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Periodic Anderson lattice : universality and specific heat anomaly

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Abstract : We have considered the Periodic Anderson lattice model and fitted the pairing state gap parameter to a power law $(T - T_c)^n$ with T near the critical temperature T_c. It has been found that n lies between 0.41 and 0.45 for almost all values of the localized level in the narrow half-filled conduction band. The specific heat shows anomalous behavior when the localized level is above the Fermi level, while it can be fitted to an exponential law when the localized level is below the Fermi level

Keywords : Periodic Anderson lattice, universality, specific heat anomaly

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Heavy Fermions and non-conventional superconductors are now two most important systems of intensive experimental and theoretical investigations [1,2,3,4]. One of the most serious contenders for the description of these systems is the Periodic Anderson lattice model [5,6] with the hamiltonian

$$H = H_0 + H',$$

$$H_0 = \sum_{k,\sigma}\left(\varepsilon_{k,\sigma} - \varepsilon_F\right)c^{\dagger}_{k,\sigma}c_{k,\sigma} + \sum_{m,\sigma}\left(E_{\sigma} - \varepsilon_F\right)a^{\dagger}_{m,\sigma}a_{m,\sigma}$$

$$+ \frac{U}{2}\sum_{m,\sigma}\left(a^{\dagger}_{m,\sigma}a_{m,\sigma}\right)\left(a^{\dagger}_{m,\bar{\sigma}}a_{m,\bar{\sigma}}\right),$$

$$H' = \frac{1}{\sqrt{N}}\sum_{k,m,\sigma}\left[V_k \exp\left(-ik.R_m\right)a^{\dagger}_{m,\sigma}c_{k,\sigma} + h.c.\right]. \tag{1}$$

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Here the c-s correspond to the conduction electrons (with momentum $\boldsymbol{k}$, spin σ and energy $\varepsilon_{k,\sigma}$), the a-s correspond to the localized electrons (at the N sites $\boldsymbol{R}_m$ with energy E_σ), U is the on-site Coulomb interaction strength, V_k is the momentum-dependent hybridization interaction and ε_F is the Fermi energy. In an earlier work [7] we had shown that on-site pairing of the localized electrons is possible in this model provided U, when dressed by the conduction electrons, is negative and satisfies a further condition. This condition depends on the relative positions of E_σ, ε_F and the magnitudes of U and V_k. In the case of a half-filled narrow band system, $\varepsilon_0 - \Delta\varepsilon/2 \le \varepsilon_{k,\sigma} \le \varepsilon_0 + \Delta\varepsilon/2$ with $\varepsilon_F = \varepsilon_0$, it was found that within an allowed region of the $(U, E_0 - \varepsilon_0)$ phase space it is possible to have on-site pairing of localized electrons given by non-zero value of the temperature-dependent gap parameter $\Delta = \langle a_{m,\sigma} a_{m,\bar{\sigma}} \rangle$ where $E_0 = \Sigma_\sigma E_\sigma / 2$.

The bare localized state parameters of the hamiltonian are dressed by the conduction electrons and these dressed quantities are denoted by the corresponding symbols with a tilde above them, like $\tilde{E}_0$ and $\tilde{U}$. In terms of the dimensionless reduced variables $t = k_B T / |\tilde{U}|, e = \tilde{E}_0 / |\tilde{U}|$ we had previously obtained [7] the temperature dependence of the gap parameter Δ (Figure 1) for different values of e, dependence of the critical temperature t_c on e^2, re-entrant behaviour in large magnetic field and the nature of the transition from normal to pairing phase.

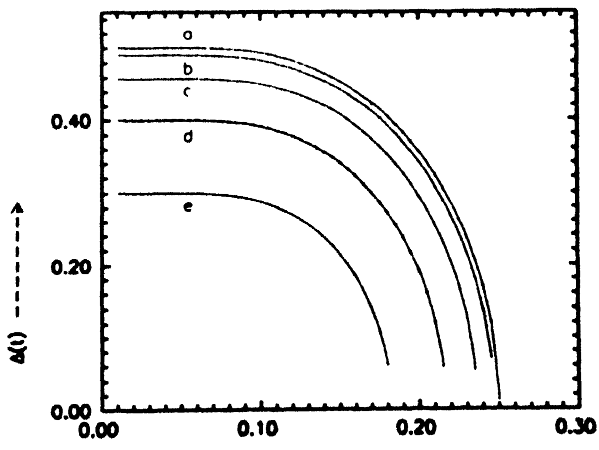

Figure 1. Gap parameter $\Delta(t)$ as a function of t for $e = 0.0$ (a), 0.1 (b), 0.2 (c), 0.3 (d) and 0.4 (e).

We are here interested to investigate whether there is any universality in the transition. Such universal scaling properties have been observed [8–10] for Hall coefficient and thermoelectric power in the normal state of Bi-2212 and Tl-2212 systems. In case of any phase transition universality is one of the first properties that is first looked into. In Figure 2, we have plotted $\Delta(t)/\Delta(0)$ as a function of t/t_c for $e = 0.0, 0.1, 0.2, 0.3$ and 0.4. The figure suggests that there is at least an approximate universality. To see it more clearly

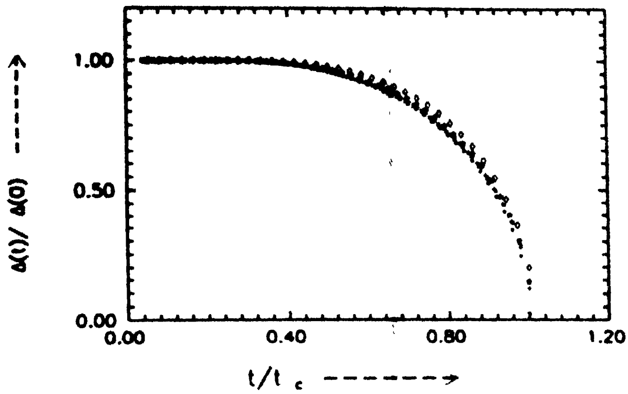

Figure 2. Reduced gap parameter $\Delta(t)/\Delta(0)$ as a function of t/t_c for $e = 0{\cdot}0$, 0 1, 0 2, 0 3 and 0.4.

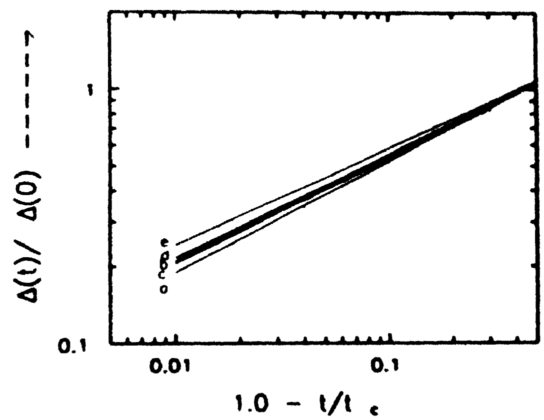

Figure 3. Power law fitting $\Delta(t)/\Delta(0) = A(1\ 0 - t/t_c)^n$ for $e = 0.0$ (*a*), 0.1 (*b*), 0.2 (*c*), 0.3 (*d*) and 0 4 (*e*)

we have fitted in Figure 3 $\Delta(t)/\Delta(0) = A(1.0 - t/t_c)^n$ for t near t_c with the best fit values of A and n given in Table 1. At low temperature for t near 0 we have fitted in

Table 1. Best fit values of A and n in the fitting $\Delta(t)/\Delta(0) = A(1\ 0 - t/t_c)^n$ for t near t_c for different values of e

e	A	n
0 0	1 46348	0 451741
0 1	1 38678	0 410222
0.2	1 41512	0.421230
0.3	1.41323	0 408642
0.4	1.39814	0.378980

Figure 4 $\Delta(t)/\Delta(0) = 1.0 - A\exp(-\alpha t_c/t)$ with the best fit values of A and α given in Table 2. The values of n given in Table 1 show considerable deviation from Ginzburg-Landau value.

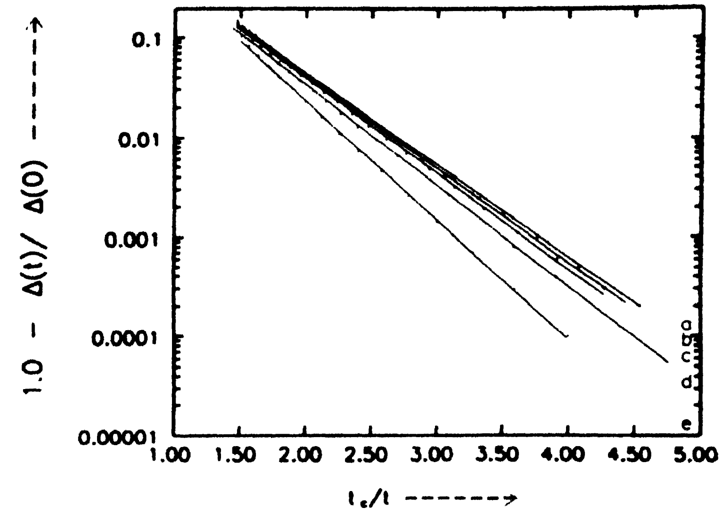

Figure 4. Exponential fitting $\Delta(t)/\Delta(0) = 1.0 - A\exp - \alpha t_c/t$ for $e = 0.0$ (a), 0.1 (b), 0.2 (c), 0.3 (d) and 0.4 (e)

Table 2. Best fit values of A and α in the fitting $\Delta(t)/\Delta(0) = 1.0 - A\exp(-\alpha t_c/t)$ when t is near 0 for different values of e

0.0	3.18547	2.13348
0.1	3.27402	2.17336
0.2	3.44061	2.22653
0.3	3.62535	2.33737
0.4	6.02010	2.77457

The specific heat for the system shows quite interesting feature. The values calculated from eq. (39) of Ref. [7] for positive values of e have been shown in Figure 5

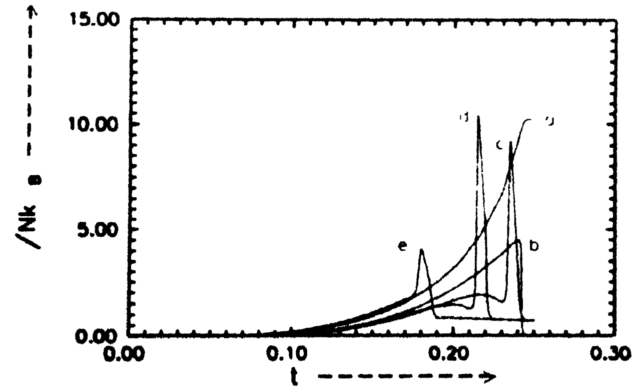

Figure 5. Specific heat $C(t)/Nk_B$ as a function of t for $e = 0.0$ (a), 0.1 (b), 0.2 (c), 0.3 (d) and 0.4 (e).

and those for negative values of e have been shown in Figure 6. While for the negative values of e the curves are similar to those for systems with gaps in the energy spectrum, for

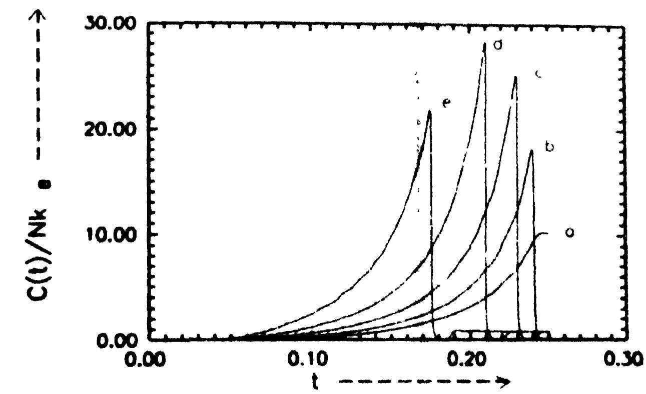

Figure 6. Specific heat $C(t)/Nk_B$ as a function of t for e = 0.0 (a), –0.1 (b), –0.2 (c), –0.3 (d) and –0.4 (e).

positive values of e there are humps before the peak and the succeeding drop. This behaviour has been reported [11,12] in experiments performed on $Ba_{1-x}K_xBiO_3$ and $Bi_{1-x}Pb_xBaO_3$. For negative values of e specific heat attains a constant value in the normal phase after the drop as in classical physics, the constant value being independent of e. The specific heat data for negative values of e could not be fitted to a single power law $C(t)/Nk_B = A(1.0 - t/t_c)^n$. But fitting to exponential laws.

1. $C(t)/Nk_B = A\ \exp{-\alpha(1.0 - t/t_c)}$ shown in Figure 7 with best fit values of A and α given in Table 3, and

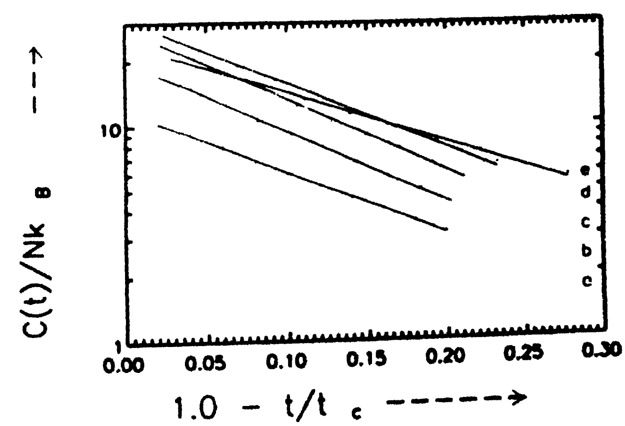

Figure 7. Exponential fitting $C(t)/Nk_B = A\exp{-\alpha(1.0 - t/t_c)}$ for e = 0.0 (a), –0.1 (b), –0.2 (c), –0.3 (d) and –0.4 (e).

Table 3. Best fit values of A and α in the fitting $C(t)/Nk_B = A\exp-\alpha(1\ 0 - t/t_c)$ when t is near t_c for different values of e.

e	A	α
0 0	11.7515	6.63387
–0 1	19.9804	7.59467
–0.2	28.4975	7 68435
–0.3	31.3607	6 94682
–0.4	24.3347	5.38330

2. $C(t)/Nk_B = A\exp-\alpha\left(t_c/t - 1.0\right)$ shown in Figure 8 with best fit values of A and α given in Table 4

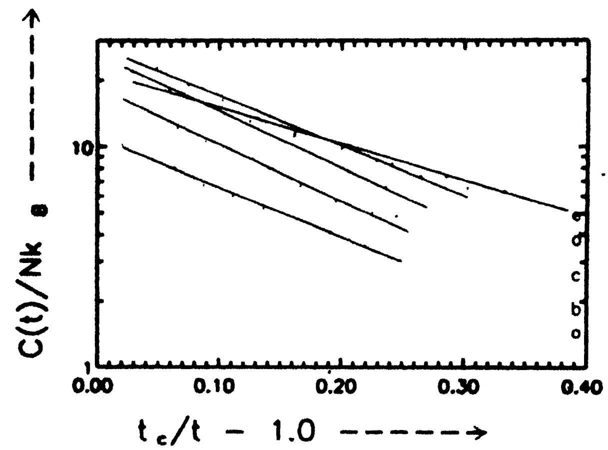

Figure 8. Exponential fitting $C(t)/Nk_B = A\exp-\alpha(t_c/t - 1\ 0)$ for e = 0.0 (a), –0.1 (b), –0.2 (c), –0.3 (d) and –0.4 (e).

Table 4. Best fit values of A and α in the fitting $C(t)/Nk_B = A\exp-\alpha(t_c/t - 1.0)$ when t is near t_c for different values of e.

		α
0.0	11.0289	5.19188
–0.1	18.4818	5.89484
–0.2	26.1624	5.89660
–0.3	28.5635	5.18112
–0.4	21.9252	3.76084

is possible. Of these two fittings, the first one seems to be slightly better. This points to a non-conventional type of transition. But the almost equality of the values of α again indicates at least an approximate universality. It should be pointed out that all the calculations have been done for zero external magnetic field. A point should be noted about the Figures 5–8. The specific heat has really been plotted with the numerical estimate of the derivative of the Helmholtz' free energy as the ratio of two differences. In reality in Figure 6 there is a jump in the specific heat at the transition point.

This analysis confirms the general feeling that Heavy Fermionic and non-conventional superconducting systems have many peculiar features which are not observed in ordinary systems.

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