi level and \( \gamma \) has a discontinuity.}
\end{figure}
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