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Superconducting Fluctuations and Spin Relaxation Rate of Quasi-One-Dimensional Compounds*

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The nuclear spin-lattice relaxation rate $1/T_1$ in weakly coupled parallel superconducting chains is calculated within a renormalized scheme. Using self-consistently calculated values for correlation length and order parameter, the T dependence of $1/T_1$ above T_c is obtained for different values of interchain coupling ϵ. For a wide range of ϵ the fluctuation-induced enhancement of T_{1n}/T_1 never exceeds 10%.

In this Letter we report a microscopic calculation of the nuclear spin-lattice relaxation rate ($1/T_1$) in quasi-one-dimensional clean superconductors. The renormalization of the fermion propagators by the order-parameter spatial fluctuations $\Delta(\vec{r})$ is taken into account consistent with the Ward identity. The crossover from one- to three-dimensional critical behavior is treated using self-consistent Hartree approximation for the fluctuation propagator. In contrast to a previous calculation[1] our results indicate a weak ($\simeq 10\%$) enhancement of $1/TT_1$ above T_c. Moreover the T dependence of $1/TT_1$ is found to exhibit two types of behavior: (1) For very weak interchain coupling $1/TT_1$ shows a peak above T_c (of the three-dimensional ordering), explaining the anomaly observed experimentally[2] in an annealed sample of Nb_3Al. (2) For somewhat larger values of the coupling parameter the fluctuations produce only a tail above T_c and we expect a peak of the usual bulk behavior below T_c, behavior which has been also reported in other A-15 compounds.[2,3]

We consider a model of weakly coupled superconducting parallel chains (in the x direction) described by a free-energy density functional[4]

$$F/\Omega = A(T)|\Delta(\vec{r})|^2 + \tfrac{1}{2}B|\Delta(\vec{r})|^4 + C|\partial\Delta(\vec{r})/\partial x|^2 + \epsilon C[|\partial\Delta(\vec{r})/\partial y|^2 + |\partial\Delta(\vec{r})/\partial z|^2]. \tag{1}$$

The coefficients $A(T)$, B, and C are given by

$$A(T)=N_0(T/T_{c0}-1)\equiv N_0(t-1);\quad B=N_0 b_0/(k_B T_{c0})^2;\quad b_0=1/(1.76)^2;\quad C=N_0\xi_0^2; \tag{2}$$

where N_0, ξ_0, and T_{c0} represent the bulk density of states at the Fermi level, the correlation length along the chain, and the BCS transition temperature. The interchain coupling is denoted by ϵ. Using a self-consistent Hartree approximation[5] we have

$$\sigma=B\langle|\Delta(\vec{r})|^2\rangle=(B/\Omega)\sum_q\{A(T)+\sigma+C[q_x^2+\epsilon(q_y^2+q_z^2)]\}^{-1}. \tag{3}$$

Defining the temperature-dependent inverse correlation length $\kappa(T)$ as $C\kappa(T)^2=A(T)+\sigma$, we perform the q integration in Eq. (3) by introducing transverse momentum (q_y, q_z) cutoff π/a, where a is the interchain distance ($a\simeq 5$ Å). Consequently we obtain

$$x^2-(t-1)=(2b_0t/\gamma\epsilon)(a/\pi\xi_0)^2\{[x^2+\epsilon(\pi\xi_0/a)^2]^{1/2}-x\}, \tag{4}$$

where $x(t)=\xi_0\kappa(T)$ and $\gamma=2N_0S\xi_0k_BT_{c0}$, S being the cross-sectional area of the chain. We note that the solutions of Eq. (4) go smoothly to the pure one-dimensional case ($\epsilon=0$) in the limit $\epsilon\to 0$. The plot of the solutions of Eq. (4) is given in Fig. 1(a) for $\gamma=5$ and $\xi_0/a=10$, values appropriate for Nb_3Al.[2,6] In the one-dimensional case ($\epsilon=0$) there is no phase transition at finite T; however for finite ϵ we see the appearance of a three-dimensional ordering with finite $T_c<T_{c0}$. The ratio $T_c/T_{c0}=t_c(\gamma,\epsilon)$ for different values of γ as a function of ϵ is exhibited in Fig. 1(b). It is interesting to note the scaling relation for the function $t_c(\gamma,\epsilon)$,

$$t_c(\alpha\gamma,\epsilon)=t_c(\gamma,\alpha^2\epsilon), \tag{5}$$

which is valid for any finite value of α. Numerical evidence indicates that this relation is an exact scaling law; the same relation appears to follow for T_c/T_{c0} calculated in the mean-field approximation by Scalapino, Imry, and Pincus[7] for weakly coupled chains. From Eq. (4) we estimate the temperature T_{cr} of crossover from three- to one-dimensional behavior by putting $x(T_{cr})\simeq\epsilon^{1/2}(\pi\xi_0/a)$ and solving for T_{cr} graphically using curves such as given by Fig. 1(a). The corresponding values of $\langle|\Delta|^2\rangle$ for the same values of γ, ϵ, and (ξ_0/a) used in Fig. 1(a), are plotted in the inset of Fig. 3. The curves for $\epsilon\neq 0$ are terminated at $T_c(\epsilon)$ on the BCS curve.

Using the above calculated values of $\kappa(T)$ and $\langle|\Delta|^2\rangle$ we calculate the relaxation rate $1/T_1$. Using the zero-frequency "one-dimensional" fluctuation propagator[8]

$$R(q)=2\kappa(T)\langle|\Delta|^2\rangle/[q^2+\kappa(T)^2] \tag{6}$$

we calculate the self-energy of the fermion propagator given by Fig. 2(a) and we obtain the following expression for the renormalized fermion

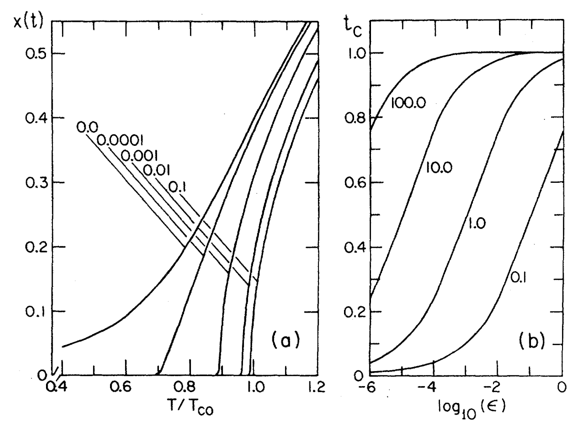

FIG. 1. (a) The temperature dependence of the dimensionless inverse correlation length $x(t)=\xi_0\kappa(T)$ in Hartree approximation for $\gamma=5$ and $\xi_0/a=10$. The curves are labeled by the interchain coupling values of ϵ. (b) The reduced transition temperature $t_c(\gamma,\epsilon)=T_c/T_{c0}$ as a function of ϵ for different families of γ.

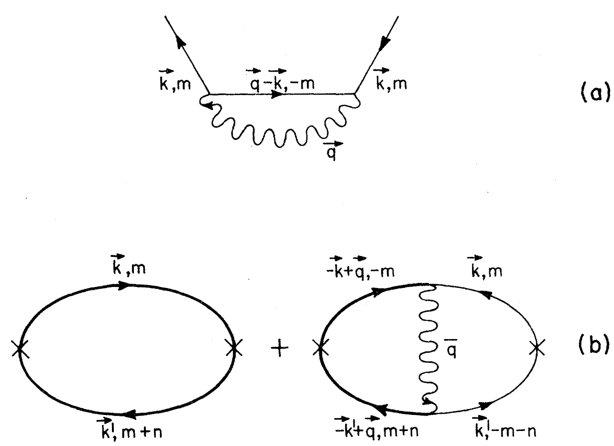

FIG. 2. (a) Pair-fluctuation contribution to the fermion self-energy; (b) diagrammatic expansion of $\chi_{zz}(\vec{q},\omega_n)$. Heavy lines, fermion propagator renormalized with the self-energy of (a); light lines, bare fermion propagator; wavy lines, one-dimensional pair-fluctuation propagator defined by Eq. (6).

propagator:

$$G(\vec{k},\omega)=\left(\omega-\epsilon_{\vec{k}}-\frac{\langle|\Delta|^2\rangle}{\omega+\epsilon_{\vec{k}}+i\sigma_\omega V_F\kappa(T)}\right)^{-1}, \quad (7)$$

where $\epsilon_{\vec{k}}$ and V_F are the electron kinetic energy and Fermi velocity; $\sigma_\omega=\mathrm{sgn}(\mathrm{Im}\omega)$. The factor $[V_F\kappa(T)]^{-1}$ plays a role of the electron lifetime induced by the fluctuations.[9] The nuclear spin-lattice relaxation rate $1/T_1$ is given by

$$1/T_1\propto(T/\omega)\mathrm{Im}\sum_q[\chi_{zz}(q,\omega_N)]_{i\omega_N\to\omega+i0}, \quad (8)$$

where $\chi_{zz}(q,\omega)$ is the dynamic electron-spin susceptibility. Consistent with the approximation used in Eq. (6) for the self-energy and with the Ward identity, the susceptibility is calculated from the diagrams of Fig. 2(b). Performing the k, q, and ω_m summation followed by an analytic continuation ($i\omega_n\to\omega_N+i0$) we obtain in the $\omega_N\to 0$ limit the following result:

$$(T_{1n}/T_1)=\int_{-\infty}^{\infty}dx\left(-\frac{\partial f}{\partial x}\right)\left\{\left[\mathrm{Re}\frac{z}{(z^2-\langle|\Delta|^2\rangle)^{1/2}}\right]^2+\langle|\Delta|^2\rangle\left[\mathrm{Re}\frac{1}{(z^2-\langle|\Delta|^2\rangle)^{1/2}}\right]^2 - \left[\frac{V_F\kappa(T)}{2}\right]\mathrm{Im}\frac{\langle|\Delta|^2\rangle}{(z^2-\langle|\Delta|^2\rangle)[z^*+(z^2-\langle|\Delta|^2\rangle)]^{1/2}}\right\}, \quad (9)$$

where $z=x+iV_F\kappa(T)/2$ and $f(x)$ is the Fermi function. Note that in the limit $\kappa(T)\to 0$ the expression (9) goes over to the well-known BCS result, characterized by the first two terms. The additional term acts to remove the high-temperature divergence (of $1/T_1$) reported previously for the zero-dimensional superconductors using the same approximation (zero frequency in the fluctuation propagator).[10] In the present one-dimensional case there is a finite damping of the fermion propagators at high temperatures due to large values of $\kappa(T)$ [see Eq. (7)] which prevents the above mentioned divergence.

The values of T_{1n}/T_1 for $\gamma=5$, $\xi_0/a=10$, and various values of ϵ as a function of $t=T/T_{c0}$ are plotted in Fig. 3. In the purely one-dimensional case ($\epsilon=0$) there is no enhancement of the relaxation rate of the superconductor relative to the normal metal (in fact $1/TT_1$ remains always below $1/TT_{1n}$). This in contrast with a previous calculation[1] which shows an enhancement diverging as $T\to T_{c0}$. The physical reason for our finite result is the proper renormalization of fermion progagators and the use of self-consistently calculated values for $\kappa(T)$ and $\langle|\Delta|^2\rangle$.[11]

For finite values of ϵ the plots in Fig. 3 are again (like for $\langle|\Delta|^2\rangle$ in the inset) terminated at the actual three-dimensional transition temperature $T_c(\epsilon)$. The curves exhibit two different types of behavior as a function of ϵ: (1) For $\epsilon\lesssim 5\times10^{-4}$ there is an enhancement which peaks *above* T_c; this anomalous behavior was actually found in experiments on annealed Nb_3Al.[2,12] (2) For values of $\epsilon\gtrsim 10^{-4}$ there is only a fluctuation-induced tail which may go over into a peak below T_c. In fact, such behavior seems to be corroborated by the measurements[2] on unannealed Nb_3Al which show a peak below T_c, peak which we believe is of usually three-dimensional BCS origin (see the experimental points in Fig. 3).[13]

In conclusion, we believe that our renormalized calculation is suitable to describe the effect of the superconducting fluctuations in the one-dimensional crossover regime above T_c. Inclusion of finite frequencies of the order-parameter fluctuations is not expected to produce drastic changes of our results in the vicinity of T_c. In the three-dimensional case when a real phase transi-

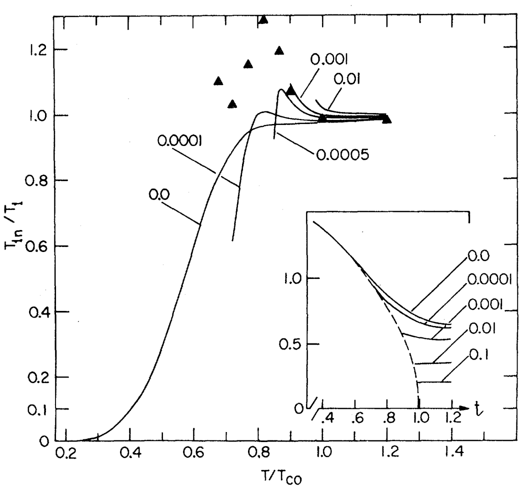

FIG. 3. The temperature dependence of the relaxation rate of a quasi-one-dimensional superconductor relative to a normal metal for $\gamma=5$ and $\xi_0/a=10$. The curves are labeled by the values of ϵ. The experimental points (▲) are taken from Ref. (2) for an unannealed Nb_3Al sample (with $T_c=18.7$°K) and are fitted by the $\epsilon=0.001$ curve with $t_c=0.9$. Inset, the corresponding curves for $(\langle|\Delta|\rangle)^{1/2}/k_BT_{c0}$ used in the calculation of T_{1n}/T_1.

tion occurs [$\kappa(T) \to 0$], only the static fluctuations are important. Far away from T_c the values of $X(t)$ become bigger and finite frequencies as well as finite q values will give a significant contribution to T_{1n}/T_1. However, an exact treatment of the fluctuation propagator with finite frequencies may appear much more difficult to handle analytically. A calculation of the relaxation rate which involves the three-dimensional fluctuations is in progress and we expect to cover temperatures both above and below T_c. However, more experiments on quasi-one-dimensional superconductors are needed to give more reliable information about the values of the interchain coupling ϵ and crossover temperature T_{cr}.

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