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Scaling in BCS to Bose crossover problem in different partial waves *

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Scaling in BCS to Bose Crossover Problem in Different Partial Waves*

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The BCS superconductivity to Bose condensation crossover problem is studied in two dimensions in S, P, and D waves with a finite-range separable potential at zero temperature. The gap parameter and the chemical potential as a function of Cooper-pair binding B_c exhibit universal scaling. In the BCS limit the results for coherence length ξ and the critical temperature T_c are appropriate for high-T_c cuprate superconductors and also exhibit universal scaling as a function of B_c.

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A collection of electrons (Fermions), interacting via a weak residual interaction at very low temperature and high density, exhibits pairing instability. Overlapping Cooper pairs [1] are formed spontaneously according to the Bardeen-Cooper-Schreiffer (BCS) theory of superconductivity [2]. For usual superconductors, the BCS theory yields $\xi k_F \sim 1000$ and $2\Delta/(k_B T_c) = 3.52$ in agreement with experiments, where k_F is the Fermi momentum, k_B the Boltzmann constant, Δ the gap parameter, T_c the critical temperature and ξ the coherence length.

In the opposite limit of strong residual interaction, nonoverlapping diatomic Bosonic molecules emerge as bound states of Fermion pairs [3,4]. At sufficiently low density and temperature, these composite objects act as an ideal gas of Bosons with $\xi k_F \sim 0$, which may undergo phase transition. In three dimensions this phase transition is the usual Bose condensation [3,5]. In two dimensions one can have a superfluid transition under appropriate conditions [6,7]. Hence the two extreme limits of the same system exhibit two interesting phenomena.

Leggett [3] emphasized the importance of the abovementioned BCS superconductivity to Bose condensation crossover problem. This problem has gained new impetus after the discovery of high-T_c cuprate superconductors with certain general properties [5,7–10]. These superconductors have a very small coherence length: $\xi k_F \sim 10$ [8,9], and exhibit a linear scaling between T_c and T_F known as the Uemura scaling [11], where T_F is the Fermi temperature.

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The small value of ξ suggests that its superconducting phase might be understood as one in the abovementioi crossover regime [5,7,8,10].

Many high-T_c superconductors have a conducting structure similar to a two-dimensional layer of carriers [8,10,1 which suggests the use of two-dimensional models. The mathematical complications of the crossover problem is a simpler in two dimensions than in one or three dimensions [5,7–9]. Hence in order to understand the subtleties of t problem, the present study is limited to two dimensions.

In the S wave crossover problem in three dimensions, Leggett considered N electrons, each of mass m and of spaci l, interacting via a weak short-range potential of range $r_0(<< l)$. The scattering length a satisfies $|a| >> r_0$. varying the ratio l/a, the BCS and the Bose limits could be attained. When suitably scaled, most of the propert of the system are insensitive to the details of the potential and are universal functions of the dimensionless varial l/a. In three dimensions $l \sim k_F^{-1}$ and hence one could use the equivalent variable $1/(k_F a)$. For the S wave probl in two dimensions with a very short-range attractive potential, the presence of a two-body bound state in vacuum the necessary and sufficient condition for pairing instability [4,8]. Hence the convenient dimensionless variable cou be B_2/E_F with B_2 the two-body binding in vacuum, $E_F \equiv k_B T_F \equiv \hbar^2 k_F^2/(2m)$ the Fermi energy.

The usual treatment of BCS employs a potential in momentum space with a constant value for momentum betwe $2m(E_F - E_D)/\hbar^2$ and $2m(E_F + E_D)/\hbar^2$ and zero elsewhere with E_D the Debye energy. This implies a modera range of the interaction. This potential is a physically motivated phonon induced electron-electron one [2]. T objective of the present work is to find out to what extent the universal nature [4,7,8] of the solution of the crossov problem is modified after introducing a smooth potential of medium range in place of the above potential. For sor of the high-T_c materials, experiments suggest non-S wave Cooper pairing [8,9]. This is why we have also extend the discussion of universality to the crossover problem in P and D waves.

The energy B_2 is not really the ideal variable for studying universality in the crossover problem in two dimensic for non-S partial waves, because in P and D waves one could have Cooper pairing, and hence BCS superconductivi in the absence of a two-body bound state in vacuum [8]. The appropriate reference variable for studying the crosso problem in all cases, including the three-dimensional problem [12], is the Cooper pair binding B_c. For the zero-ra S wave model of Ref. [8] $B_2 = B_c$. Previously, there have been studies of the crossover problem in terms of poten strength or scattering length.

We studied the crossover problem with a finite-range separable potential and specially, the dependence of the universal behavior of the crossover problem on the range of the interaction potential. We found that the universal behavior of the crossover problem does not significantly change with the change of the range of potential. We calculated the zero-temperature chemical potential μ and gap parameter Δ in the entire crossover region, and ξ and T_c in the BCS region for different values of the range parameter. We found robust universal scaling in each case valid over several decades of Cooper pair binding. We did not find similar scaling when μ, Δ, T_c, and ξ were considered as a function of potential strength or of binding B_2 [12]. The present model also produced an appropriate T_c/T_F ratio and a small ξ in the BCS region in accord with experiments on high-T_C cuprate superconductors.

The two-body problem, the Cooper and BCS models all exhibit ultraviolet divergences for zero range potential and require renormalization to produce finite results [8]. For non-S partial waves, the nature of these divergences is more complicated and there is no general prescription for renormalization. The present study with finite-range potential leads to a well-defined mathematical problem without the necessity for renormalization.

We consider a two-body system, each of mass m, in the center of mass frame [8]. The single [two] particle energy is given by $\epsilon_q = \hbar^2 q^2/(2m)$ $[2\epsilon_q]$, where q is the wave number. We consider the following attractive separable short-range potential $V_{pp'} = -\lambda f_p f_{p'}$. The angular momentum ($L$) dependence of all the variables will not be explicitly shown. This potential leads to pairing instability for any λ, L and f_p [12]. In even (odd) partial waves pairing occurs in singlet (triplet) state. The corresponding t matrix is

$$T_{pp'}(2E) = f_p f_{p'}[-\lambda^{-1} - \sum_q f_q^2 (2E - 2\epsilon_q)^{-1}]^{-1}$$

where $2E$ is the parametric relative energy. The condition for a bound state at energy $2E = -B_2$ is

$$\lambda^{-1} \equiv \sum_q f_q^2 (B_2 + 2\epsilon_q)^{-1}. \tag{0.1}$$

The Cooper pair problem for two electrons above the filled Fermi sea for this potential is given by [1,2] $\lambda^{-1} = \sum_{q>k_F} f_q^2 (2\epsilon_q - 2\hat{E})^{-1}$, with Cooper binding $B_c \equiv 2E_F - 2\hat{E}$. Using Eq. (0.1), the Cooper problem is written as

$$\sum_q f_q^2 (B_2 + 2\epsilon_q)^{-1} - \sum_{q>k_F} f_q^2 (2\epsilon_q - 2\hat{E})^{-1} = 0. \tag{0.2}$$

Leggett [3] provided a generalization of the BCS model valid for a crossover from large to small coherence lengths at zero temperature. The finite temperature (T) version of this problem is given by the following BCS gap and number

equations [4]

$$\Delta_p = -\sum_q V_{pq} \frac{\Delta_q}{2E_q} \tanh \frac{E_q}{2k_B T}, \tag{0.3}$$

$$N = \sum_q \left[1 - \frac{\epsilon_q - \mu}{E_q} \tanh \frac{E_q}{2k_B T}\right], \tag{0.4}$$

with $E_q = [(\epsilon_q - \mu)^2 + \Delta_q^2]^{1/2}$ and μ ($\neq E_F$). At finite temperatures the coupled system of equations (0.3) and (0.4) is only valid in the weak coupling BCS region characterized by positive μ/E_F. In the strong coupling Bose region, characterized by negative μ/E_F, due to the existence of preformed composite Bosons at finite temperatures above T_c the number equation (0.4) breaks down [5,7]. Actually, the physical process changes as one moves from the BCS to Bose limit. In the BCS limit the formation of Cooper pairs at $T = T_c$ signals superconductivity, whereas in the Bose limit the preformed composite Bosons may undergo a superfluid phase transition at $T = T_c$ under appropriate conditions [6,7]. At zero temperature Eqs. (0.3) and (0.4) are valid in the whole crossover region [8].

With the present potential, Δ_q of Eq. (0.3) behaves as $\Delta_q \equiv \Delta f_q$. Equation (0.3) then becomes

$$\lambda^{-1} = \sum_q f_q^2 \frac{1}{2E_q} \tanh \frac{E_q}{2k_B T}, \tag{0.5}$$

where $E_q = [(\epsilon_q - \mu)^2 + \Delta^2 f_q^2]^{1/2}$. Using Eqs. (0.1) and (0.2), Eq. (0.5) can be rewritten as

$$\sum_{q>k_F} \frac{f_q^2}{\epsilon_q - \hat{E}} - \sum_q \frac{f_q^2}{E_q} \tanh \frac{E_q}{2k_B T} = 0. \tag{0.6}$$

Equation (0.6) is valid independent of the existence of a two-body bound state in vacuum.

Equations (0.4) and (0.6) can be explicitly written as

$$\int_{E_F}^{\infty} d\epsilon_q \frac{f_q^2}{\epsilon_q - \hat{E}} - \int_0^{\infty} d\epsilon_q \frac{f_q^2}{E_q} \tanh \frac{E_q}{2k_B T} = 0, \tag{0.7}$$

$$\int_0^{\infty} d\epsilon_q \left[1 - \frac{\epsilon_q - \mu}{E_q} \tanh \frac{E_q}{2k_B T}\right] = 2E_F. \tag{0.8}$$

Equations (0.7) and (0.8) permit following analytic solutions for S wave ($L = 0$) zero-range potential given by $f_q = 1$. At $T = 0$, $\Delta = (2B_c E_F)^{1/2}$ and $\mu = E_F - B_c/2$ [8]. At $T = T_c$ ($\Delta = 0$) in the BCS limit ($\mu \approx E_F$) we find the analytic solutions: $\mu + 2k_B T_c \ln[2\cosh(\mu/(2k_B T_c)] = 2E_F$ and $T_c/T_F = \sqrt{2}\exp(\gamma)(B_c/E_F)^{1/2}/\pi$ where $\gamma = 0.57722$. In this case $2\Delta/(k_B T_c) = 2\pi/\exp(\gamma) \approx 3.528$.

Next Eqs. (0.7) and (0.8) are solved numerically in S ($L = 0$), P ($L = 1$), and D ($L = 2$) waves with form factors $f_q = q^L[\alpha/(q^2 + \alpha)]^{(L+1)/2}$ where α is the range parameter. We studied the crossover problem in the entire

domain at $T = 0$ and calculated the dimensionless order parameter $\mathrm{D} \equiv \Delta/E_F^{(1-L/2)}$ and the chemical potential μ/E_F as functions of B_c/E_F for different L and α. The order parameters are shown in Figs. 1 (a), 1 (b), and 1 (c) for S, P, and D waves, respectively. In Fig. 2 we exhibit μ/E_F in these cases. The coherence length defined by $\xi^2 = \langle\psi_q|r^2|\psi_q\rangle/\langle\psi_q|\psi_q\rangle$ with the pair wave function $\psi_q = \Delta_q/(2E_q)$ was numerically calculated using $r^2 \equiv -\nabla_q^2$. The calculated $(\xi k_F)^2$ are shown in Fig. 3 as a function of B_c/E_F. The S wave Pippard coherence length $(= \hbar k_F/(\pi m\Delta))$ is also shown in Fig. 3 for comparison. We also calculated T_c in the BCS domain by setting $\Delta_q = 0$ in Eqs. (0.7) and (0.8). The calculated T_c/T_F is also plotted in Fig. 1 for different partial waves.

Before presenting a discussion of the results we mention two limitations of the present model. First, for non-S waves the zero-range limit ($\alpha \to \infty$) cannot be taken because of the appearance of strong ultraviolet divergences. For S wave, this limiting solution is analytically known [8]. Secondly, the size of the two-body bound state in vacuum with this potential behaves as $B_2^{-1/2}$ (α^{-1}) when $B_2/2 <$ ($>$) α^2. Hence the size of this bound state as well as the Cooper pair becomes unrealistic for $B_2/2 > \alpha^2$. Consequently, for very large B_c/E_F, the ideal Bose limit of nonoverlapping Bosons is not realized for small α. Hence the present study is limited to a potential of intermediate ranges: $\alpha/E_F \sim 1 - 10$.

From Fig. 1 we find that both D and T_c/T_F exhibit universal behavior as functions of B_c/E_F in different partial waves. In the BCS region they exhibit linear scaling valid over about four to five decades. The scaling exponents are roughly constant for all L and α: $\mathrm{D} \sim (B_c/E_F)^{1/2}$, $T_c/T_F \sim (B_c/E_F)^{1/2}$. For an ideal Bose gas there is no condensation in two dimensions and hence one might think that T_c should reduce to zero as B_c/E_F increases in the Bose region. However, because of a weak residual interaction between Bosons, this system may undergo superfluid transition with quasi long range order below a fixed small T_c/T_F independent of B_c/E_F [7]. The T_c for this transition can only be found in numerical model studies. Hence all T_c/T_F of Fig. 1 should reduce quickly and attain a small constant value as B_c increases in the Bose region [7]. We find that both T_c/T_F and D increase with decreasing α and L. The ratio $2\mathrm{D}/(T_c/T_F) \equiv 2\Delta E_F^{L/2}/(k_B T_c)$ increases as α decreases and/or L increases. For example, for $\alpha/E_F = 1$ (2, 5) this ratio is 4.93 (4.31, 3.87) for $L = 0$, 7.07 (5.29, 4.21) for $L = 1$, and 10.0 (6.37, 4.39) for $L = 2$. The corresponding universal gap-to-T_c ratio $2\Delta_{k_F}/(k_B T_c)$ for $\alpha/E_F = 1$ (2, 5) is 3.50 (3.52, 3.53) for $L = 0$, 3.54 (3.53, 3.51) for $L = 1$, and 3.53 (3.47, 3.35) for $L = 2$.

From Fig. 2 we find that the zero-temperature μ has a linear dependence on B_c for all α and L almost over the

entire crossover region. The minor deviation from linearity occurs for small μ. We present this dependence u
$B_c/E_F = 40$. For larger B_c/E_F, μ is essentially given by the zero-range analytic S wave solution: $\mu = E_F - B_2/$

From Fig. 3, for all α and L, we have the universal scaling $(\xi k_F)^2 \sim (B_c/E_F)^{-1}$ valid over three decades of B_c in BCS domain. The corresponding S wave Pippard coherence length satisfies the same scaling. The parameter $(\xi$ decreases as L and/or α decreases. In the extreme Bose domain, this scaling should also hold in all cases. The analy zero-range S wave solution has this scaling [8,9]. However, because of the unphysical nature of the present poten model in the extreme Bose limit, this scaling is not observed in our study. For a fixed B_c/E_F, Fig. 1 leads to a scal of T_c with T_F for all α and L. This scaling was observed by Uemura et al. [11] for high-T_c superconductors. Fr Fig. 1 we find for S, P, and D waves, Uemura's experimental value $T_c/T_F \simeq 0.05$ leads to a B_c/E_F in the dom 0.01–0.001, which implies the weak coupling BCS limit. From Fig. 1 we find that, for $\alpha/E_F = 5$, $T_c/T_F = 0.05$ le to $B_c/E_F = 0.0032$ (0.0079, 0.0135) for S (P, D) waves. From Fig. 3 the above Cooper pair bindings give ξk_F in all partial waves. This implies a universal correlation between T_c/T_F and ξk_F in all partial waves.

In conclusion, we studied the BCS superconductivity to Bose condensation crossover problem in different part waves for a finite-range separable potential. We found robust scaling relations involving the order parameter, chemi potential, coherence length and critical temperature as a function of Cooper pair binding. In the BCS domain present results may simulate typical high-T_c values for the coherence length ξ, and T_c. They also exhibit the T_c ver T_F linear correlation (at a fixed B_c/E_F) as observed by Uemura [11]. The consequence of these findings in describ the high-T_c superconductors in two dimensions in not all too obvious. Though we have exhibited the results a specific separable potential model, we verified that the general trend is maintained as form factors are chan Hence we do not believe our findings to be so peculiar as to have no general validity. A preliminary study of three-dimensional crossover problem employing the same separable potential in different partial waves as a func of B_c/E_F also leads to similar universal scaling [12]. A detailed account of that will be reported elsewhere.

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Figure Captions:

1. $\log_{10}(2D)$ and $\log_{10}(T_c/T_F)$ versus $\log_{10}(B_c/E_F)$ plots for (a) S ($L = 0$), (b) P ($L = 1$), and (c) D ($L = 2$) waves, denoted by full and dashed-dotted lines, respectively, where $D = \Delta/E_F^{(1-L/2)}$. T_c is calculated in the weak coupling or the BCS regime as the finite temperature version of the Leggett equations are valid only in this regime.

2. μ/E_F versus B_c/E_F plots for different partial waves and α. The curves are labelled by partial wave(s) and α.

3. $(\xi k_F)^2$ versus B_c/E_F plots for different partial waves and α: dashed lines – S ($L = 0$) wave results, dotted lines – P ($L = 1$) wave results, dashed-dotted lines – D ($L = 2$) wave results, and full lines – the S wave Pippard coherence lengths. The curves are labelled by partial wave(s) and α.

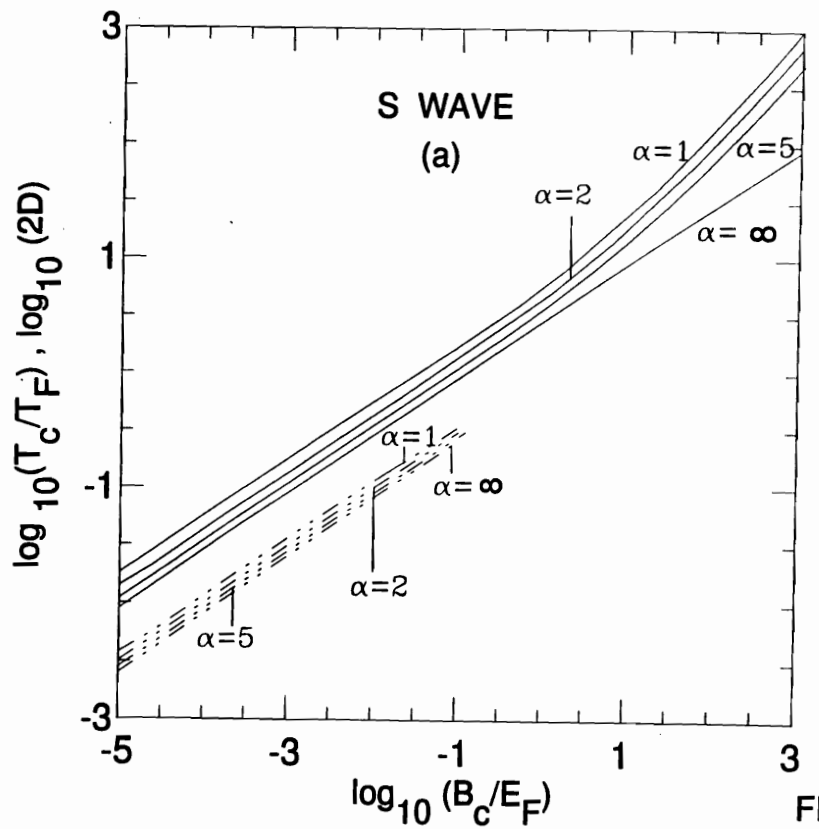


FIG 1

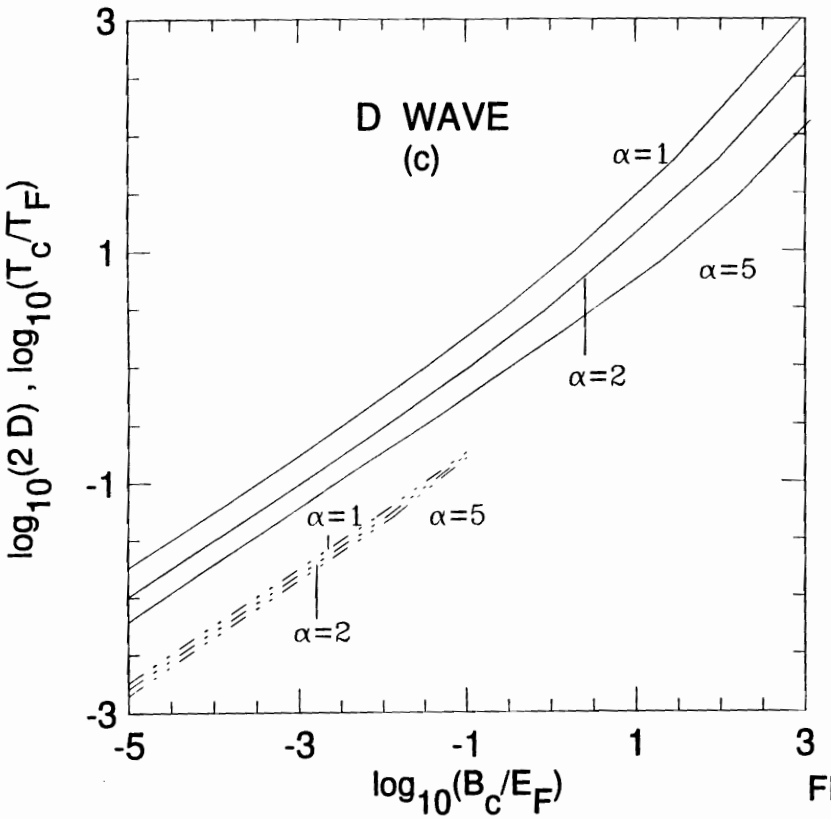
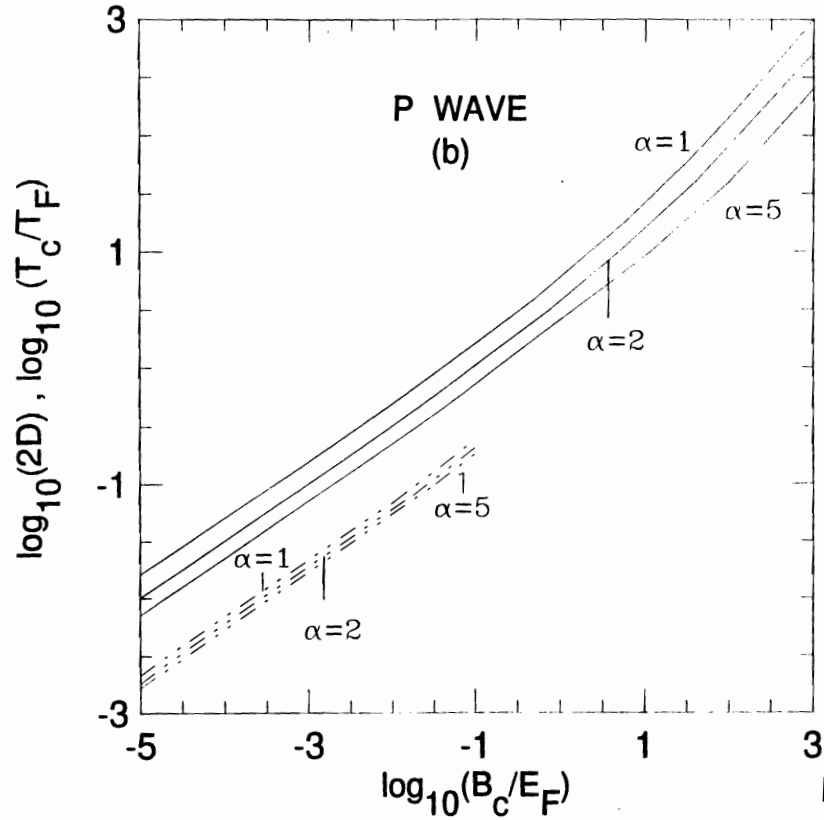

D WAVE
(c)
α=1
α=5
α=2
α=1
α=5
α=2
3
1
-1
-3
-5
-3
-1
1
3
log10(2 D) , log10(Tc/TF)
log10(Bc/EF)

FIG 1


P WAVE
(b)
α=1
α=5
α=2
α=5
α=1
α=2
3
1
-1
-3
-5
-3
-1
1
3
log10(2D) , log10 (Tc/TF)
log10(Bc/EF)

FIG

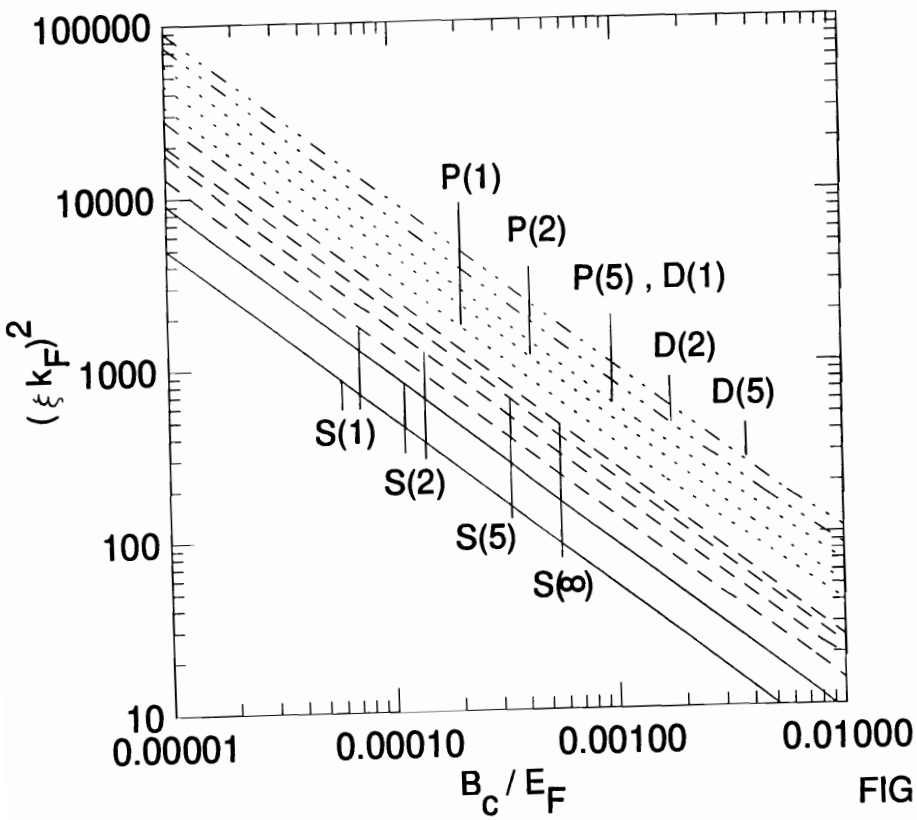

100000
10000
1000
100
10
0.00001
0.00010
0.00100
0.01000
$(\xi k_F)^2$
B_c / E_F
P(1)
P(2)
P(5) , D(1)
D(2)
D(5)
S(1)
S(2)
S(5)
S(∞)

FIG 3

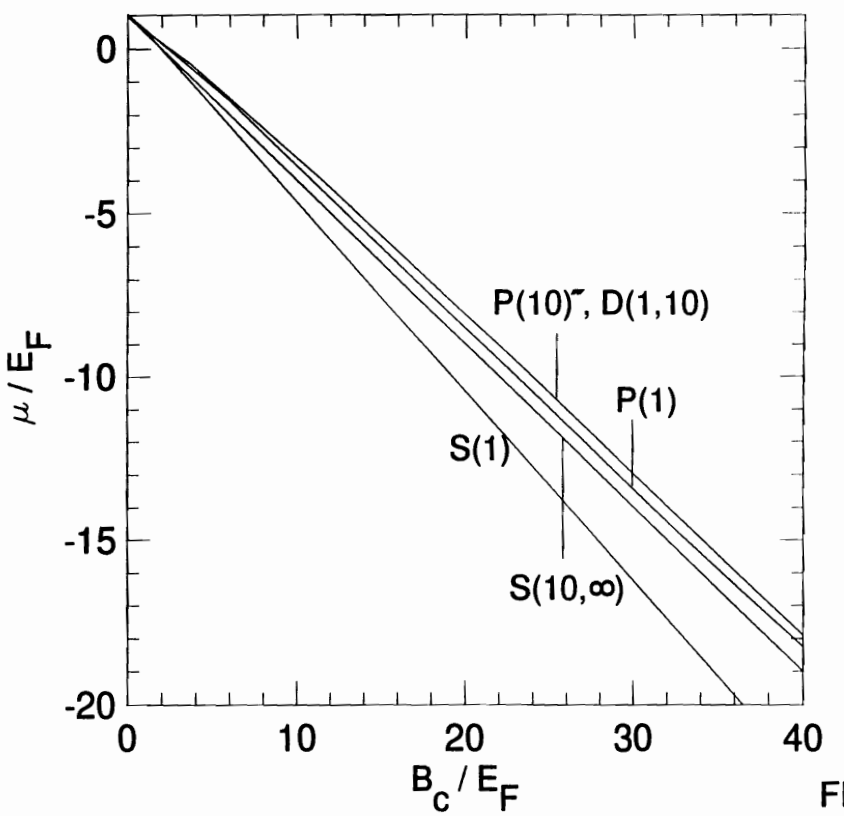

0
-5
-10
-15
-20
0
10
20
30
40
μ / E_F
B_c / E_F
P(10), D(1,10)
P(1)
S(1)
S(10,∞)

FIG 2