Small $T_{1}^{-1}$ coherence peak near $T_c$ in unconventional BCS superconductors

David Parker$^{1,2}$ and Stephan Haas$^{1}$

$^{1}$Department of Physics and Astronomy, University of Southern California, Los Angeles, CA 90089-0484 USA
$^{2}$Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, D-01187 Dresden, Germany

(Dated: June 25, 2018)

It is usually believed that a coherence peak just below $T_c$ in the nuclear spin lattice relaxation rate $T_1^{-1}$ in superconducting materials is a signature of conventional s-wave pairing. In this paper we demonstrate that any unconventional superconductor obeying BCS pure-case weak-coupling theory should show a small $T_{1}^{-1}$ coherence peak near $T_c$, generally with a height between 3 and 15 percent greater than the normal state $T_{1}^{-1}$ at $T_c$. It is largely due to impurity and magnetic effects that this peak has not commonly been observed.

PACS numbers:

It is well known that conventional superconductors obeying BCS weak-coupling theory generally show a large coherence peak in the nuclear spin lattice relaxation rate $T_1^{-1}$ below $T_c$. This is a direct consequence of the large quasi-particle density-of-states found for $E \geq 1.0$ at the gap edge. It is commonly believed, and experimentally largely true, that unconventional superconductors show no coherence peak near $T_c$. However, a simple quantitative argument shows that if the BCS weak-coupling pure case theory applies, a small coherence peak below $T_c$ must exist.

Consider the BCS weak-coupling equation for the nuclear spin lattice relaxation rate $T_1^{-1}$ for unconventional superconductors:

$$\frac{(T_1)^{-1}}{(T_1 T)^{-1}} \bigg|_{T=T_c} = \int_0^\infty dE \frac{N^2(E) \text{sech}^2(E/(2T))/2T}{2T} \hspace{1cm} (1)$$

The $\text{sech}^2(E/(2T))$ acts as an attenuation factor and dominates the low-temperature $T_1^{-1}$, yielding exponentially activated behavior for s-wave superconductivity and power-law behavior for unconventional superconductivity. However, as $T \to T_c$ all of the structure in $N(E)$ (i.e. DOS different from unity) is shifted to lower energies, since $N(E) = N(E/\Delta)$ and $\Delta \to 0$. See Figure 1 for a depiction of this behavior for the 3-d $^3$He A-phase order parameter $\Delta(k) = \Delta \sin \theta$. All of the structure in $N(E)$ falls in the region where $E/2T \ll 1$, so that for this structure the exponential damping factor becomes essentially irrelevant. Define $F(E) = N(E) - 1$. Note that by the density-of-states sum rule, $\int_0^\infty F(E)dE = 0$. Now substituting in for $N(E)$ we find

$$\frac{(T_1)^{-1}}{(T_1 T)^{-1}} \bigg|_{T=T_c} = \int_0^\infty dE \frac{1}{2} \frac{F(E)}{2T}$$

(2)

The first term trivially yields 1. The second term, $\int_0^\infty dE \frac{F(E)}{2T} \text{sech}^2(E/(2T))/2T$ can be evaluated by noticing that as $\Delta \to 0$, $F(E)$ is only significantly different from 0 in regions where the argument of the $\text{sech}^2$ is small, so that to an excellent approximation near $T_c$ this integral is equal to $\int_0^\infty F(E) dE = 0$. The final term, $\int_0^\infty dE \frac{F(E)}{2T} \text{sech}^2(E/(2T))/2T$, is positive, and so in the immediate neighborhood of $T_c$, $(T_1)^{-1}/(T_1 T)^{-1} \bigg|_{T=T_c} > 1$, implying the existence of a peak. It is this redistribution of $N(E)$ away from an energy-constant ($= N_0$) density-of-states, represented by $F^2(E)$, that is responsible for the peak in $T_1^{-1}$ near $T_c$. The larger this effect, the larger the peak.

This redistribution is intimately tied in with the nodal structure of $\Delta(k)$. This can be seen directly from the BCS expression for the density-of-states $N(E/\Delta) \equiv N(x) = \text{Re} \left( \frac{\pi^2}{2} x^2 \right)$, where $x = \sqrt{1 - (E/\Delta)^2}$, and $\Delta$ denotes an average over the Fermi surface and f contains the angular dependence of the order parameter, (i.e. $\Delta(k) = \Delta_0 f(k)$). The contribution of the nodes is most easily parametrized by $< f^2 >$, with larger values indicating less nodal order parameters. For example, an s-wave order parameter has $< f^2 > = 1$, while a 2d d-wave order parameter (containing line nodes) has $< f^2 > > 0.5$. Gap functions $f$ with larger $< f^2 >$, indicating effectively small or absent nodes, have a comparatively smaller region of phase space contributing to the integral, for $x < 1$. These gap functions will therefore show depleted low-energy density-of-states, and by the sum rule must have enhanced spectral weight in the peak at $E = \Delta$. Both effects will tend to enhance the $T_1$ peak just below $T_c$.

These behaviors are illustrated in Figure 2, which depicts densities-of-states and $T_1^{-1}$ for a series of 3-d order parameters $\Delta(k) = 1 - \cos^2(\theta)$, with $\theta$ the polar angle. As n increases, the low-energy DOS is depleted and the coherence-peak DOS enhanced, with a concomitant increase in the $T_1$ peak near $T_c$. For these cases, $< f^2 >$ increases monotonically from $\frac{\pi^2}{4} \simeq 0.533$ for $n=2$ to 0.866 for $n=10$.

FIG. 1: Diagram depicting attenuation factor and quasi-particle density-of-states for $T \simeq 0.98 T_c \simeq 0.5 \Delta_0, \Delta = 0.2 \Delta_0$, 3-d $^3$He A-phase order parameter.

Results.- In Figure 3 are depicted the coherence peaks near $T_c$ for several unconventional order parameters: d$_{x^2-y^2}$-wave, the $^3$He A-phase order parameter (for which $\Delta(k) = \Delta_0 \sin \theta$), and the p-wave 3-dimensional order parameter $\Delta(k) = \Delta_0 \cos \theta$, as well as the quasiparticle density-of-states for these order parameters. Note that a small peak just below $T_c$ is evident even for the last order parameter, whose
The analysis of the preceding paragraph demonstrates that it is largely the second moment of the DOS around an energy-constant DOS (i.e. not necessary for the formation of a peak.

The quasiparticle density-of-states shows no divergence at $E = \Delta$. The analysis of the preceding paragraph demonstrates that it is largely the second moment of the DOS around an energy-constant DOS ($\approx N_0$) that produces the small peak just below $T_c$. While a large or divergent DOS at $E = \Delta$ clearly enhances the coherence peak near $T_c$, it is not necessary for the formation of a peak.

For the three cases described above, it is possible to derive an analytic expression for $T_1^{-1}$ just below $T_c$, and compare with the numerical results. The quasiparticle density-of-states for each of the three order parameters can be computed analytically, and one finds the following well known results:

$$\text{d-wave: } N(x) = \frac{2}{\pi^2} K_0 \left( \sqrt{x} \right), x < 1; \quad \text{d-wave: } N(x) = \frac{2}{\pi} x K_0 \left( \sqrt{x} \right), x > 1$$

$$\text{$^3$He A - phase: } N(x) = \frac{x}{2} \log \left( \frac{1 + x}{1 - x} \right)$$

In other words, very near $T_c$, we can express the ratio $(T_1^{-1})/(T_1^{-1})_{T=T_c}$ as simply $1 + \alpha \Delta(T)/T$, where $\alpha$ is an order parameter-dependent constant, and this expression yields reasonably good agreement with the numerical results. In order to better model the behavior near $T_c$ we have calculated analytically the next order term and found excellent agreement, as indicated in the plot below. Below 0.98 $T_c$, this approximation becomes less accurate.

Discussion.- The foregoing analysis shows that BCS weak-coupling pure-case unconventional superconductors should exhibit a small $T_1^{-1}$ coherence peak just below $T_c$. Yet a literature survey on this topic [1, 2, 3, 5, 10, 11, 12, 14, 15, 16, 17, 18, 20, 21, 22, 23, 24, 25, 26, 27] has uncovered just two materials - CePt$_3$Si and (TMTSF)$_2$PF$_6$-which show such a peak. The question therefore arises as to why such peaks are not commonly observed.
To address this question, we have conducted an analysis of the effect of resonant impurity scattering upon this $T_{c}^{-1}$ peak, for a two dimensional d-wave order parameter. It is well known that such impurity scattering truncates the DOS peak at $E = \Delta$ and in addition generate substantial low-energy density-of-states. Both of these effects would tend to reduce the size of the coherence peak. It turns out that for these reasons the appearance of this peak is extraordinarily sensitive to impurity scattering. Depicted below are four $T_{c}^{-1}$ curves for d-wave superconductivity: zero impurity scattering, and three cases of small impurity scattering: $\Gamma/\Delta_{00} = 0.01, 0.02$ and 0.03. Within the unitary limit this last concentration is roughly 7 percent of the critical impurity concentration required to destroy superconductivity. This and would result in a depression of $T_{c}$ of this order. As is clear from the plot, the height of the peak is greatly diminished even by the rather low impurity scattering rates modeled here.

Given that materials in the unitary limit typically have superconductivity destroyed by an impurity concentration on the order of a few percent, the foregoing analysis indicates that an impurity concentration of just 0.25 percent is sufficient to largely destroy this peak. Such a concentration is well within the range of observation. In order to observe this peak samples of the highest possible quality are clearly essential, with impurity concentration less than 0.1 percent. It would also be advantageous to perform low-temperature specific heat measurements on the same samples as this would allow accurate assessment of the prediction of a finite relaxation rate at $T=0$, via a measurement of the residual density of states.

An additional effect complicating the observance of this peak is the frequent occurrence of magnetism in the heavy-fermion and high-$T_{c}$ cuprate materials upon which most of the measurements have been performed. The combination of magnetism and the extreme sensitivity of this peak to the presence of impurities in the unitary limit makes its observation difficult in the heavy-fermion and cuprate superconductors. However, the recently discovered noncentrosymmetric superconductor Li$_2$Pt$_3$B$_{12}$ shows no signs of magnetism or strong electron correlation, and appears to be unconventional on at least one band, based upon magnetic penetration depth data. This material may therefore be an ideal material in which to search for this small $T_{c}^{-1}$ peak. Another possibility for experiment is the class of organic superconductors, which may not necessarily have the sensitivity to impurities characteristic of the heavy-fermion and cuprate materials. Indeed, the organic superconductor (TMTSF)$_2$PF$_6$ has already shown a small peak below $T_{c}$. To summarize, here we have demonstrated that any unconventional superconductor obeying BCS pure-case theory should show a small coherence peak in the nuclear spin lattice relaxation rate $T_{c}^{-1}$ just below $T_{c}$. It is likely due to magnetic and impurity effects that this peak has not generally been observed in unconventional superconductors.

**Acknowledgment**

We are indebted to K. Maki for useful suggestions.

---

[1] J.R. Schrieffer, “Theory of Superconductivity”, (Addison-Wesley: New York), 1988.
[2] H. Won and K. Maki, Phys. Rev. B 49, 1397 (1994).
[3] P.J. Hirschfeld, P. Wölfle and D. Einzel, Phys. Rev. B 37, 83 (1988).
[4] M. Sigrist and K. Ueda, Rev. Mod. Phys. 63, 239 (1991).
[5] M. Yogi, Y. Kitaoka, S. Hashimoto, T. Yasuda, R. Settai, T.D. Matsuda, Y. Haga, Y. Onuki, P. Rogl, and E. Bauer, Phys. Rev. Lett. 93, 027003 (2004).
[6] H. Kotegawa, M. Yogi, Y. Imamura, Y. Kawasaki, G.-q. Zheng, Y. Kitaoka, S. Ohsaki, H. Sugawara, Y. Aoki, and H. Sato, Phys. Rev. Lett. 90, 027001 (2003).
[7] C. Tien and L.M. Jiang, Phys. Rev. B 40, 229 (1989).
[8] K. Ishida, H. Mukuda, Y. Kitaoka, Z.Q. Mao, Y. Mori and Y. Maeno, Phys. Rev. Lett. 84, 5387 (2000).
[9] D.E. MacLaughlin, C. Tien, L.C. Gupta, J. Aarts, F.R. de Boer, and Z. Fisk, Phys. Rev. B 30, 1577 (1984).
[10] G.-q. Zheng, K. Tanabe, T. Mito, S. Kawasaki, Y. Kitaoka, D. Aoki, Y. Haga, and Y. Onuki, Phys. Rev. Lett. 86, 4664 (2001).
[11] T. Fujimoto, G.-q. Zheng, Y. Kitaoka, R.L. Meng, J. Cmaidalka, and C. W. Chu Phys. Rev. Lett. 92, 047004 (2004).
[12] N. J. Curro, T. Caldwell, E. D. Bauer, L. A. Morales, M. J. Graf, Y. Bang, A. V. Balatsky, J. D. Thompson and J. L. Sarrao, Nature 434, 622 (2005).
[13] K. Ishida, Y. Kawasaki, K. Tabuchi, K. Kashima, Y. Kitaoka, and K. Asayama, C. Geibel and F. Steglich, Phys. Rev. Lett. 82, 5353 (1999).
[14] K. Kanoda, K. Miyagawa, A. Kawamoto and Y. Nakazawa, Phys. Rev. B 54, 76 (1996).
[15] S.M. DeSoto, C.P. Slichter, A.M. Kini, H.H. Wang, U. Geiser and J.M. Williams, Phys. Rev B 52, 10364.
[16] H. Kotegawa, S. Kawasaki, A. Harada, Y. Kawasaki, K. Okamoto, G.-q. Zheng, Y. Kitaoka, E. Yamamoto, Y. Haga, Y. Onuki, K.M. Itoh, and E. H. Haller, J. Phys: Cond. Matt. 15, S2043 (2003).
[17] Y. Kohori, Y. Yamato, Y. Iwamoto, T. Kohara, E.D. Bauer, M.B. Maple, J.L. Sarrao, Phys. Rev B 64, 134526 (2001).
[18] Y. Kawasaki, S. Kawasaki, M. Yashima, T. Mito, G.-q. Zheng, Y. Kitaoka, H. Shishido, R. Settai, Y. Haga and Y. Onuki, J. Phys. Soc. Jpn. 72, 2308 (2003).
[19] M. Kato, C. Michioka,, T. Waki, Y . Itoh, K. Yoshimura, K. Ishida, H. Sakurai, E. Takayama-Muromachi, K. Takada and T. Sasaki, J. Phys.: Cond. Matt. 18, 669 (2006).
[20] D.E. MacLaughlin, C. Tien, W.G. Clark, M.D. Lan, Z. Fisk, J.L. Smith and H.R. Ott, Phys. Rev. Lett. 53, 1833 (1984).
[21] Y. Iwamoto, K. Ueda and T. Kohara, Solid State Comm. 113, 615 (2000).
[22] H. Sakai, Y. Tokunaga, T. Fujimoto, S. Kambe, R.E. Waldstedt, H. Yasuoka, D. Aoki, Y. Homma, E. Yamamoto, A. Nakamura,
Y. Shiokawa, K. Nakajima, Y. Arai, T.D. Matsuda, Y. Haga and Y. Onuki, J. Phys. Soc. Jpn. 74, 1710 (2005).

[23] K. Matsuda, Y. Kohori and T. Kohara, Phys. Rev. B 55, 223 (1997).

[24] C. Tien and M.D. Lan, Chin. J. Phys. 26, S152 (1988).

[25] S. Kawasaki, G.-q. Zheng, H. Kan, Y. Kitaoka, H. Shishido, and Y. Onuki, Phys. Rev. Lett. 94, 037007 (2005).

[26] T. Mito, S. Kawasaki, G.-q. Zheng, Y. Kawasaki, K. Ishida, Y. Kitaoka, D. Aoki, Y. Haga and Y. Onuki, Phys. Rev. B 63, 220507 (2001).

[27] I.J. Lee, S.E. Brown, W.G. Clark, M.J. Strouse, M.J. Naughton, W. Kang, and P.M. Chaikin, Phys. Rev. Lett. 88, 017004 (2002).

[28] A.A. Abrikosov and L.P. Gorkov, Sov. Phys. JETP 12, 1243 (1961).

[29] K. Maki, in “Lectures on the Physics of Highly Correlated Electron Systems”, AIP Conference Proceedings 438, Salerno, Italy, 1997.

[30] M.J. Graf, R.J. Keizer, A. de Visser, and J.J.M. Franse, Physica B 259-261, 666 (1999).

[31] P. Badica, T. Kondo and K. Togano, J. Phys. Soc. Jpn. 74, 1014 (2005).

[32] H.Q. Yuan, D.F. Agterberg, N. Hayashi, P. Badica, D. Vandervelde, K. Togano, M. Sigrist and M.B. Salamon, Phys. Rev. Lett. 97, 017006 (2006).