EFFECT OF ENERGY DEPENDENCE
ON SUPERCONDUCTIVITY

SOME EFFECTS OF ENERGY DEPENDENCE IN THE ELECTRONIC DENSITY OF STATE ON SUPERCONDUCTIVITY

by

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ABSTRACT

Based on the assumption of unusual fine structure in the electronic density of states close to the Fermi energy, new approximate analytic expressions for the critical temperature, and the gap parameter at absolute zero are obtained. We have represented approximately the rapid variation in $N(\varepsilon)$ by a Lorentzian form of width a and strength g superimposed on a constant background $N(0)$. Further, we have assumed that the Fermi energy falls off the center of the peak. The solutions we have obtained for T_c and $\Delta(0)$ are significantly modified from the BCS solutions although for a & $b >> k_BT_c$ and $\omega_D >> \Delta(0)$ the ratio $2\Delta(0)/k_BT_c$ remains unchanged and equal to 3.54. Mathematical studies have been done for the evaluation of the condensation energy. The shift in the chemical potential as the temperature increases above the absolute zero was calculated and it was found that the correction term due to raising the temperature is negligible and can be ignored without the introduction of any significant error. A modified finite-temperature BCS gap equation has been solved mathematically in which we have obtained a significantly new modified approximate analytic expression for $\Delta(T)$ valid in the limit when $T \rightarrow T_c$. The use of the equation for $\Delta(T)$ helps to evaluate the discontinuity in the electronic specific

heat at the critical temperature. Finally it has been shown that in the low-temperature limit the specific heat is proportional to $e^{-\Delta(0)/k_B T}$ as in BCS theory.

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CHAPTER I

INTRODUCTION

Since several intermetallic compounds possessing the A-15 crystal structure have been found to exhibit exceptionally high T_c 1), for this reason these materials are practically important materials to study since many large scale applications of superconductivity are expected for the 1981's and beyond. In addition to high transition temperatures, it was discovered that these materials possess anomalies in electronic and elastic properties. It was reported by Batterman and Barrett 2) that V_3Si undergoes a structural transformation at temperatures not far above T_c. Shortly afterward the elastic instability of this material was reported by Testardi et al. 3).

Unfortunately as a class and as a phenomenon there are few materials for which so much detailed information is now available due to the fact that these materials have a very complex crystal structure and all involve transition metal elements. Their electronic structure is very complicated and only recently have some preliminary results become available from band structure calculations. Little is known of their lattice dynamics and knowledge of electron-phonon interaction in these materials is even more sketchy.

Attempts have been made to account for the high value of T_c of the A- 5 compounds. The theoretical explanations generally proposed are based on the assumption of unusual fine structure in the electronic density of states at the Fermi level. In 1961 Clogston and Jaccarino$^{4)}$ were the first to suggest the presence in these materials of a peak in the density of electronic states close to which the Fermi level was situated.

The occurrence of high T_c in the A-15 compounds which is of critical importance motivates us to search for the reason why these materials have high T_c compared to the simple metals and try to explain and treat such interesting phenomenon qualitatively and quantitatively. We begin in Chapter II by giving a brief discussion of the weak coupling theory of superconductivity and presenting some facts about A-15 compounds emphasizing their chemical structure which we do believe is an important characteristic of the A-15 leading to a large electron-phonon interaction. Based on these facts about A-15 compounds, a density of state peak model has been suggested with which we shall work in the subsequent chapters were we develop the fundamental equations and calculate some of the thermodynamic properties. In Chapter III we present the mathematics developed for obtaining simple analytic expressions for the critical temperature, the gap parameter at absolute zero $\Delta(0)$, the chemical potential and the condensation energy for the case when the electronic density of states can be represented approximately by a Lorentzian peak of width a, superimposed on a constant background.

In Chapter IV the discontinuity in the electronic specific heat at the critical temperature T_c and its temperature dependence at low temperature are calculated mathematically. In fact this study of the electronic specific heat is a natural extension of our other work to an analytic solution of the modified BCS finite-temperature gap equation for temperatures just below the critical one. In the last chapter we present our conclusions and give the results we have obtained for the theoretical model involving an energy dependent electronic density of states.

CHAPTER II

SUPERCONDUCTIVITY IN A-15 COMPOUNDS

The purpose of this chapter is to discuss very briefly the BCS theory of superconductivity and to display some of the most important recent facts about A-15 compounds. We will start by giving a brief discussion of BCS theory.

In the BCS$^{5)}$ formulation of the theory of superconductivity, it was assumed that in a metal there is an attractive force between pairs of conduction electrons caused by virtual phonon exchange and the repulsive force due to the screened coulomb interaction. For superconductivity to occur the combined effect of the two forces has to be attractive. Further it was assumed that the ground state is constructed by correlating zero momentum singlet electron pairs $(k\uparrow, -k\downarrow)$ neglecting all other electron-electron interactions which are not present in the solution of normal metal problems. The application of this pairing hypothesis results in the reduction of many body problem to a soluble problem which is believed to contain the qualitative features necessary for a description of superconductivity. This theoretical formulation leads to an integral equation for Δ_k which is given by

$$\Delta_k = \frac{1}{\Omega} \sum_{k'} V_{k,k'} \frac{\Delta_{k'}}{2E_{k'}} \{1-2f(\beta E_k)\} \qquad (2.1)$$

where $E_{k'} = (\varepsilon_{k'}^2+\Delta_{k'}^2)^{1/2}$, $\varepsilon_k = (\hbar^2 k^2/2m)-\mu$, μ is the chemical potential, and $V_{kk'}$ is the matrix element for the scattering of a pair of electrons from state $(k\uparrow,-k\downarrow)$ to $(k'\uparrow,-k'\downarrow)$. $V_{kk'}$ is composed of two terms; the first describing the attractive electron-electron interaction mediated by phonons and the second resulting from the screened Coulomb repulsion. In order to calculate measurable quantities, BCS may chose a very simple model in which the interaction $V_{k,k'}$ is assumed to be isotropic i.e. independent of angles and can be replaced by a constant attractive interaction $-V$ within a characteristic energy $h\omega_D$ of the Fermi surface such that

$$V_{k,k'} = \begin{cases} -V & \text{for } |\varepsilon_k|, |\varepsilon_{k'}| \leq \hbar\omega_D \\ 0 & \text{otherwise} \end{cases}$$

By assuming a constant density of states within an energy $\hbar\omega_D$ of the Fermi energy, the summation in equation (2.1) can be replaced by an integral

$$1 = \frac{N(0)V}{2} \int_{-\hbar\omega}^{\hbar\omega} d\varepsilon \, \frac{\{1-2f(\beta E)\}}{E} \qquad (2.2)$$

where $N(0)$ is the density of electron states for one spin direction at the Fermi surface, $E = (\varepsilon^2+\Delta^2)^{1/2}$ and $\Delta_k = \Delta$ for $|\varepsilon_k| \leq \hbar\omega_D$ and $\Delta_k = 0$ otherwise. To find the temperature

T_c at which the transition takes place and the gap parameter at absolute zero, $\Delta(0)$, equation (2.2) has to be solved analytically. Analytic solution for this integral equation gives the following two equations for T_c and $\Delta(0)$ in the weak coupling limit, $N(0)V \ll 1$.

$$kT_c = 1.13\, \hbar\omega_D\, e^{-1/N(0)V} \tag{2.3}$$

and

$$\Delta(0) = 2\hbar\omega_D\, e^{-1/N(0)V} \tag{2.4}$$

Hence in this model the ratio of the energy gap at the absolute zero, to kT_c is a universal constant,

$$2\Delta(0)/kT_c = 3.53$$

independent of the interaction V and of the particular superconductor.

In the BCS theory it was assumed that - as it has been mentioned above - the density of electronic states is constant over the energy range $E_f \pm \hbar\omega_D$ in which it is proportional to the square root of the energy with all states below the Fermi energy E_f are occupied, but in a real metal, specifically the A-15 compounds,the electronic density of states can be much more complicated as can be the Fermi surface between occupied and unoccupied states. The fact of unusual fine structure in the electronic density of states close to which the Fermi level is located on the scale of the Debye energy ω_D has been reported many times[6,7,8,9]. Further, recent self consistent pseudopotential band structure calculations in Nb_3Ge by Ho et al.[11], give several peaks in the electronic density of states with width of the order of 70 mev with the Fermi energy E_f falling near the center of the peak.

We turn now to some important facts about A-15 compounds, and more specifically the crystal structure which we will focus our attention on it. They all have the chemical formula A_3B. There exists over 70 members in the A-15 family. They show anomalies (for some members) in the magnetic susceptibility, Knight shift, elastic constants, electrical resistivity, thermal conductivity, specific heat etc. The relevant part of the periodic table is shown in table (2.1) where the three possible groups of A elements are IVB (Ti,Zr,Hf), VB (V,Nb,Ta) and VIB (Cu,Mo,W). The A-15 structure is shown in Fig. (2.1) for the compound formula A_3B. For the high T_c superconductivity, the A atom is a transition metal atom, usually V or Nb. The B atom is often (but not always) a nontransition metal atom, e.g., Si,Ge,Al,Ga and Sn. The B atoms occur at the bcc sites, while the A atoms occur on the cube faces in pairs with the atoms of each pair separated by half the unit cell length.

A possible relation of the unique properties of the A-15 materials to the crystal structure was first pointed out by Weger (1964)[12]. The transition metal A atoms in this structure form three orthogonal linear chains

Table (2.1)

Periodic Table

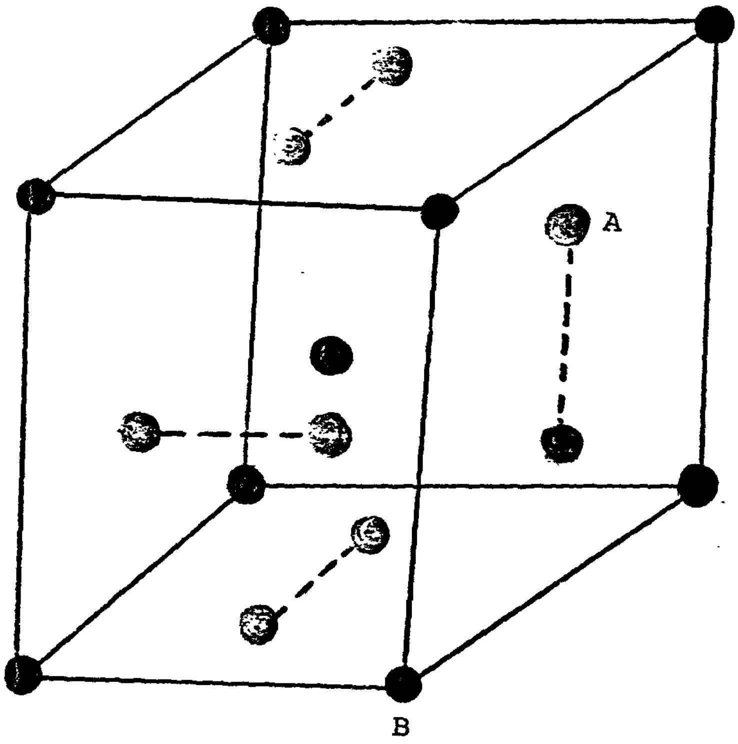
										C		O	F
IVB	VB	VIB							Al	Si	P		
Ti	V	Cr			Co	Ni		Zn	Ga	Ge	As		
Zr	Nb	Mo	Tc	Ru	Rh	Pd		Cd	In	Sn	Sb	Te	
Hf?	Ta	W	Re	Os	Ir	Pt	Au	Hg	Gl	Pb	Bi		

element appearing as A

element appearing as B

Fig. (2.1)

The A-15 cystal structure for the compound formula A_3B. For high T_c superconductors, A is the transition metal atom and B is usually (but not always) a nontransition metal atom.


A
B

Weger (1964) has argued that the electronic band structure of these materials has unusual features which reflect the quasi-one-dimensional nature of these A atom chains. There is in fact evidence from alloying studies confirming the improtance of the A sublattice. It is found that both the high-T_c superconductivity as well as some of the anomalous behavior disappear more rapidly for alloy substitutions on the A sublattice than the B sublattice. In terms of the A-A distance along the chains the A-B distance is 1.12 and the closest A-A distance between the two chains is 1.23. The simplest model is then, that of weakly interacting perpendicular A atom chains with the distance between A atoms along the chain small compared to the cube dimensions.

In Table (2.2)$^{(10)}$ we represent a striking result. From a survey of the existing literature it has been found that for a given element, say Nb, the A-A distance in a chain is not very dependent on the B element. In that case for 13 possible B atoms, the A-A distance is 2.60±0.03 Å. Further we note that this is smaller than the Nb-Nb distance in metallic Nb which is 2.85 Å or .25 Å larger. Thus, we expect the bound between Nb atoms in the chain to be more covalent like than metallic. In a metal, to a first approximation, the free electrons fill the space between the ions more or less in a uniform fashion. If the ion-ion distance is reduced, more electrons must find their way between the ion

Table (2.2)

A-15's ARRANGED BY A ATOM

Group	No. of Compounds	A-Atom	Intra-chain A-A dist. (All distances)	Inter-chain A-A dist. in Å	Metallic A-A dist.	Metallic less Intra-Chain
	8	Ti	2.57 .05	3.16	2.91	.34
IVB	6	Zr	2.80 .03	3.44	3.16	.36
		Hf				
	19	V	2.41 .04	2.96	2.63	.22
VB	13	Nb	2.60 .03	3.20	2.85	.25
	4	Ta	2.61 .04	3.21	2.85	.24
	10	Cr	2.61 .04	2.85	2.49	.17
VlB	12	Mo	2.48 .03	3.05	2.72	.24
	2	W	2.48 .04	3.05	2.73	.25

charge so as to increase the screening otherwise the structure would not be stable. This is an important characteristic fact about these materials. A charge density plot shown in Fig. (2.2) for V_3Si confirms this picture. We note mountains of screening charge around the V ions and ridges of charge between the mountains. Highly directional bounds are clearly seen. We believe that this is an important characteristic of the A-15 leading to a large electron-phonon interaction and consequently to high T_c. The localization of the conduction electrons in the region between the V ions in the chain implies that they interact strongly with them.

Experiments carried out recently by Ghosh and Strogin$^{12)}$ on the normal state electronic specific heat and on the upper critical magnetic field H_{c2}, reveal that when the A-15 compounds (Nb_3Sn, Nb_3Al, Nb_3Ge, V_3Si and MO_3Ge) are damaged by irradiation there exist large variations in the electronic density of states. They believe that the reason for this great variation on irradiation is due to the fact that the density of electronic states is a rapidly changing function of energy near E_f perhaps exhibiting a peak of the order of 100°. Basically such a situation could be represented approximately by a Lorentzian form superimposed on a constant background, specifically

$$N(\varepsilon) = N(0)\{1 + \frac{g}{\pi} \frac{a}{a^2+(\varepsilon-b)^2}\}$$

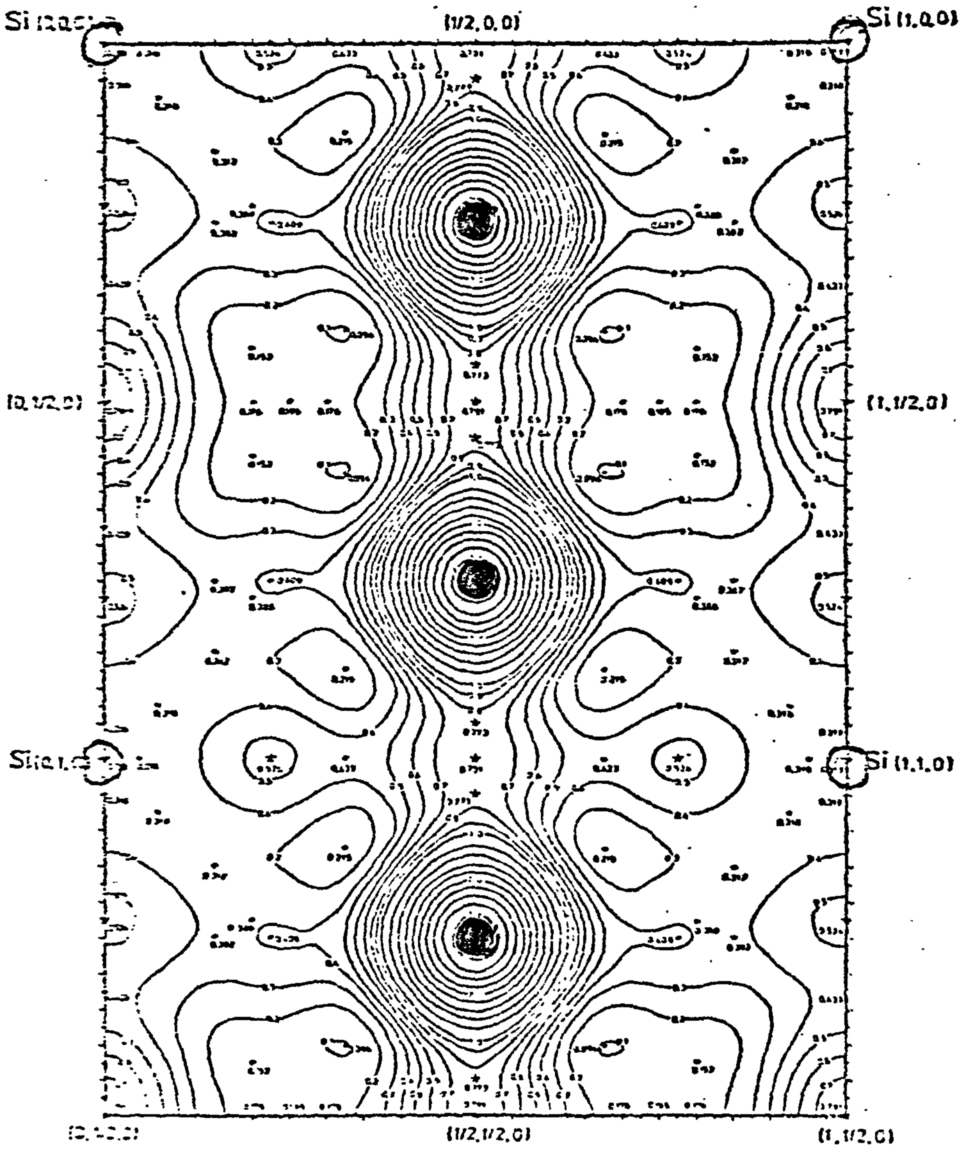
where g is the strength of the Lorentzian peak, a its half

Fig. (2.2)

A charge density plot for V_3Si.

Fig. (2.2)

V_3Si



● V

○ Si

width and b is the center of the Lorentzian. This is the model of the electronic density of states which we will study extensively in this thesis.

CHAPTER III

A THEORETICAL CALCULATION OF THE GAP, THE CRITICAL TEMPERATURE, THE CHEMICAL POTENTIAL AND THE CONDENSATION ENERGY WITH ENERGY DEPENDENT ELECTRONIC DENSITY OF STATES

In this chapter we present analytic expressions for the gap $\Delta(0)$, the critical temperature τ_c, the chemical potential and the condensation energy valid in the case when the electronic density of states $N(\varepsilon)$ varies significantly around the Fermi energy on the scale of the Debye energy ω_D.

3.1 The critical temperature

It is given by the solution of the following equation:

$$1 = V \int_{-\omega_D}^{\omega_D} N(\varepsilon) \frac{\{1-2f(\beta_c\varepsilon)\}}{2\varepsilon} d\varepsilon \qquad (3.1)$$

where V is the pairing potential and $f(\beta_c\varepsilon)$ is the Fermi Dirac temperature factor $1/(e^{\beta_c\varepsilon}+1)$ with $\beta_c = \frac{1}{T_c}$ (in units with $\hbar = k_B = 1$).

To solve analytically for the critical temperature it is convenient to take for $N(\varepsilon)$, a Lorentzian form of width a and strength g superimposed on a constant background of height N(0). Further, the Fermi energy is assumed to fall off the center of the peak. Specifically

$$N(\varepsilon) = N(0)\{1 + \frac{g}{\pi}\,\frac{a}{a^2+(\varepsilon-b)^2}\} \tag{3.2}$$

At the Fermi energy $N(\varepsilon_f = 0) = N(0)(1+D)$ with $D = \frac{g}{\pi a}\,\frac{a^2}{(a^2+b^2)}$ giving the height of the peak (right at the Fermi energy) relative to the background and at the center of the peak $N(\varepsilon=b) = N(0)(1+d)$ with $d = \frac{g}{\pi a}$ giving the height of the centre of the peak relative to the background. The parameter D we have introduced plays an important role in what follows.

With reference to equation (3.2), equation (3.1) can be rewritten as

$$\frac{1}{N(0)V} = \int_0^{\omega_D} \frac{\{1-2f(\beta_c\varepsilon)\}}{\varepsilon}\,d\varepsilon + \frac{ga}{2\pi}\int_{-\omega_D}^{\omega_D} \frac{\{1-2f(\beta_c\varepsilon)\}}{\varepsilon}\,\frac{1}{a^2+(\varepsilon-b)^2}\,d\varepsilon$$

$$= \ell n\{\frac{1.13\omega_D}{T_c}\} + \frac{ga}{2\pi}\int_{-\omega_D}^{\omega_D} d\{\frac{1}{2(a^2+b^2)}\,\ell n(\frac{\varepsilon^2}{a^2+(\varepsilon-b)^2}) +$$

$$\frac{(b/a)}{(b^2+a^2)}\tan^{-1}(\frac{\varepsilon-b}{a})\}(1-2f(\beta_c\varepsilon))d\varepsilon \tag{3.3}$$

Performing an integration by parts in the last integral gives

$$\frac{1}{N(0)V} = \ell n[\frac{1.13\omega_D}{T_c}] + \frac{ga}{2\pi}\Bigg[\Bigg|\,[\frac{1}{2(a^2+b^2)}\,\ell n[\frac{\varepsilon^2}{a^2+(\varepsilon-b)^2}] +$$

$$\frac{b/a}{a^2+b^2}\tan^{-1}[\frac{\varepsilon-b}{a}]\Bigg](1-2f(\beta_c\varepsilon))\Bigg|_{-\omega_D}^{\omega_D} - \int_{-\omega_D}^{\omega_D}[\frac{1}{2(a^2+b^2)}\,\ell n[\frac{\varepsilon^2}{a^2+(\varepsilon-b)^2}]$$

$$+ \frac{b/a}{(a^2+b^2)}\tan^{-1}[\frac{\varepsilon-b}{a}]\Bigg]\,\frac{d}{d\varepsilon}\,(1-2f(\beta_c\varepsilon))d\varepsilon\Bigg] \tag{3.4}$$

Using the fact that

$$1-2f(\varepsilon\beta_c) \rightarrow \begin{cases} 1 & \omega_D \rightarrow \infty \\ -1 & \omega_D \rightarrow \infty \end{cases}$$

equation (3.4) can be written as

$$\frac{1}{N0)V} = \ell n\{\frac{1.13\omega_D}{T_c}\} + \frac{ga}{\pi(a^2+b^2)} \Bigg[\frac{1}{2}\, \ell n[\frac{1}{\sqrt{[(\frac{a}{\omega})^2+(\frac{\omega-b}{\omega})^2][(\frac{a}{\omega})^2+(\frac{\omega+b}{\omega})^2]}}]$$

$$+ \frac{b}{2a}\{\tan^{-1}(\frac{\omega-b}{a})-\tan^{-1}(\frac{\omega+b}{a})\} - \int_{-\omega_D}^{\omega_D} \frac{1}{4}\,\ell n(\varepsilon^2)\, \frac{d}{d\varepsilon}\,(1-2f(\beta_c\varepsilon))d\varepsilon$$

$$+ \int_{-\omega_D}^{\omega_D} \frac{1}{4}\,\ell n(a^2+(\varepsilon-b)^2)\frac{d}{d\varepsilon}(1-2f(\beta_c\varepsilon))d\varepsilon - \int_{-\omega_D}^{\omega_D} \frac{b}{2a}\tan^{-1}(\frac{\varepsilon-b}{a}) \times$$

$$\cdot \frac{d}{d\varepsilon}\,(1-2f(\beta_c\varepsilon))d\varepsilon \Bigg] \qquad (3.5)$$

Since the differential of the Fermi function $f'(\beta\varepsilon)$ is negligible except in the neighbourhood of the Fermi energy and since $b >> k_BT_c$ the integral in equation (3.5) can be done as follows

$$\frac{1}{N(0)V} = \ell n\{\frac{1.13\omega_D}{T_c}\} + \frac{ga}{\pi(a^2+b^2)} \Bigg[\ell n[\frac{1}{\sqrt{[(\frac{a}{\omega})^2+(\frac{\omega-b}{\omega})^2]^{1/2}\,[(\frac{a}{\omega})^2+(\frac{\omega+b}{\omega})^2]^{1/2}}}]$$

$$+ \frac{b}{2a}\{\tan^{-1}(\frac{\omega-b}{a})-\tan^{-1}(\frac{\omega+b}{a})\} - \int_{-\omega_D}^{\omega_D} \frac{1}{4}\,\ell n(\varepsilon^2)\frac{d}{d\varepsilon}(1-2f(\beta_c\varepsilon))d\varepsilon$$

$$+ \frac{1}{4}\,\ell n(a^2+b^2) \int_{-\omega_D}^{\omega_D} \frac{d}{d\varepsilon}(1-2f(\beta_c\varepsilon))d\varepsilon + \frac{b}{2a}\tan^{-1}\frac{b}{a}\int_{-\omega_D}^{\omega_D}\frac{d}{d\varepsilon}(1-2f(\beta\varepsilon_c))d\varepsilon\Bigg] \qquad (3.6)$$

But

$$\int_{-\omega_D}^{\omega_D} \frac{d}{d\varepsilon}\,(1-2f(\beta_c\varepsilon)) = 1-2f(\beta_c\varepsilon)\Big|_{-\omega_D}^{\omega_D} = 2$$

(to a very good approximation, since $\omega_D >> kT_c$). Therefore equation (3.6) can be reduced to

$$\frac{1}{N(0)V} = \ell n\{\frac{1.13\omega_D}{T_c}\} + \frac{ga}{\pi(a^2+b^2)}\Bigg[\ell n[\frac{1}{\sqrt{(\frac{a}{\omega})^2+(\frac{\omega-b}{\omega})^2]^{1/2}\,[(\frac{a}{\omega})^2+(\frac{\omega+b}{\omega})^2]^{1/2}}}]$$

$$+ \frac{b}{2a}\{\tan^{-1}(\frac{\omega-b}{a})-\tan^{-1}(\frac{\omega+b}{a})\} + \frac{b}{a}\tan^{-1}(\frac{b}{a}) + \frac{1}{2}\,\ell n(a^2+b^2)$$

$$- \int_{-\omega_D}^{\omega_D}\frac{1}{4}\,\ell n(\varepsilon^2)\,\frac{d}{d\varepsilon}\,(1-2f(\beta_c\varepsilon))d\varepsilon\Bigg] \qquad (3.7)$$

The last integral in equation (3.7) can be done as follows:

$$- \int_{0}^{\omega_D} \ell n\;\varepsilon\,\frac{d}{d\varepsilon}\,\{1-2f(\beta_c\varepsilon))\} \equiv 2\int_0^{\beta_c\omega} \ell n(\frac{x}{\beta_c})\frac{d}{dx}\,\{\frac{1}{e^x+1}\}\,dx$$

when a change of variable to $x = \beta_c\varepsilon$ is made. Since $\omega_D\beta_c >> 1$, therefore it can be replaced by infinity with sufficient accuracy because of the peak nature of Fermi Dirac distribution function.

Thus

$$- \int_0^{\omega_D} \ell n\varepsilon \; \frac{d}{d\varepsilon} \{1-2f(\beta_c \varepsilon)\} \equiv \int_0^{\infty} 2\ell n x \; \frac{d}{dx} \{\frac{1}{e^x+1}\} \, dx -$$

$$2\ell n\beta_c \int_0^{\infty} \frac{d}{dx} \{\frac{1}{e^x+1}\} dx \; .$$

The first integral is a number which can be written in terms of Euler's constant $\ell n \; \gamma$ as $\ell n(2\gamma/\pi)$. Since the ratio $(2\gamma/\pi)$ is 1.13. The last integral in equation (3.7) is given by $\ell n \; \{\frac{1.13}{T_c}\}$.

The temperature T_c at which the transition takes place is then given by

$$\frac{1}{N(0)V} = (1+D)\,\ell n\{\frac{1.13\omega_D}{T_c}\}+D\left[\ell n\left[\frac{\sqrt{a^2+b^2}}{\sqrt{[a^2+(\omega-b)^2]^{1/2}[a^2+(\omega+b)^2]^{1/2}}}\right] + \frac{b}{2a}\;[2\tan^{-1}(\frac{b}{a}) + \tan^{-1}(\frac{\omega-b}{a}) - \tan^{-1}(\frac{\omega+b}{a})]\right] \qquad (3.8)$$

which after rearrangement, gives

$$k_B T_c \;=\; 1.13 \; \hbar\omega_D \; H^{(\frac{D}{1+D})} \; e^{-\frac{1}{N(O)V(1+D)}} \qquad (3.9)$$

$$H = \left[\frac{\sqrt{a^2+b^2}}{\sqrt{[a^2+(\omega_D-b)^2]^{1/2}[a^2+(\omega_D+b)^2]^{1/2}}}\right]\exp\{\frac{b}{2a}\;[2\tan^{-1}(\frac{b}{a}) + \tan^{-1}(\frac{\omega-b}{a})-\tan^{-1}(\frac{\omega+b}{a})]\}$$

and

$$D = \frac{g}{\pi} \;\; \frac{a^2}{(a^2+b^2)} \; .$$

This is our final equation for the critical temperature. We note that it is the electronic density of states $N(0)(1+D)$ right at the Fermi energy that enters the exponential. Further, the pre exponential factor is modified from BCS by the quantity

$$H^{(\frac{D}{1+D})} \equiv B$$

which is new. The critical temperature is therefore B times the value of T_c (say $T_c°$) obtained by assuming $N(\varepsilon)$ to be a constant equal to its value at the Fermi energy.

3.2 The energy gap $\Delta(0)$

The gap in the quasiparticle excitation spectrum $\Delta(0)$ is given by

$$1 = \frac{V}{2}\int_{-\omega_D}^{\omega_D} d\varepsilon \, \frac{N(\varepsilon)}{\sqrt{\varepsilon^2+\Delta^2(0)}} \, . \tag{3.10}$$

Direct substitution from equation (3.2) into this equation gives

$$\frac{1}{N(0)V} = \ell n[\frac{2\omega_D}{\Delta(0)}] + \frac{ga}{2\pi}\int_{-\omega_D}^{\omega_D} \frac{d\varepsilon}{\sqrt{\varepsilon^2+\Delta^2}[a^2+(\varepsilon-b)^2]} \tag{3.11}$$

To integrate the last part in equation (3.11), the substitution $\varepsilon = \frac{x^2-\Delta^2}{2x}$ is suggested, and thus by explicit differentiation

$$d\varepsilon = \frac{1}{2}\,[1+\frac{\Delta^2(0)}{x^2}]dx$$

and in terms of the new variable x the integral of interest can be written as

$$\int_{-\omega_D}^{\omega_D} \frac{d\varepsilon}{\sqrt{\varepsilon^2+\Delta^2(0)}\,[a^2+(\varepsilon-b)^2]} \equiv \int_{\alpha}^{\gamma} \frac{4x\,dx}{4x^2a^2+[x^2-\Delta^2(0)-2bx]^2}$$

with α and γ (the new boundaries) given by

$$\alpha = -\omega_D \pm \sqrt{\omega_D^2+\Delta^2(0)} \quad \text{corresponding to } \varepsilon = -\omega_D \tag{3.12a}$$

$$\gamma = \omega_D \pm \sqrt{\omega_D^2+\Delta^2(0)} \quad \text{corresponding to } \varepsilon = \omega_D \tag{3.12b}$$

To carry out the indefinite integral $I = \int \frac{4x\,dx}{4x^2a^2+[x^2-\Delta^2(0)-2bx]^2}$ we proceed as follows

$$I = \int \frac{dx}{-ia}\,[\frac{1}{[x^2-2bx-\Delta^2(0)]+2ixa} - \frac{1}{[x^2-2bx-\Delta^2(0)]-2iax}] \tag{3.13}$$

which can be reduced to

$$I = \frac{1}{ia}\,[\int \frac{dy}{y^2-A^2} - \int \frac{d\bar{y}}{\bar{y}^2-\bar{A}^2}]$$

with

$y = x-(b+ia) \quad ; \quad A^2 = (b-ia)^2+\Delta^2(0)$

$\bar{y} = x-(b-ia) \quad ; \quad \bar{A}^2 = (b-ia)^2+\Delta^2(0)$

so that

$$I = \frac{1}{ia}\left[\frac{1}{2\sqrt{(b+ia)^2+\Delta^2(0)}}\,\ell n\left[\frac{x-(b+ia)-\sqrt{(b+ia)^2+\Delta^2(0)}}{x-(b+ia)+\sqrt{(b+ia)^2+\Delta^2(0)}}\right] - \frac{1}{2\sqrt{(b\ ia)^2+\Delta^2(0)}}\,\ell n\left[\frac{x-(b\ ia)-\sqrt{(b-ia)^2+\Delta^2(0)}}{x-(b-ia)+\sqrt{(b-ia)^2+\Delta^2(0)}}\right]\right] \qquad (3.14$$

The quantities $\sqrt{(b+ia)^2+\Delta^2(0)}$ and $\sqrt{(b-ia)^2+\Delta^2(0)}$ can be expressed as

$$\sqrt{(b+ia)^2+\Delta^2(0)} = [(b^2-a^2+\Delta^2(0)^2+4a^2b^2]^{1/4}\exp\{\tfrac{i}{2}[\tan^{-1}\frac{2ab}{b^2-a^2+\Delta^2(0)} + .5(1-\mathrm{sgn}(b^2-a^2+\Delta^2(0)))(\pi\,\mathrm{sgn}2ab)\}$$

$$\equiv F + iG \qquad (3.15)$$

Similarly

$$\sqrt{(b-ia)^2+\Delta^2(0)} \equiv F-iG \qquad (3.16)$$

with

$$F = [(b^2-a^2+\Delta^2(0))^2+4a^2b^2]^{1/4}\cos\{.5[\tan^{-1}\frac{2ab}{b^2-a^2+\Delta^2(0)} + .5(1-\mathrm{sgn}(b^2-a^2+\Delta^2(0)) \times (\pi\,\mathrm{sgn}\ 2ab)]\}\ ;$$

$$G = [(b^2-a^2+\Delta^2(0))^2+4a^2b^2]^{1/4}\sin\{.5[\tan^{-1}\frac{2ab}{b^2+a^2+\Delta^2(0)} + .5(1-\mathrm{sgn}(b^2-a^2+\Delta^2)) \times (\pi\,\mathrm{sgn}\ 2ab)]\}$$

and

$$F^2 + G^2 = \sqrt{(b^2-a^2+\Delta^2(0))^2+4a^2b^2}$$

Because of the definition given for F and G by equations (3.15) and (3.16) it is found to be convenient to express our final result for I in terms of one of them rather than in terms of both of them. This has been done by working out the relation between F and G. By definition

$$F + iG = \sqrt{(b+ia)^2+\Delta^2(0)}$$

$$F^2-G^2+2iGF = b^2-a^2+\Delta^2(0)+2iab$$

Therefore

$$F^2-G^2 = b^2-a^2 + \Delta^2(0) \tag{3.17}$$

$$GF = ab \Rightarrow G = \frac{ab}{F} \tag{3.18}$$

The solution of equation (3.17) gives

$$F^2 = [\frac{(a^2-b^2-\Delta^2(0)) \pm \sqrt{(a^2-b^2-\Delta^2(0))^2+4a^2b^2}}{2}$$

Since F is real, therefore $F^2 > 0$, and hence

$$F = \frac{1}{\sqrt{2}} \sqrt{(\Delta^2(0)+b^2-a^2) + \sqrt{(\Delta^2(0)+b^2-a^2)^2+4a^2b^2}} \tag{3.19}$$

+ve sign has been taken, since F has to be real. Then I can be written in terms of F as

$$I = \frac{-1}{a\sqrt{(b^2+\Delta^2(0)-a^2)^2+4a^2b^2}}\{\frac{ab}{2F}\ \ell n[\frac{F^2(x-b-F)^2+a^2(F+b)^2}{F^2(x-b+F)^2+a^2(F-b)^2}] +$$

$$F[\tan^{-1}(\frac{a(F+b)}{F(x-b-F)}) + .5[1-\mathrm{sgn}F(x-b-F)]\mathrm{sgn}a(F+B)\pi$$

$$-\tan^{-1}(\frac{a(F+b)}{F(x-b+F)}) - .5[1-\mathrm{sgn}F(x-b+F)]\mathrm{sgn}(F-b)\pi\} \qquad (3.20)$$

where we have used equation (3.14) and the relation

$\ell n(A\pm iC) = \frac{1}{2}\ \ell n(A^2+C^2)\pm i[\tan^{-1}(\frac{C}{A}) + .5(1-\mathrm{sgn}A)\mathrm{sgn}C\pi]$.

The complete exact solution for the gap in the quasi-particle excitation spectrum $\Delta(0)$ is then given by

$$\frac{1}{N(0)V} = \ell n[\frac{2\omega_D}{\Delta(0)}] + \frac{ga}{2\pi}\Big|I\Big|_{\alpha}^{\gamma} \qquad (3.21)$$

with I, α and γ given respectively by equations (3.20) and (3.12).

Since $\varepsilon = \frac{x^2-\Delta^2(0)}{2x}$ is a double valued function, choosing +ve sign or -ve sign solutions for α and γ will give the same answer. As a consequence of this we have used the +ve sign solutions for α and γ in the following steps.

The last equation simplifies considerably if we assume that $a >> \Delta(0)$, $b >> \Delta(0)$ and $\omega_D >> \Delta(0)$. By taking into account these facts the expression for F can be approximated as follows

Direct substitution from equations (3.23), (3.24) and (3.25) into equation (3.20) and then into equation (3.21) gives

$$\frac{1}{N(0)V} = \ell n[\frac{2\omega_D}{\Delta(0)}] - \frac{g}{\pi a}\frac{a^2}{(a^2+b^2)}[\frac{1}{4}\ell n[\frac{(2\omega_D-2b)^2+4a^2}{(2\omega_D+\frac{b}{2}\Delta^2(0)\delta)^2+(\frac{a}{2}\Delta^2(0)\delta)^2} \times$$

$$\frac{\Delta^4(0)[(\frac{1}{2\omega_D}+\frac{b}{2}\delta)^2+(a\delta/2)^2]}{(\frac{1}{2}\frac{\Delta^2}{\omega_D}-2b)^2+4a^2}] + \frac{b}{2a}\{\tan^{-1}(\frac{a}{\omega_D-b}) + .5(1-\mathrm{sgn}(\omega_D-b)\pi\,\mathrm{sgn}a$$

$$\tan^{-1}[\frac{2ab}{b(\frac{\Delta^2(0)}{2\omega_D}-2b)}] - .5[1-\mathrm{sgn}b(\frac{\Delta^2(0)}{2\omega_D}-2b)]\pi\,\mathrm{sgn}(2ab) -$$

$$\tan^{-1}[\frac{a(b\Delta^2(0)\delta/2}{b(2\omega_D+b\Delta^2(0)\delta/2)}] -.5[1-\mathrm{sgn}b(2\omega_D+b\Delta^2(0)\delta/2)\pi\,\mathrm{sgn}a(b\Delta^2(0)\delta/2)$$

$$+ \tan^{-1}[\frac{ab\Delta^2(0)\delta/2}{b(\frac{\Delta^2(0)}{2\omega_D}+\Delta^2(0)b\delta/2)}] + .5[1-\mathrm{sgn}b(\frac{\Delta^2(0)}{2\omega_D}\Delta^2(0)b\delta/2)]\pi\,\mathrm{sgn}$$

$$\times (ab\Delta^2(0)\delta/2)\} \qquad (3.26)$$

It is a fact that the quantities $(\Delta^2(0)/a^2+b^2)$ or $(\Delta^2(0)/\omega_D)$ are almost negligible with respect to unity which generally allows us to neglect such terms without the introduction of any large error.

Therefore

$$\frac{1}{N(0)V} = \ell n[\frac{2\omega_D}{\Delta(0)}]D\{\ell n[(\frac{2\omega_D}{\Delta(0)}) \frac{\sqrt{a^2+b^2}}{\sqrt{[(\omega_D-b)^2+a^2]^{1/2}[(\omega_D+b)^2+a^2]^{1/2}}}]$$

$$- \frac{b}{2a}\ [\tan^{-1}(\frac{a}{\omega_D-b}) + .5[1-\text{sgn}(\omega_D-b)]\pi \text{sgna} + \tan^{-1}(\frac{a}{b})$$

$$- \pi + \tan^{-1}(\frac{a\omega_d}{a^2+b^2+b^{\omega}D})]\}$$

which after rearrangement, gives

$$\Delta(0) = 2\omega_D E^{\frac{D}{D+1}} \exp[\frac{1}{N(0)V(1+D)}] \qquad (3.27)$$

with

$$E = \frac{\sqrt{a^2+b^2}}{\sqrt{[(\omega_D-b)^2+a^2]^{1/2}[(\omega_D+b)^2+a^2]^{1/2}}} \exp\{\frac{-b}{2a}\ [\tan^{-1}(\frac{a}{\omega_D-b}) +$$

$$.5[1-\text{sgn}(\omega_D-b)]\pi\text{sgn}(a)+\tan^{-1}(\frac{a}{b})-\pi +$$

$$\tan-1\ \frac{a\omega_D}{a^2+b^2+b\omega_D}]\}\ .$$

Equation (3.27) is our final equation for the gap parameter at the absolute zero. Similar to the T_c calculation, we note that, it is the electronic density of states N(0)(1+D) right at the Fermi energy, that enters in the exponential. Further the pre exponential factor is modified from BCS by the quantity $E^{\frac{D}{1+D}}$. Numerical calculation for the ratio $2\Delta(0)/k_BT_c$ reveals that this ratio remains unchanged and equal to the BCS value of 3.54 which implies $E = H$. To prove this analytically we proceed as follows:

If $\omega_D-b > 0$, the expression for E becomes

$$E = Z\exp\{\frac{-b}{2a}\{\tan^{-1}\frac{a}{\omega_D-b} + \tan^{-1}\frac{a}{b} - \pi + \tan^{-1}\frac{a\omega_D}{a^2+b^2+b\omega_D}\}\} \qquad (3.28)$$

where

$$Z = \frac{\sqrt{a^2+b^2}}{\sqrt{[(\omega_D-b)^2+a^2]^{1/2}[(\omega_D+b)^2+a^2]^{1/2}}}$$

If $\omega_D-b < 0$ the expression for E becomes

$$E = Z\exp\{\frac{-b}{2a}\{\tan^{-1}\frac{a}{\omega_D-b} + \tan^{-1}\frac{a}{b} + \tan^{-1}\frac{a\omega_D}{a^2+b^2+b\omega_D}\}\} \qquad (3.29)$$

In the analytic expression for T_c we have

$$H = Z\exp\{\frac{b}{2a}\{2\tan^{-1}\frac{b}{a} + \tan^{-1}\frac{\omega_D-b}{a} - \tan^{-1}\frac{\omega_D+b}{a}\}\}. \qquad (3.30)$$

This expression can be written as

$$H = Z\exp\{\frac{b}{2a}\{\frac{\pi}{2} - \tan^{-1}\frac{a}{\omega_D-b} + \frac{\pi}{2} - \tan^{-1}\frac{a}{b} + \tan^{-1}\frac{b}{a} - \tan^{-1}\frac{\omega_D+b}{a}\}\} \qquad (3.31)$$

where we have used the identity

$$\tan^{-1} x \pm \tan^{-1} y = \tan^{-1}\frac{z\pm y}{1\mp xy}$$

$$\text{for } \left|\tan^{-1} x + \tan^{-1} y \le \frac{\pi}{2}\right|$$

equation (3.31) can be written as

$$H = z\exp\{\frac{-b}{2a}\{\tan^{-1}\frac{a}{\omega_D-b} + \tan^{-1}\frac{a}{b} - \pi + \tan^{-1}\frac{a\omega_D}{a^2+b^2+b\omega_D}\}\} \qquad (3.32)$$

where this equation is valid when $\omega_D-b > 0$. Similarly when $\omega_D-b < 0$ we can prove that

$$H = Z\exp\{\frac{-b}{2a}\{\tan^{-1}\frac{a}{\omega_D-b} + \tan^{-1}\frac{a}{b} + \tan^{-1}\frac{a\omega_D}{a^2+b^2+b\omega_D}\}\} \qquad (3.33)$$

which proves analytically that $E = H$. Thus the ratio $2\Delta/k_B T_c$ remains at its B.C.S value.

For the purpose of numerical calculation, the Newton-Raphson method has been used in solving equations (3.1) and (3.10) for T_c and $\Delta(0)$. Convergence to within 10^{-8} was obtained after two or four iterations (on the average). In addition to this, the approximate analytic solutions for T_c and $\Delta(0)$, equations (3.9) and (3.27) have been evaluated numericall. The results of these numerical calculations are illustrated in the following Figs. where we plot the exact and the approximate solutions for T_c and $\Delta(0)$ against b.

In Figs. (3.1.a), (3.1.b) and (3.1.c), the calculated values for T_c are plotted against b for $a = 5$, 10 and 15 mev, $N(0)V = .15$, $g = 5.5$ mev, and $\omega_D = 35$ mev. A set of three graphs for the same values of a and ω_D but for $N(0)V = .25$ are shown in Figs. (3.2). In addition Figs. (3.3.a) and (3.3.b) show T_c against b for $a = 5$ and 10 mev, $N(0)V = .25$ and $\omega_D = 20$ mev. Similar to the work done for T_c we have produced another set of graphs for the exact and approximate solutions for $\Delta(0)$ for the same values of a, N(0)V and ω_D mentioned above.

It can be seen very clearly from these graphs that T_c or $\Delta(0)$ decrease very rapidly as a function of b specifically in the region as b ranges from 0 to ω_D. In this case we are within the peak in the electronic density of states, then it starts to saturate beyond $b \simeq \omega_D$ and reaches the BCS value. Good agreement between the exact and the approximate solutions for $\Delta(0)$ and T_c can be clearly seen, except in a few cases (Figs. 3.2.a and (3.5.a)). The agreement is not so good at small values of a and b which can be attributed to the neglect of the higher order terms in the approximation we have made for T_c and $\Delta(0)$.

In Figs. (3.7) and (3.8) we plot the ratio $2\Delta(0)/T_c$ corresponding to the exact solution for T_c and $\Delta(0)$ which shows this ratio remains unchanged and equal to the BCS value 3.53 except for unrealistically small values of a and b which are not of great interest.

The graphs we have shown for the critical or for the gap parameter $\Delta(0)$ indicate that our analytic approximate solutions for both are good enough for all practical purposes of interest. They deviate mainly for small values of a and b which are in any case not physically realizable. This motivates us to go back and look at the pre exponential factor - in the analytic T_c equation - including the energy dependence of the electronic density of states. This factor may be rewritten in the more convenient form as

$$B = H^{\left\{\frac{d}{1+d+\bar{b}^2}\right\}}$$

with

$$H = \sqrt{\frac{1+\bar{b}^2}{\{1+(\bar{\omega}-\bar{b})^2\}^{1/2}\{1+(\bar{\omega}+\bar{b})^2\}^{1/2}}}\; e^{\frac{\bar{b}}{2}\{\tan^{-1}(\bar{\omega}-\bar{b})-\tan^{-1}(\bar{\omega}+\bar{b})+2\tan^{-1}\bar{b}\}}$$

Fig. (3.1.a)

A plot of T_c (mev) versus b (mev) for the exact (——) and the approximate (•••••) solutions for T_c for $a = 5$ mev, $\omega_D = 35$ mev and $N(0)V = .15$.

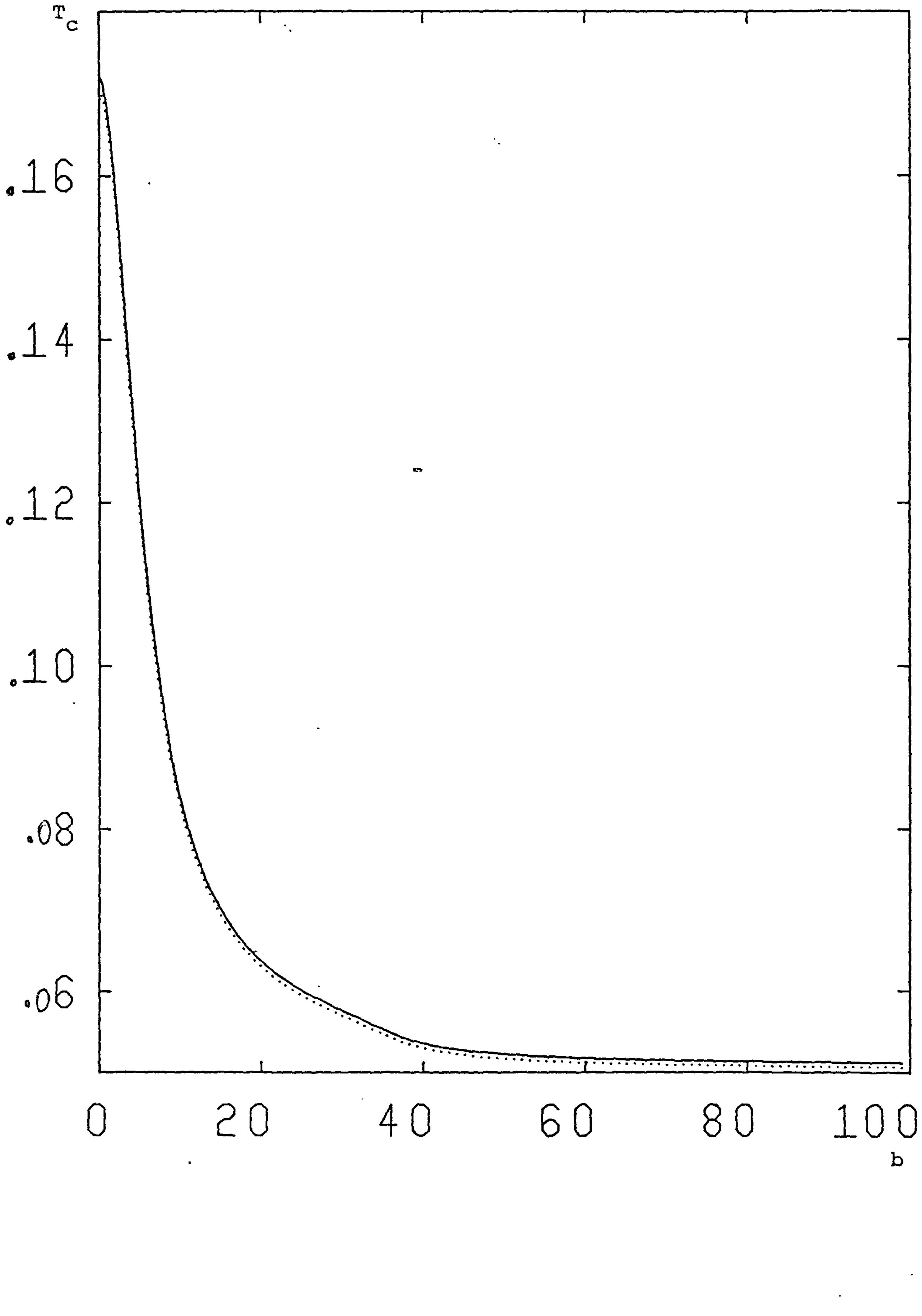

T_c
.16
.14
.12
.10
.08
.06
0
20
40
60
80
100
b

Fig. (3.1.b)

A plot of T_c (mev) versus b (mev) for the exact (——) and the approximate (·····) solutions for T_c for $a = 10$ mev, $\omega_D = 35$ mev and $N(0)V = .15$.

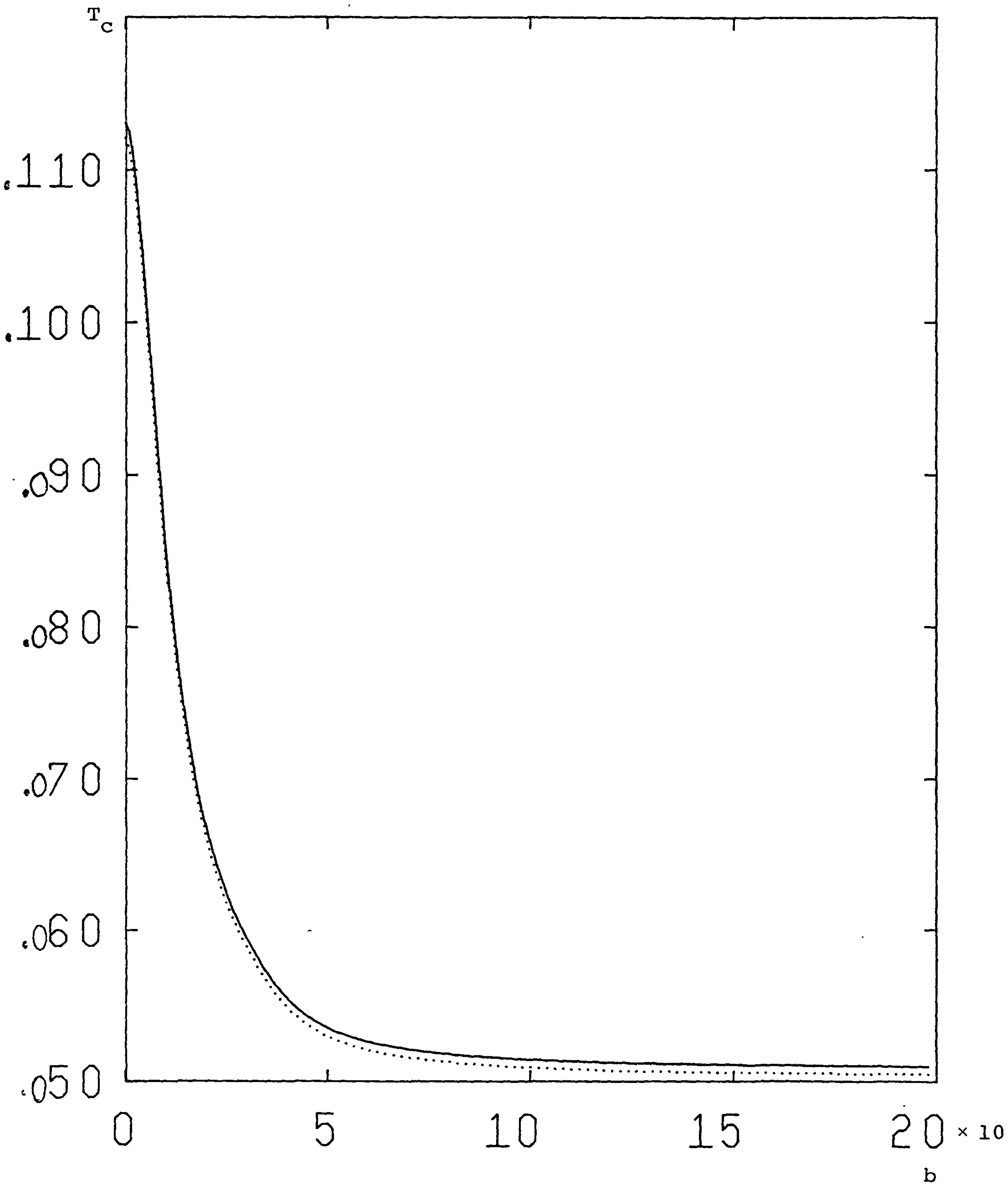
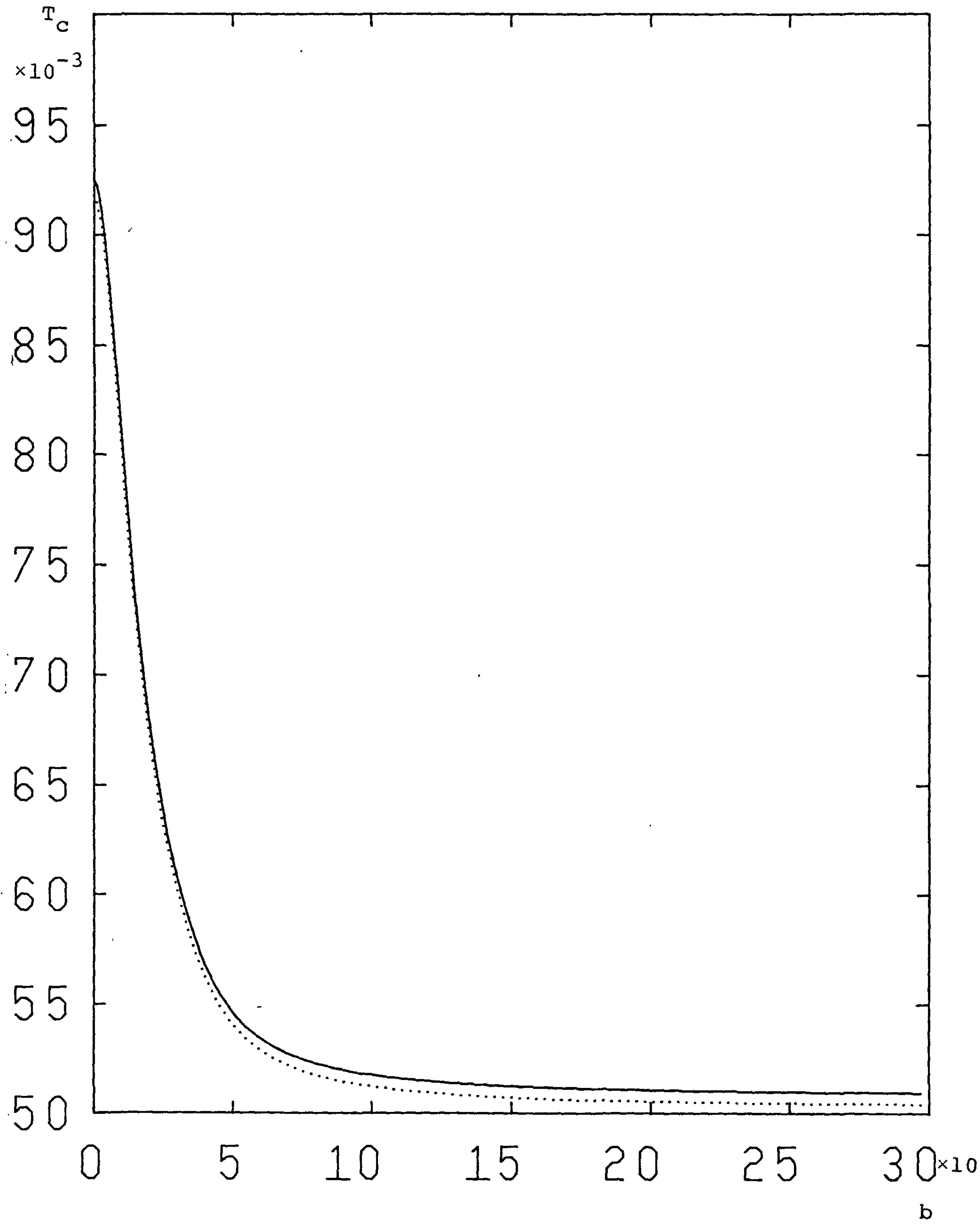

T_c
.110
.100
.090
.080
.070
.060
.050
0
5
10
15
20
× 10
b

Fig. (3.1.c)

A plot of T_c (mev) versus b (mev) for the exact (———) and the approximate (•••••) solutions for T_c for $a = 15$ meV, $\omega_D = 35$ mev and $N(0)V = .15$.



T_c
$\times 10^{-3}$
95
90
85
80
75
70
65
60
55
50
0
5
10
15
20
25
30
$\times 10$
b

Fig. (3.2.a)

A plot of T_c (mev) versus b (mev) for the exact (———) and the approximate (•••••) solutions for T_c for $a = 5$ mev, ω_D = 35 meV and N(0)V = .25.

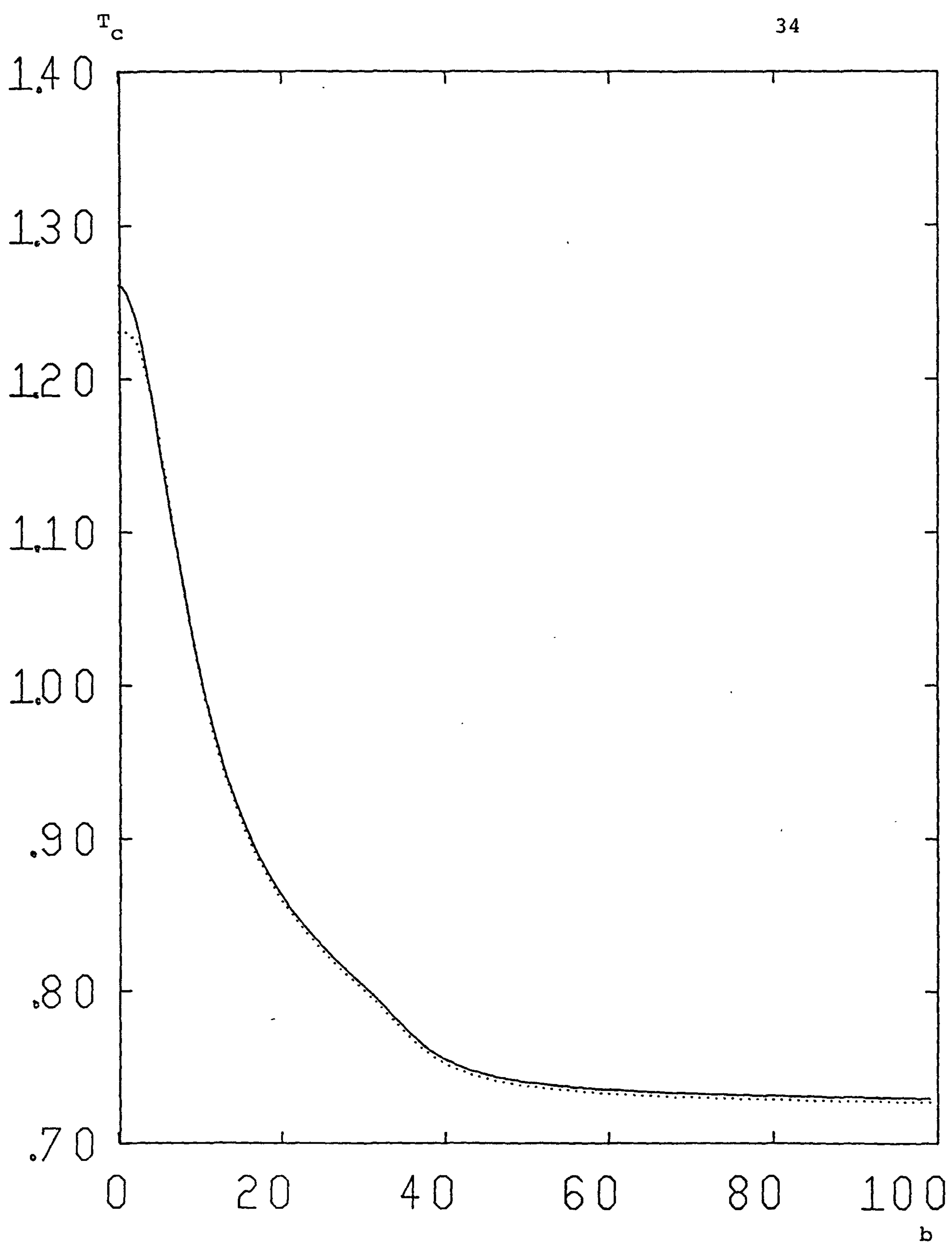

T_c
1.40
1.30
1.20
1.10
1.00
.90
.80
.70
0
20
40
60
80
100
b

Fig. (3.2b)

A plot of T_c (mev) versus b (mev) for the exact (———) and the approximate (·····) solutions for T_c for $a = 10$ mev, $\omega_D = 35$ mev and $N(0)V = .25$.

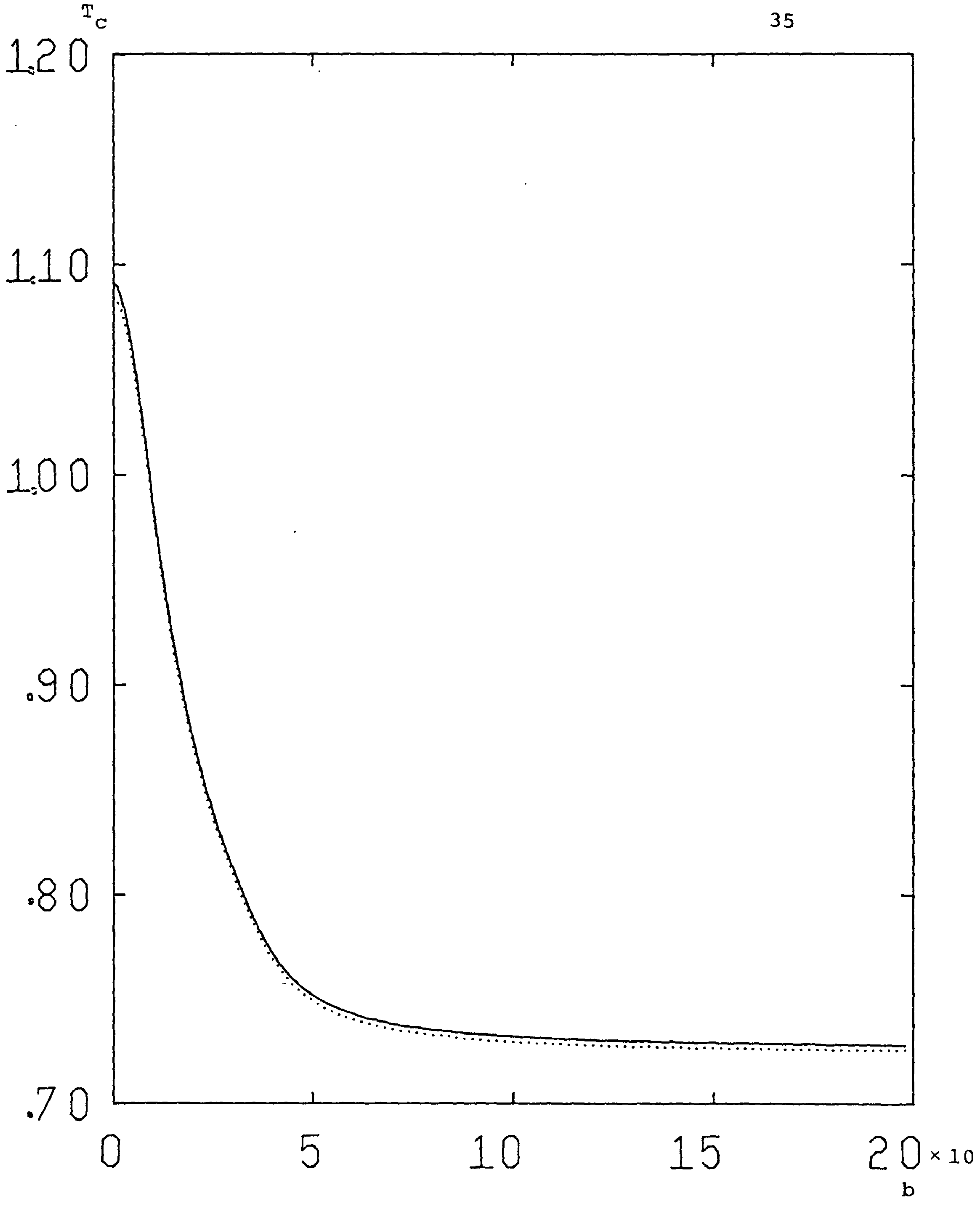

T_c
1.20
1.10
1.00
.90
.80
.70
0
5
10
15
20
× 10
b

Fig. (3.2c)

A plot of T_c (mev) versus b for the exact (———) and the approximate (•••••) solutions for T_c for a = 15 mev, ω_D = 35 mev and N(0)V = .25.

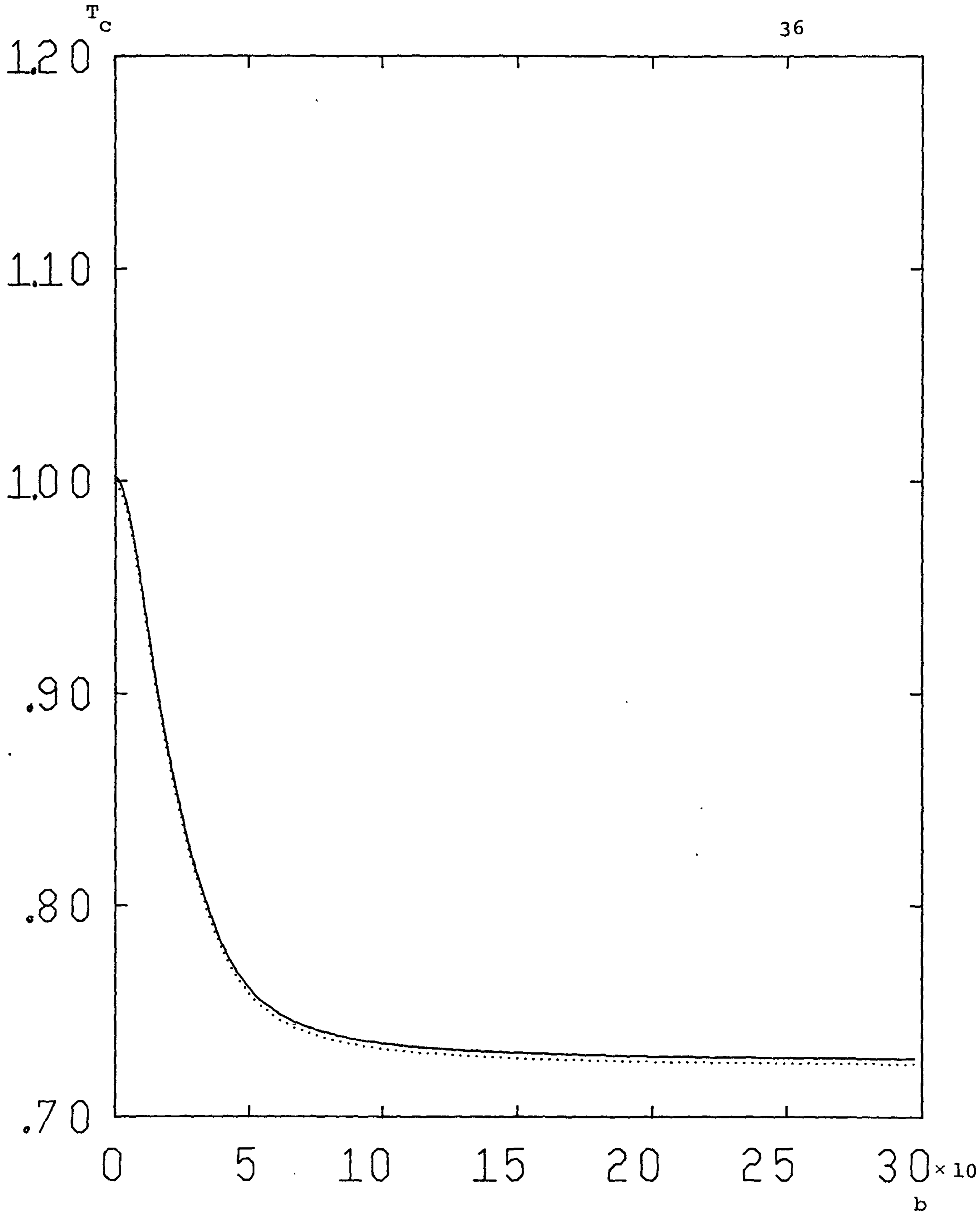

T
c
1.20
1.10
1.00
.90
.80
.70
0
5
10
15
20
25
30
× 10
b

Fig. (3.3.a)

A plot of T_c (mev) versus b (mev) for the exact (———) and the approximate (•••••) solutions for T_c for a = 5 mev, ω_D = 20 mev and N(0)V = .25.

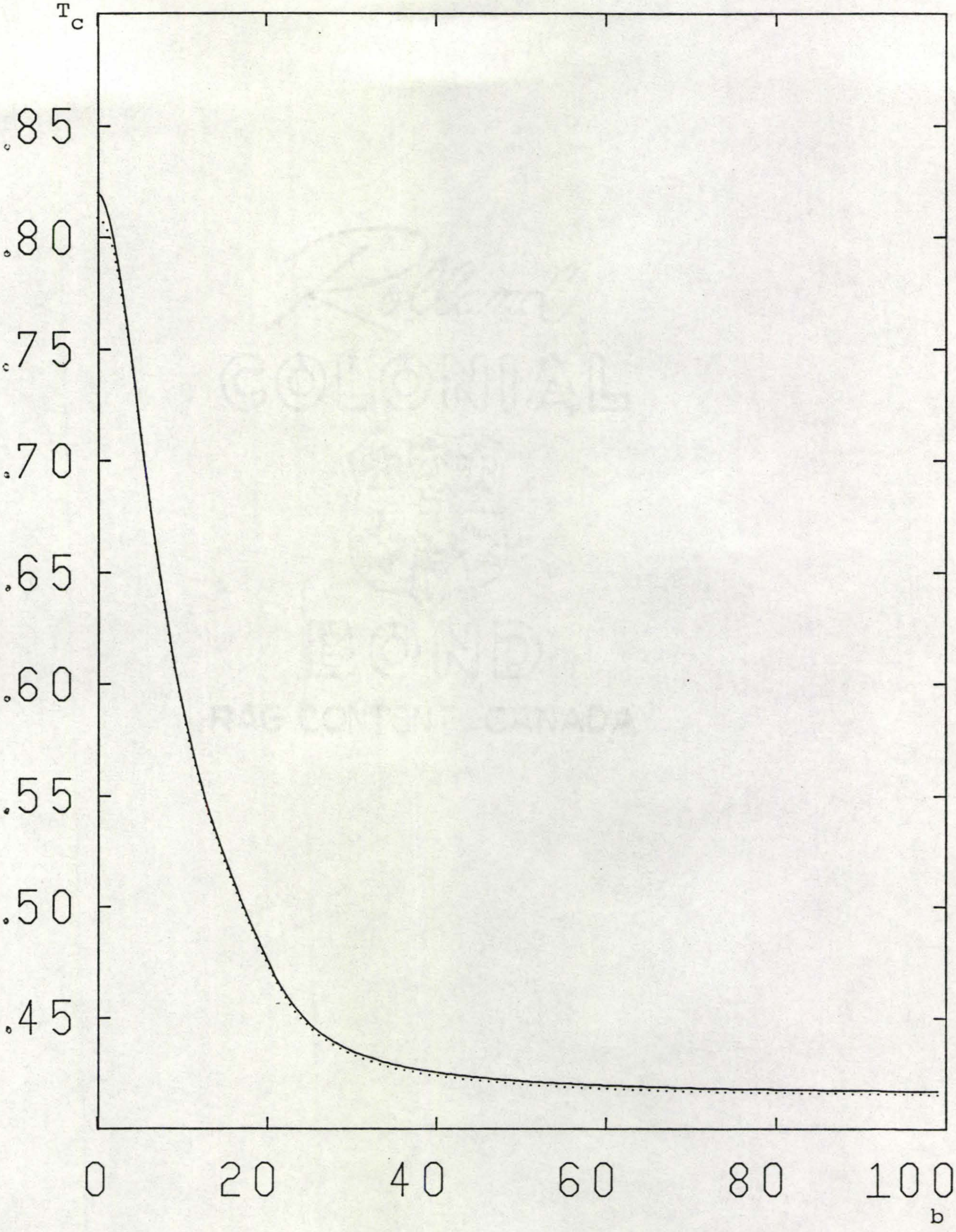

T_C
.85
.80
.75
.70
.65
.60
.55
.50
.45
0
20
40
60
80
100
b

Fig. (3.3.b)

A plot of T_c (mev) versus b (mev) for the exact (———) and the approximate (•••••) solutions for T_c for a = 10 mev, ω_D = 20 mev and N(0)V = .25.

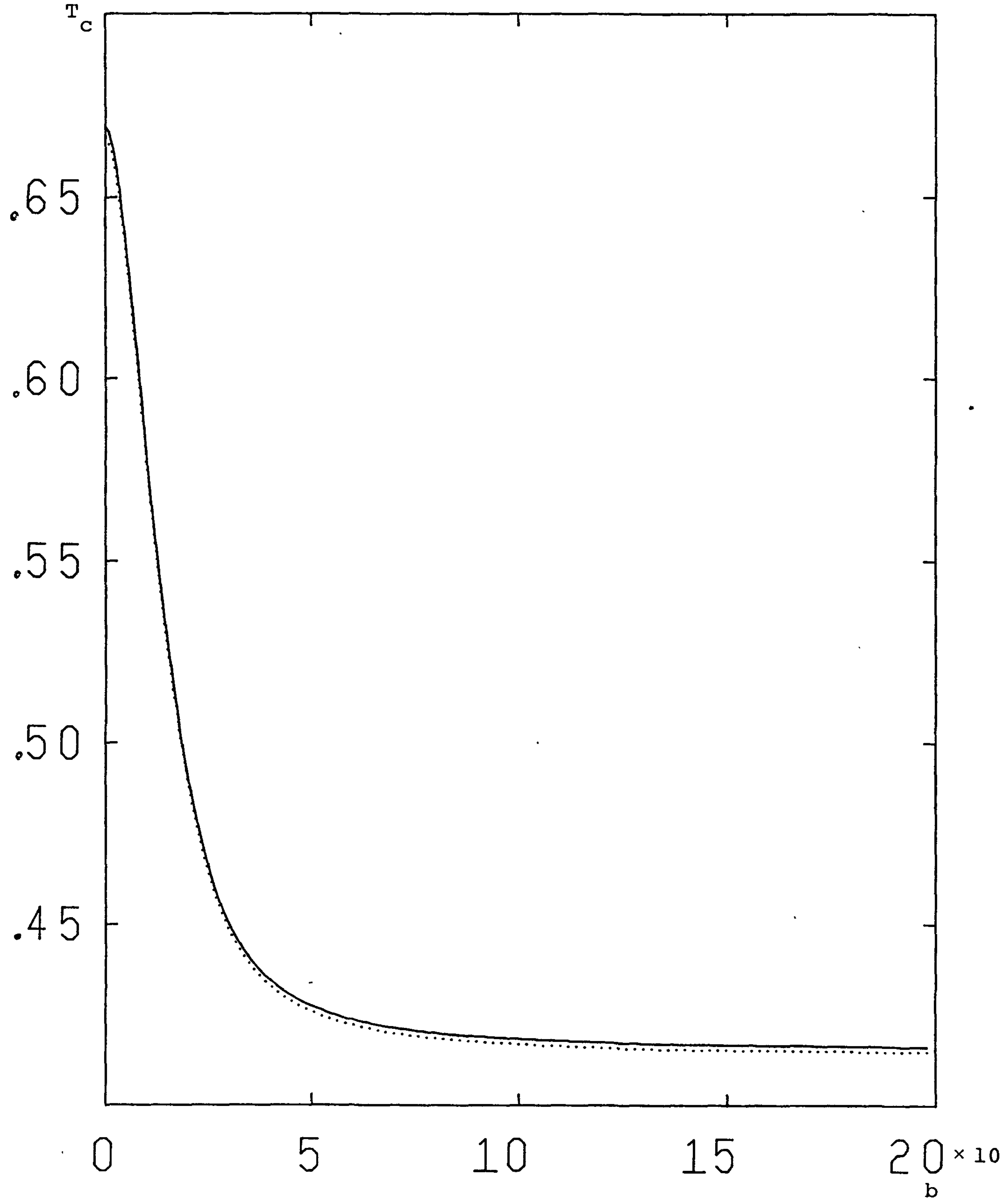

T_c
.65
.60
.55
.50
.45
0
5
10
15
20
× 10
b

Fig. (3.4.a)

A plot of $\Delta(0)$ (mev) versus b (mev) for the exact (———) and the approximate (•••••) solutions for $\Delta(0)$ for $a = 5$ mev, $\omega_D = 35$ mev and $N(0)V = .15$.

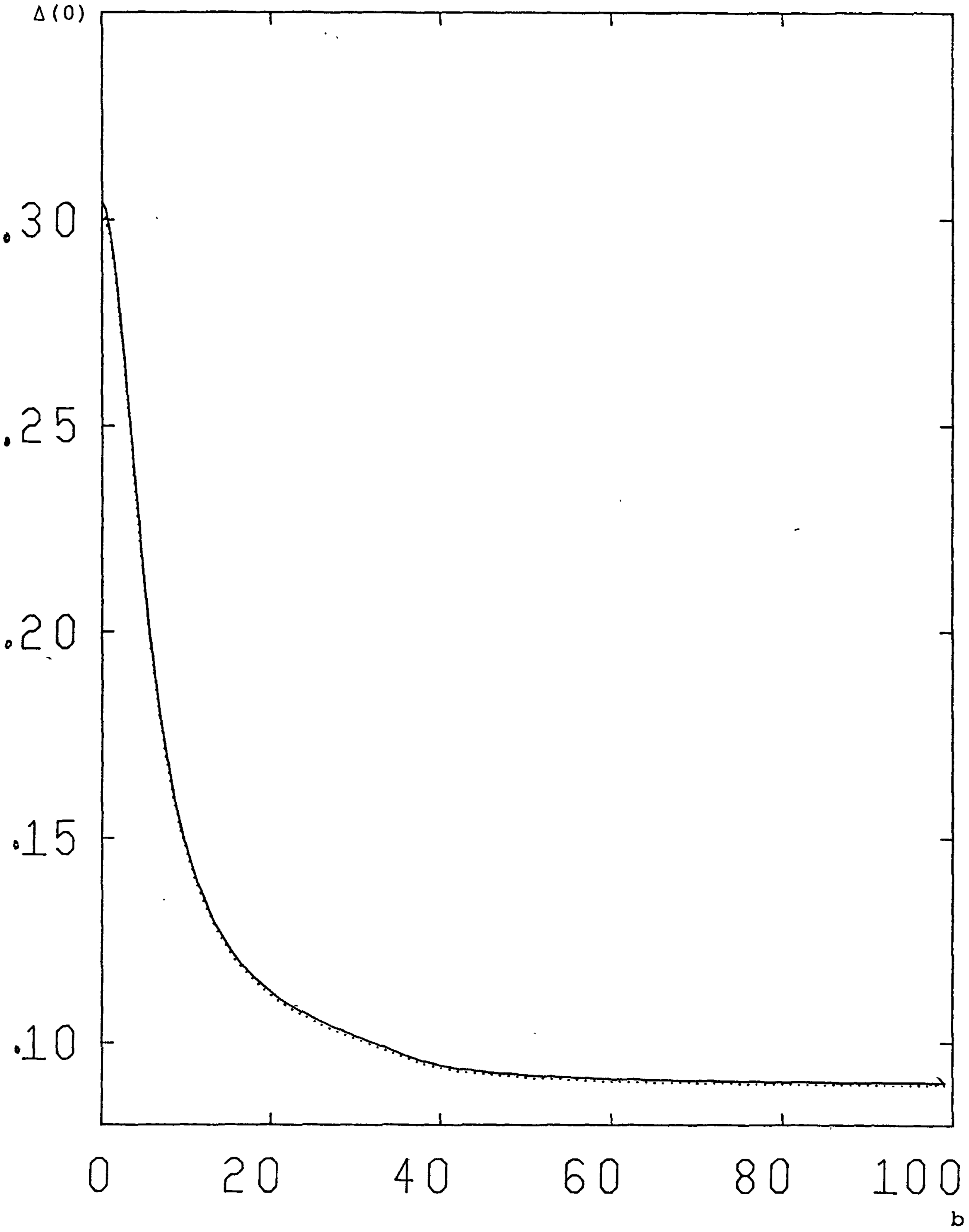

Δ(0)
.30
.25
.20
.15
.10
0
20
40
60
80
100
b

Fig. (3.4.b)

A plot of $\Delta(0)$ (mev) versus b (mev) for the exact (———) and the approximate(·····) solutions for $\Delta(0)$ for $a = 10$ mev, $\omega_D = 35$ mev and $N(0)V = .15$.

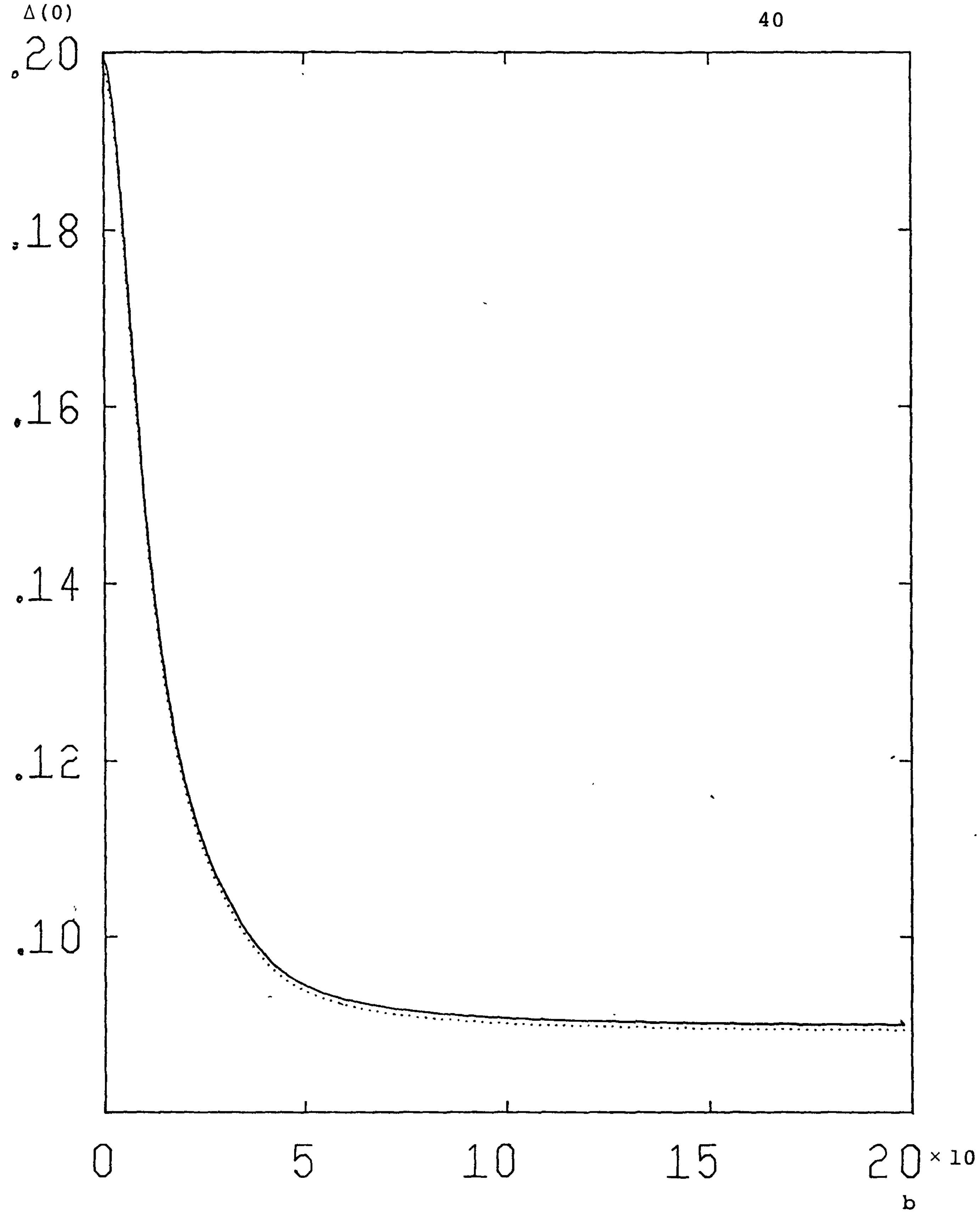

Δ(0)
.20
.18
.16
.14
.12
.10
0
5
10
15
20
× 10
b

Fig. (3.4.c)

A plot of $\Delta(0)$ (mev) versus b (mev) for the exact (———) and the approximate (·····) solutions for $\Delta(0)$ for $a = 15$ mev, $\omega_D = 35$ mev and $N(0)V = .15$.

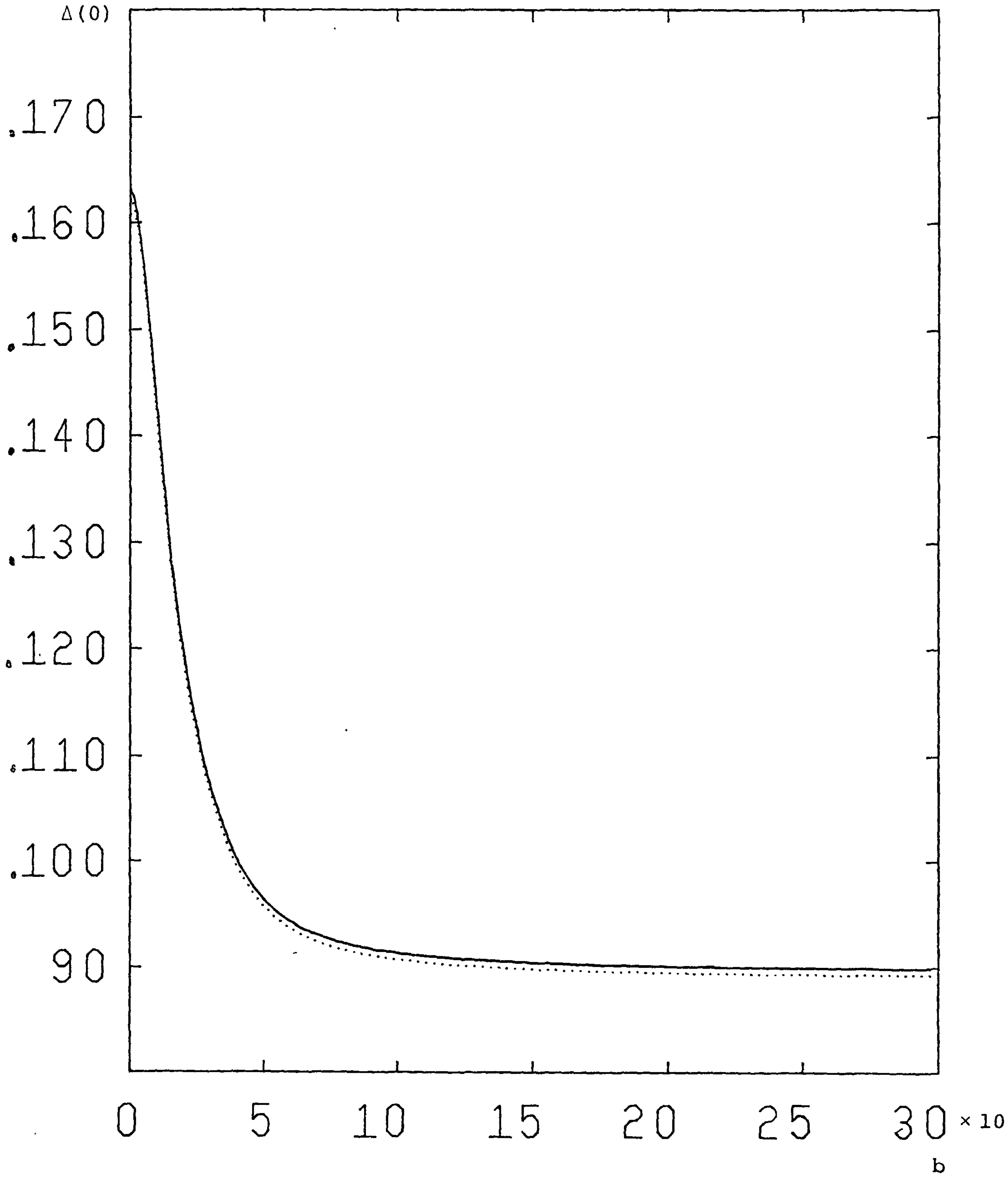

Δ(0)
.170
.160
.150
.140
.130
.120
.110
.100
90
0
5
10
15
20
25
30
× 10
b

Fig. (3.5.a)

A plot of $\Delta(0)$ (mev) versus b (mev) for the exact (———) and the approximate (•••••) solutions for $\Delta(0)$ for $a = 5$ mev, $\omega_D = 35$ mev and $N(0)V = .25$.

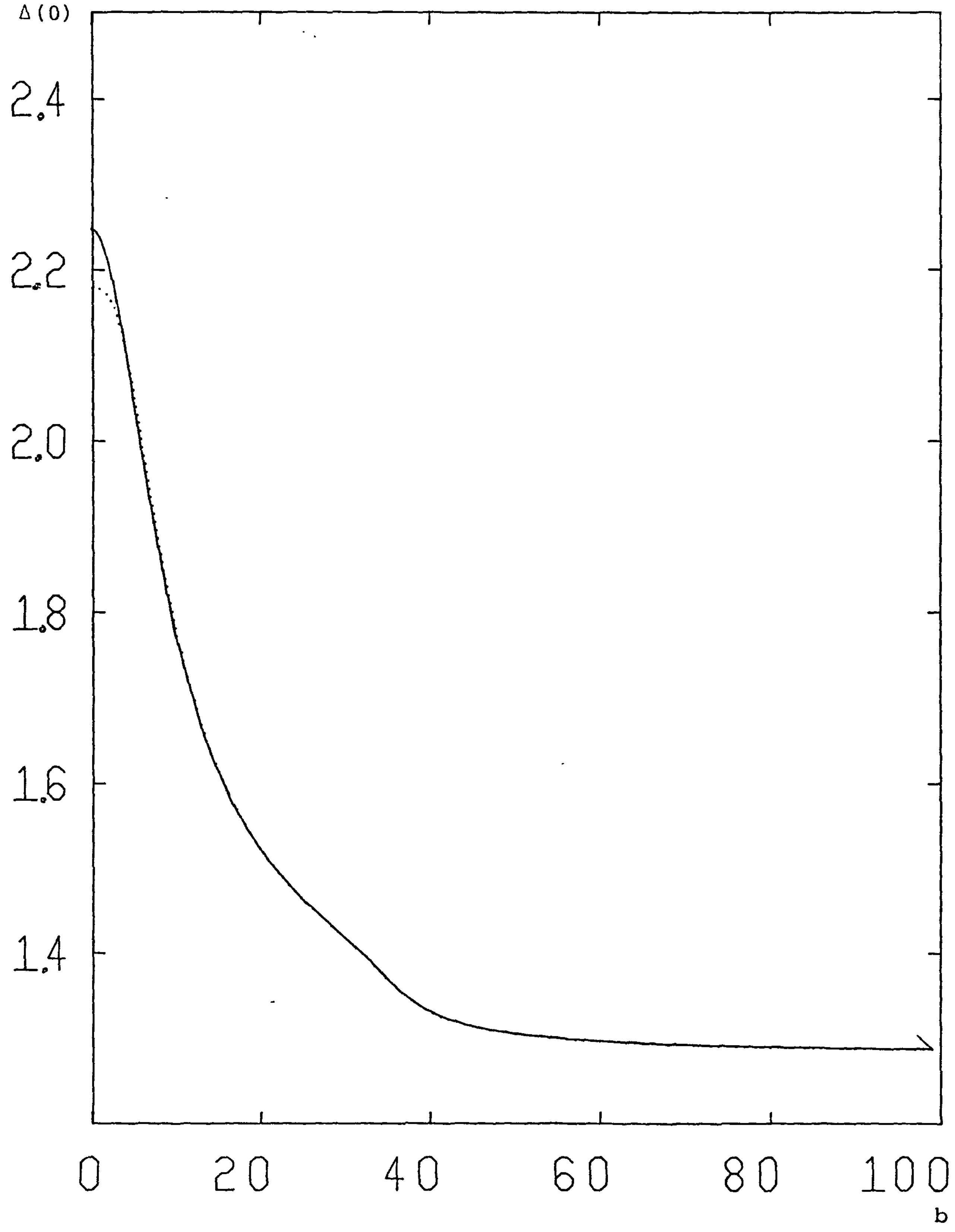

Δ(0)
2.4
2.2
2.0
1.8
1.6
1.4
0
20
40
60
80
100
b

Fig. (3.5.b)

A plot of $\Delta(0)$ (mev) versus b (mev) for the exact (———) and the approximate (······) solutions for $\Delta(0)$ for $a = 10$ mev, $\omega_D = 35$ mev and $N(0)V = .25$.

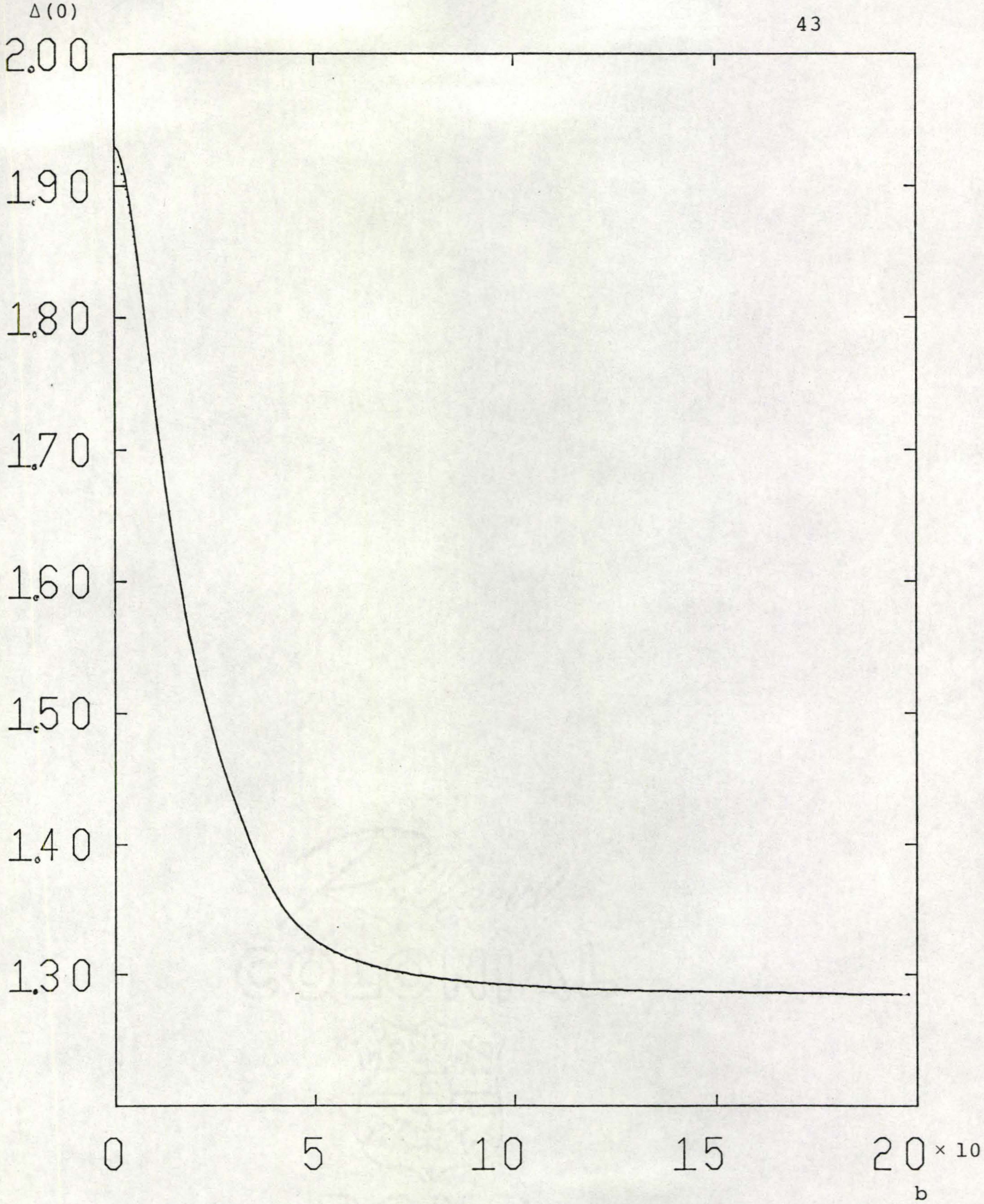

Δ(0)
2.00
1.90
1.80
1.70
1.60
1.50
1.40
1.30
0
5
10
15
20
× 10
b

Fig. (3.5.c)

A plot of $\Delta(0)$ (mev) versus b (mev) for the exact (———) and the approximate (·····) solutions for $\Delta(0)$ for $a = 15$ mev, ω_D = 35 mev and $N(0)V$ = .25.

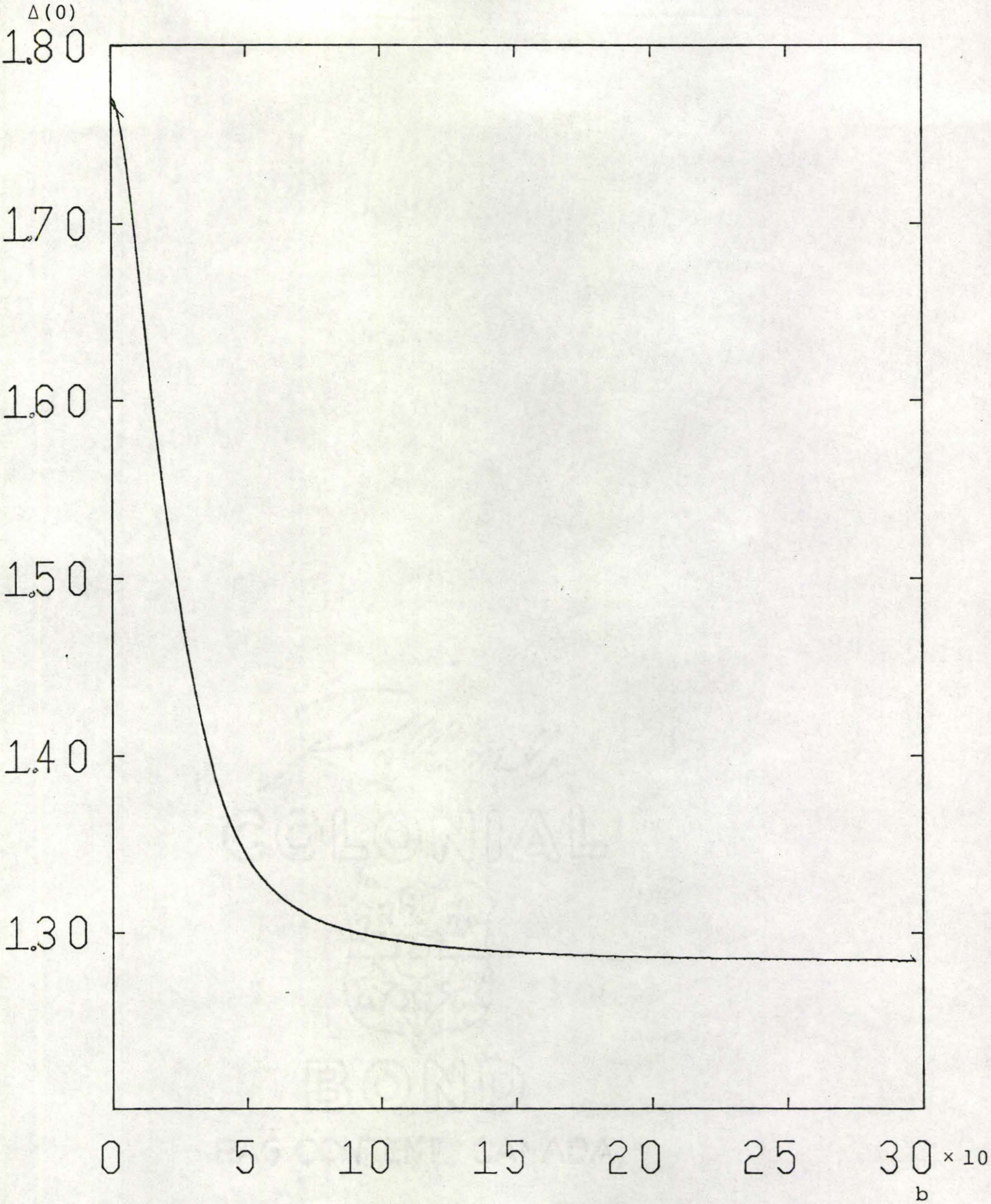

Δ(0)
1.80
1.70
1.60
1.50
1.40
1.30
0
5
10
15
20
25
30
×10
b

Fig. 3.6.a)

A plot of $\Delta(0)$ (mev) versus b (mev) for the exact (———) and the approximate (•••••) solutions for $\Delta(0)$ for $a = 5$ mev, $\omega_D = 20$ mev and $N(0)V = .25$.

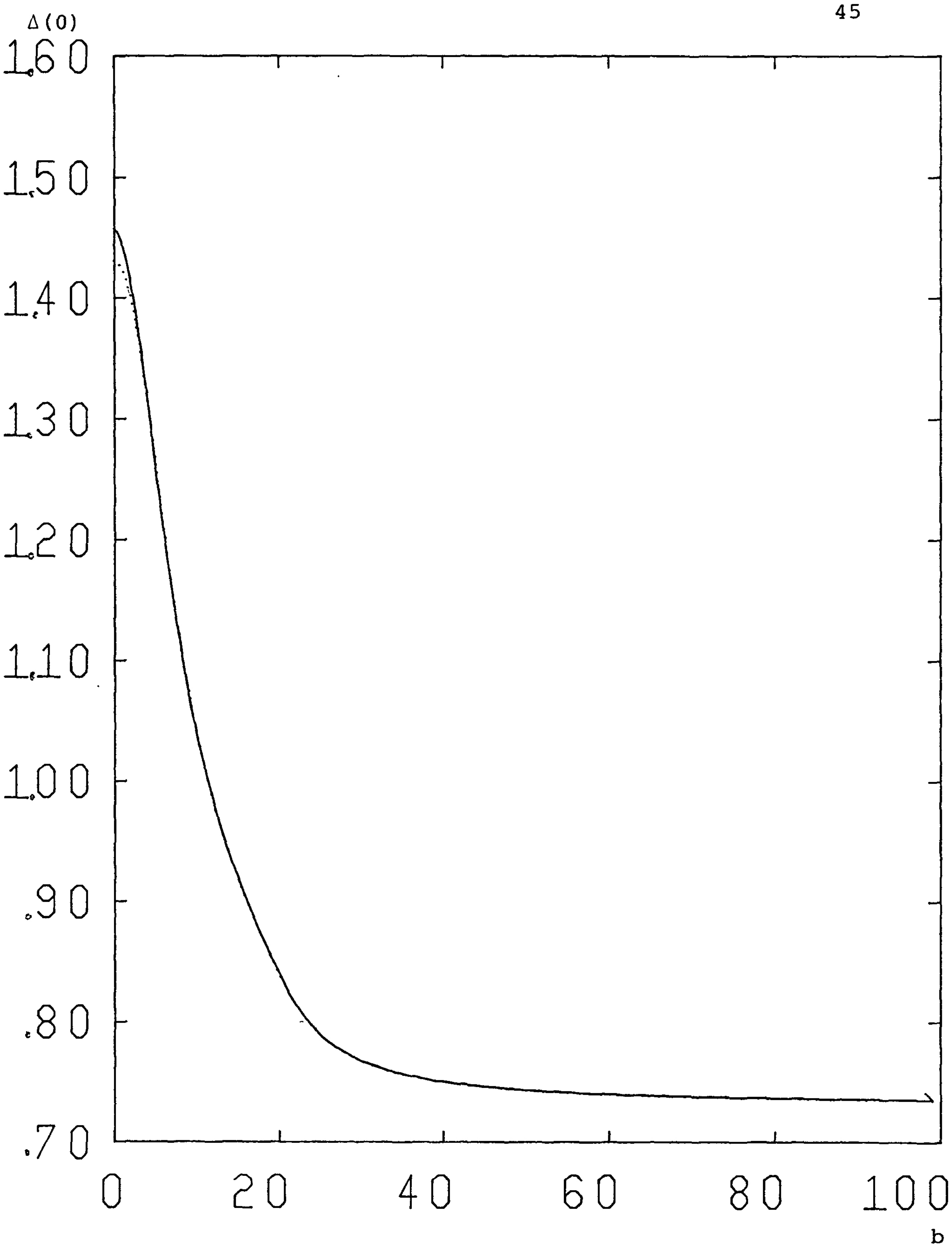

Δ(0)
1.60
1.50
1.40
1.30
1.20
1.10
1.00
.90
.80
.70
0
20
40
60
80
100
b

Fig. (3.6.b)

A plot of $\Delta(0)$ (mev) versus b (mev) for the exact (———) and the approximate (·····) solutions for $\Delta(0)$ for $a = 10$ mev, $\omega_D = 20$ mev and $N(0)V = .25$.

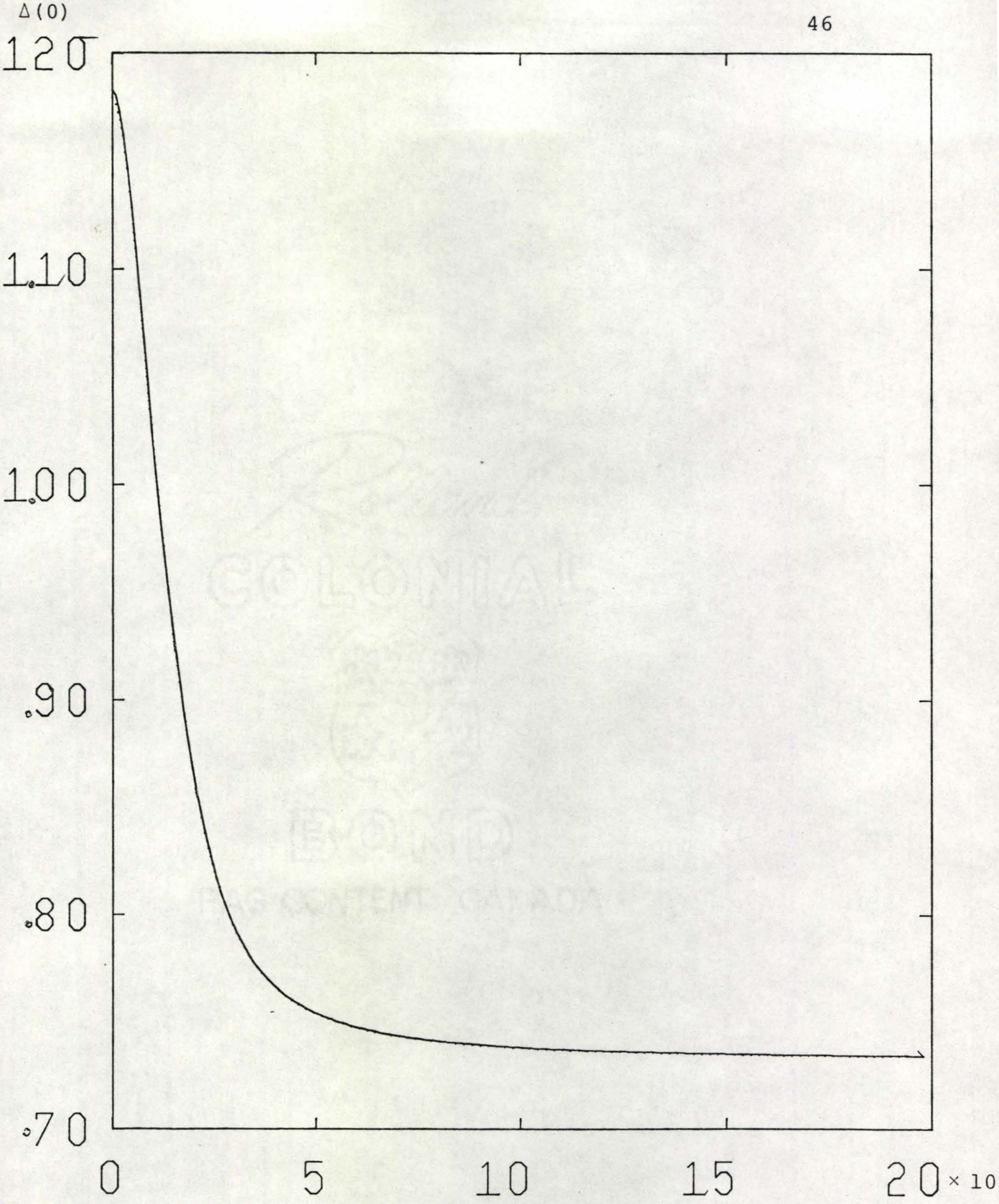

Δ(0)
1.20
1.10
1.00
.90
.80
.70
0
5
10
15
20
× 10
b

Fig. (3.7.a)

A plot of $\{2\Delta(0)/k_BT_c\}_{exact}$ versus b (mev) for a = 5 mev, ω_D = 35 mev and N(0)V = .15.

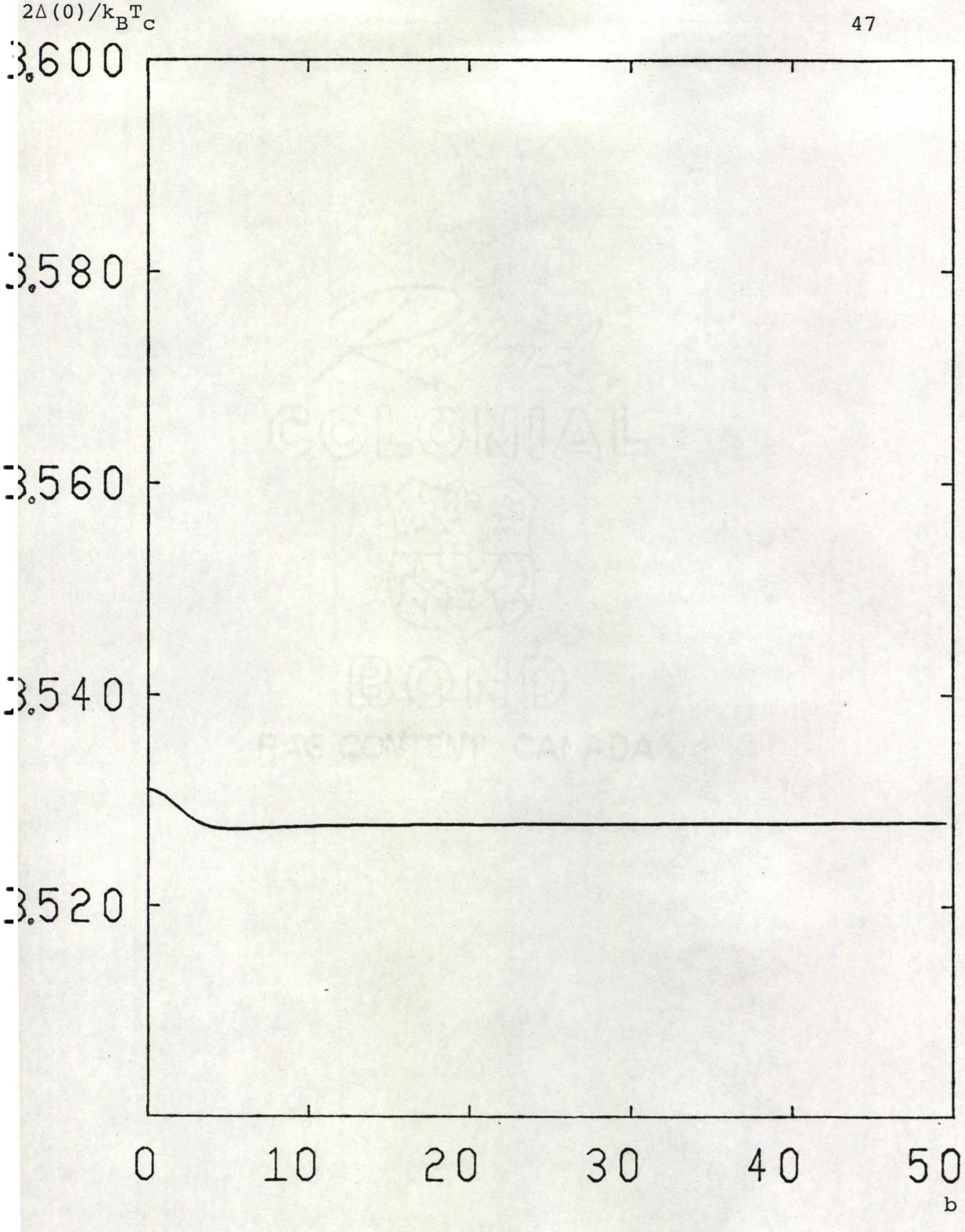

2Δ(0)/k_BT_c
3.600
3.580
3.560
3.540
3.520
0
10
20
30
40
50
b

Fig. (3.7.b)

A plot of $\{2\Delta(0)/k_B T_c\}_{exact}$ versus b (mev) for a = 10 mev, ω_D = 35 mev and N(0)V = .15.

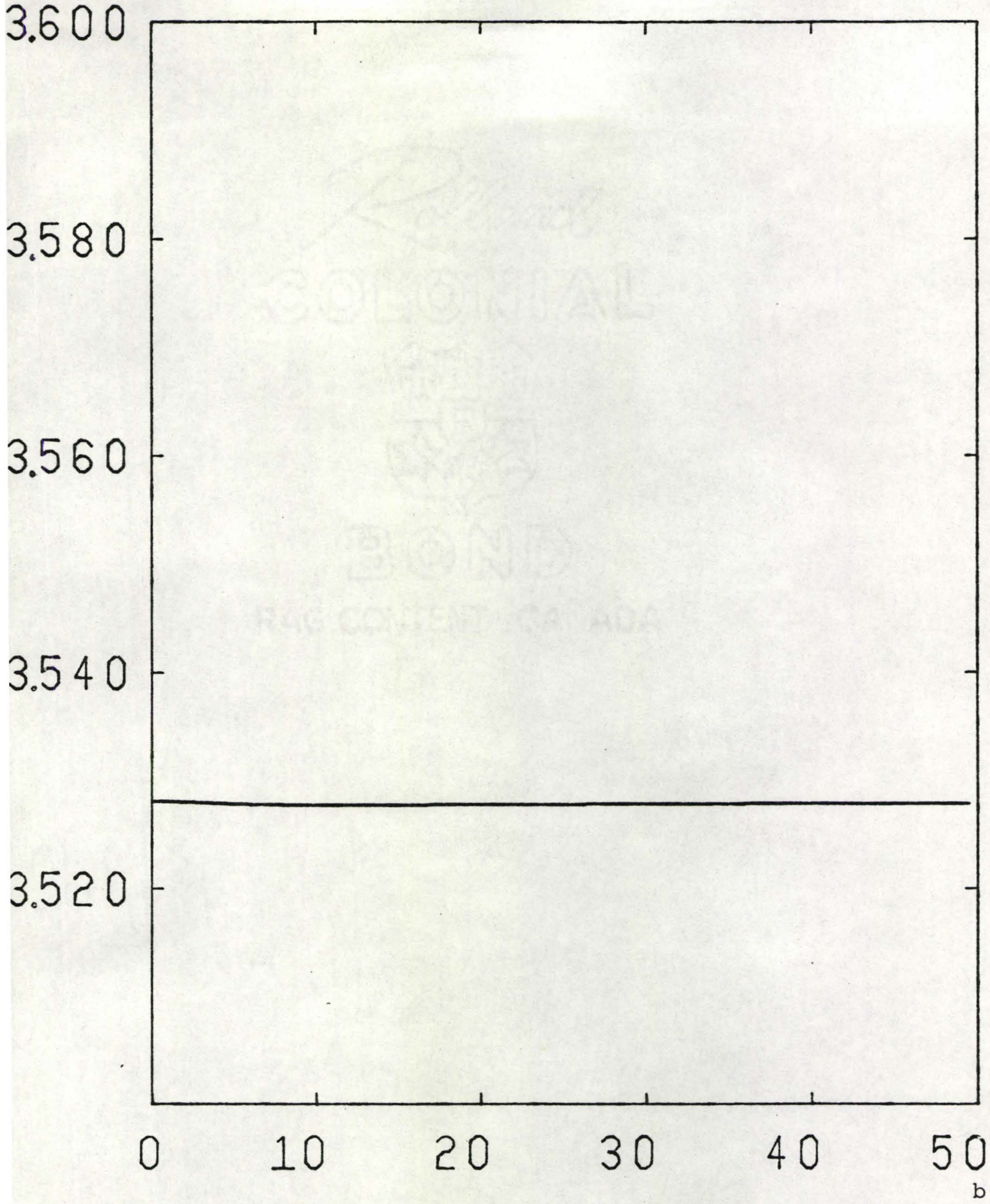

$2\Delta(0)/k_BT_c$
3.600
3.580
3.560
3.540
3.520
0
10
20
30
40
50
b

Fig. (3.7.c)

A plot of $\{2\Delta(0)/k_BT_c\}_{\text{exact}}$ versus b (mev) for a = 15 mev, ω_D = 35 mev and N(0)V = .15.

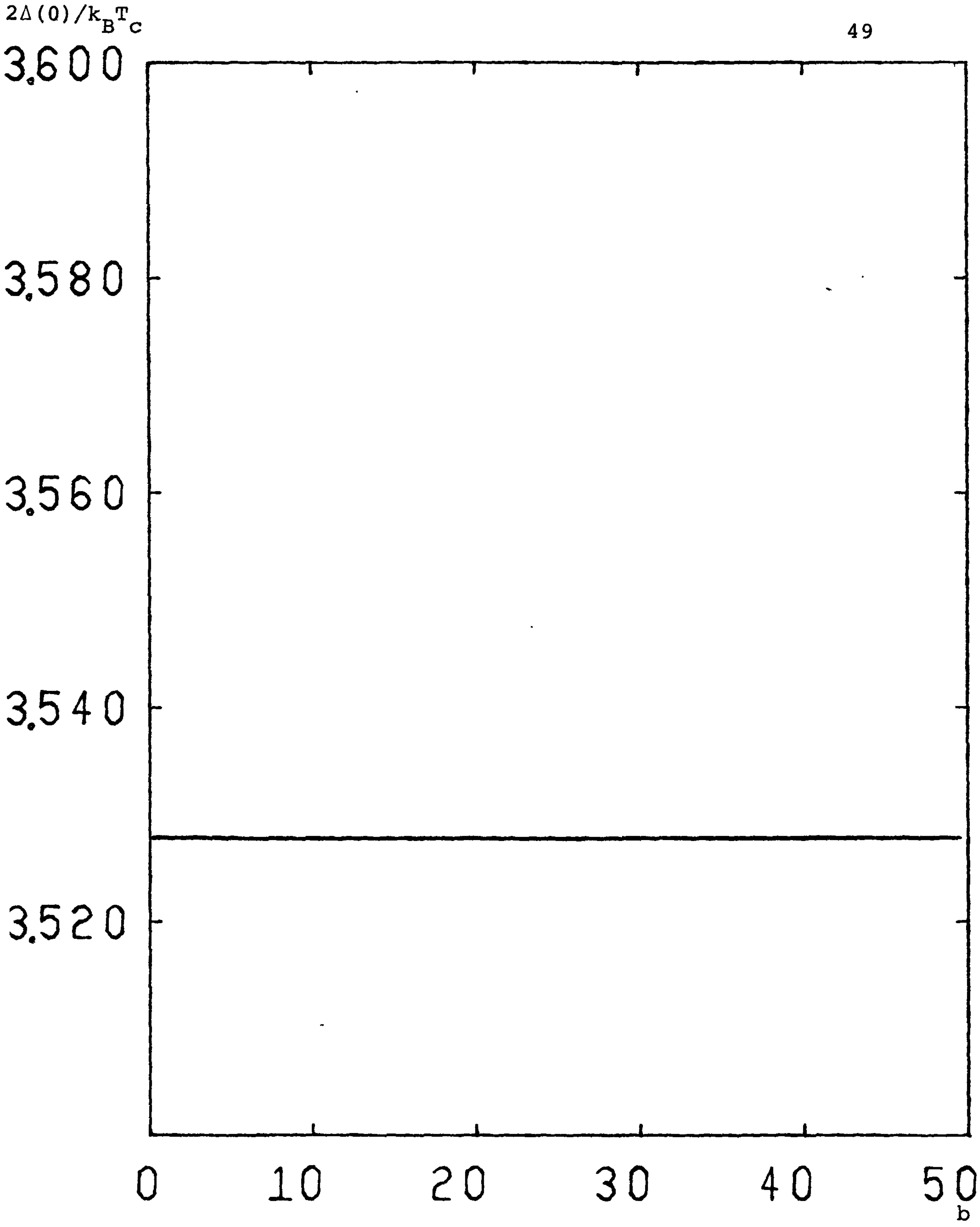

$2\Delta(0)/k_BT_c$
3.600
3.580
3.560
3.540
3.520
0
10
20
30
40
50
b

Fig. (3.8.a)

A plot of $\{2\Delta(0)/k_BT_c\}_{\mathrm{exact}}$ versus b (mev) for $a = 5$ mev, $\omega_D = 35$ mev and $N(0)V = .25$.

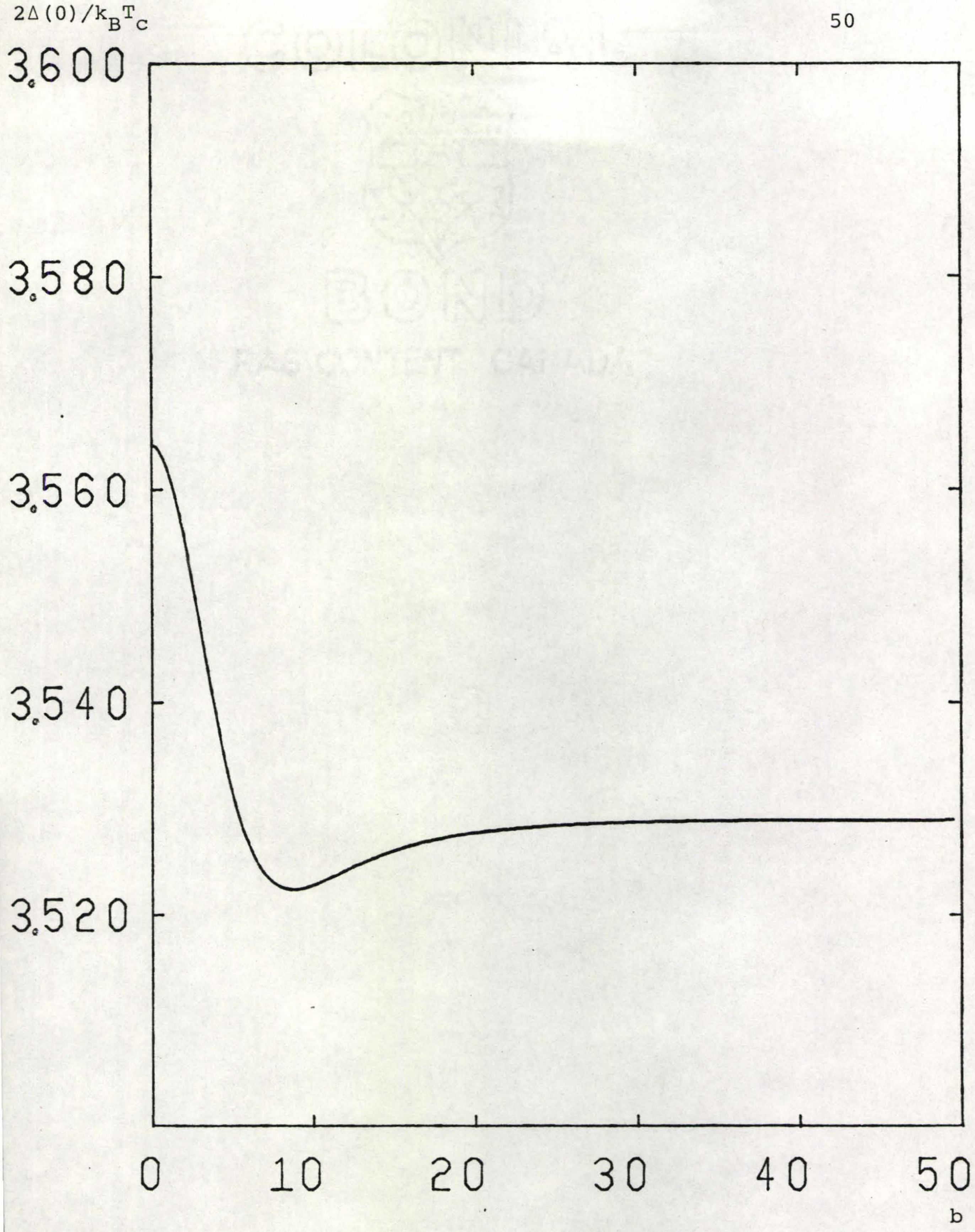

$2\Delta(0)/k_BT_c$
3.600
3.580
3.560
3.540
3.520
0
10
20
30
40
50
b

Fig. (3.8.b)

A plot of $\{2\Delta(0)/k_B T_c\}_{exact}$ versus b (mev) for $a = 10$ mev, $\omega_D = 35$ mev and $N(0)V = .25$.

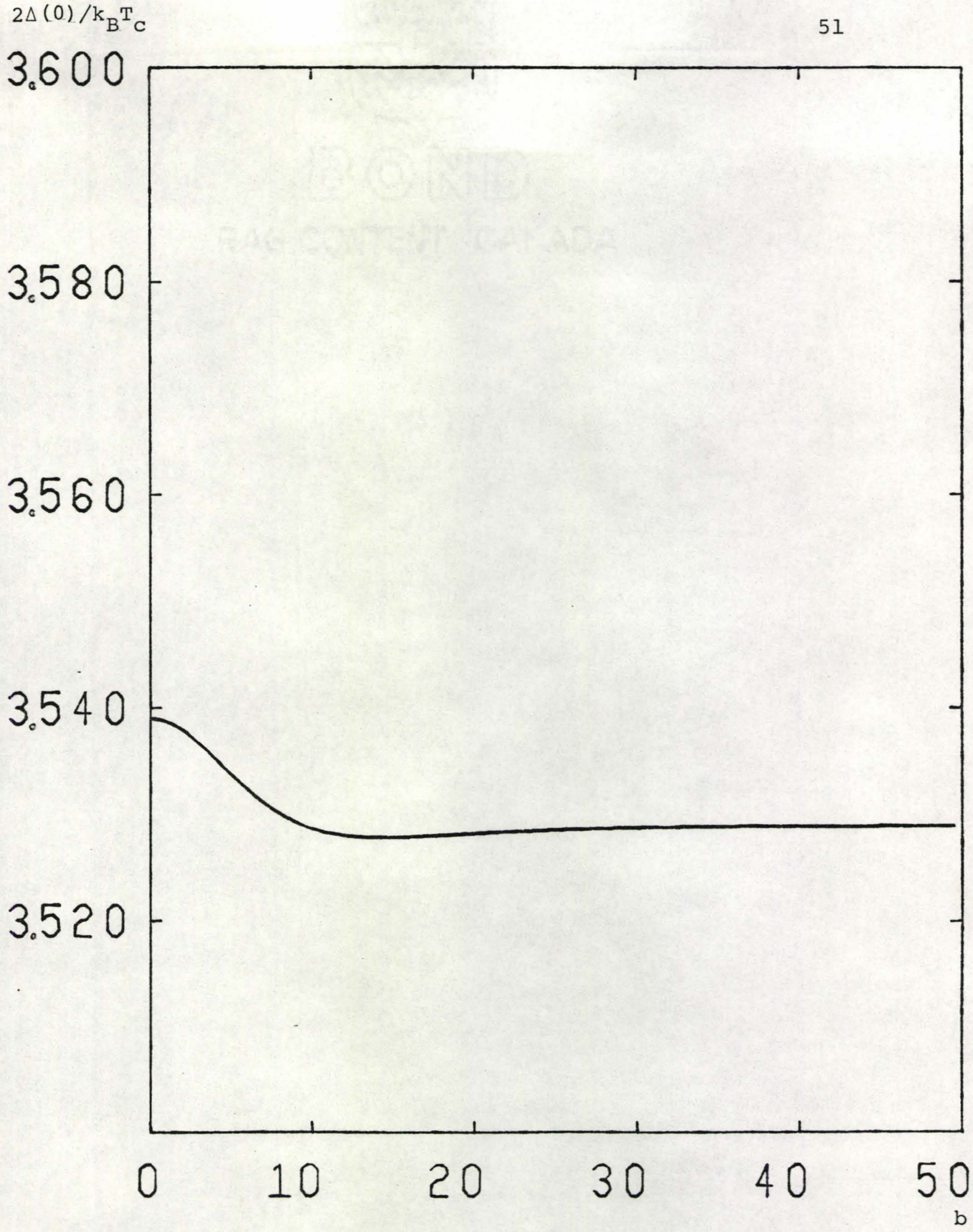
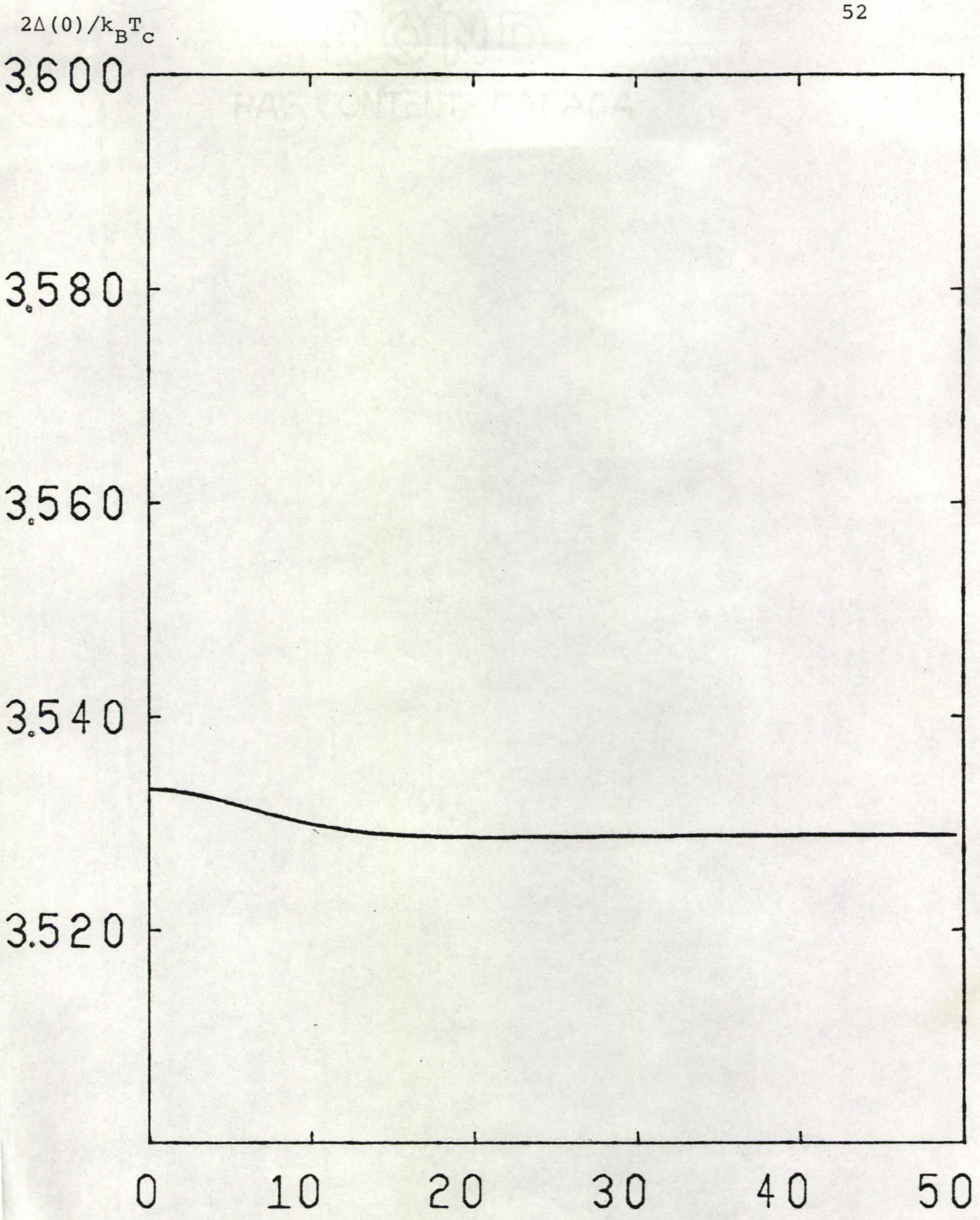

2Δ(0)/k_BT_c
3.600
3.580
3.560
3.540
3.520
0
10
20
30
40
50
b

Fig. (3.8.c)

A plot of $\{2\Delta(0)/K_B T_c\}_{exact}$ versus b (mev) for $a = 15$ mev, ω_D = 35 mev and N(0)V = .25.



$2\Delta(0)/k_BT_c$
3.600
3.580
3.560
3.540
3.520
0
10
20
30
40
50
b

in which we have introduced the new parameters $\bar{b}$, $\bar{\omega}$ and d. They are defined as:

$$\bar{b} = b/a \quad ; \quad \bar{\omega} = \omega_D/a \quad \text{and} \quad d = g/\pi a$$

so it can be seen very clearly that instead of having B as a function of four variables a, b, g and ω, we have obtained an equivalent expression for the factor B as a function of three variables only; $\bar{b}$, $\bar{\omega}$ and d. Now since this critical factor B gives us the change in T_c from the average theory (with density of state evaluated at the Fermi energy) and since it contains all the information about the energy dependence of the electronic density of states, it is appropriate to investigate the variation of $B(\bar{b},\bar{\omega},d)$ as a function of $\bar{b}$ at various values of $\bar{\omega}$ trying to cover the region required for the practical purposes of interest. Figs. 3.9, 3.10, 3.11, 3.12, 3.13 and 3.14 illustrate $B(\bar{b},\bar{\omega},d)$ against $\bar{b}$ for various values of $\bar{\omega}$ (4, 2, 1, .5 and .25) at five values for d (2,1.5,1,.75 and .35). The rapid increase in $B(\bar{b},\bar{\omega},d)$ as the parameter $\bar{b}$ is raised from zero corresponds to the rounding off of the T_c and $\Delta(0)$ curves at small values of b. The anomalous behaviour in $B(\bar{b},\bar{\omega},d)$ as a function of $\bar{b}$ for small values of $\bar{a}$ accounts for the bump we have seen in the T_c and $\Delta(0)$ graphs at small values of a. We note the fact that B rises above 1 at intermediate values of $\bar{b}$ and then saturates to 1 as expected. The numerical calculation for the factor B reveals that for small values of b and for D > 0, i.e. a

Fig. (3.9)

A plot of B ($\bar{b},\bar{\omega}$,d) versus $\bar{b}$ for d = 2 and for $\bar{\omega}$ = 4 (———), 2(•••••), 1(-----), .5(-•--•--•) and .25 (-••-••-••-).

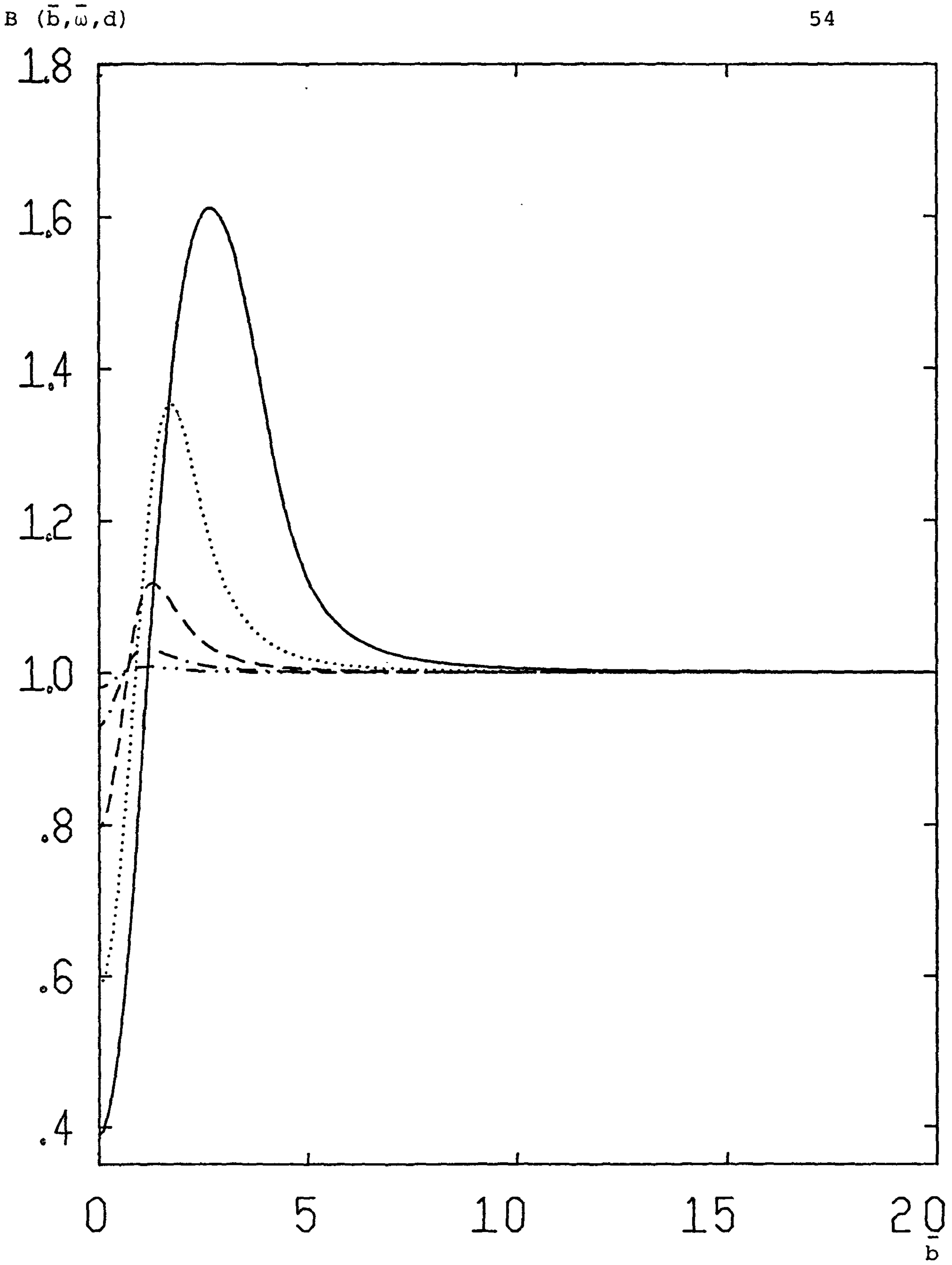

B ($\bar{b}$,$\bar{\omega}$,d)
1.8
1.6
1.4
1.2
1.0
.8
.6
.4
0
5
10
15
20
$\bar{b}$

Fig. (3.10)

A plot of B $(\bar{b},\bar{\omega},d)$ versus $\bar{b}$ for $d = 1.5$ and for $\bar{\omega} = 4$ (———), 2(•••••), 1(-----), .5(-•--•--•-) and .25 (-••-••-••-).

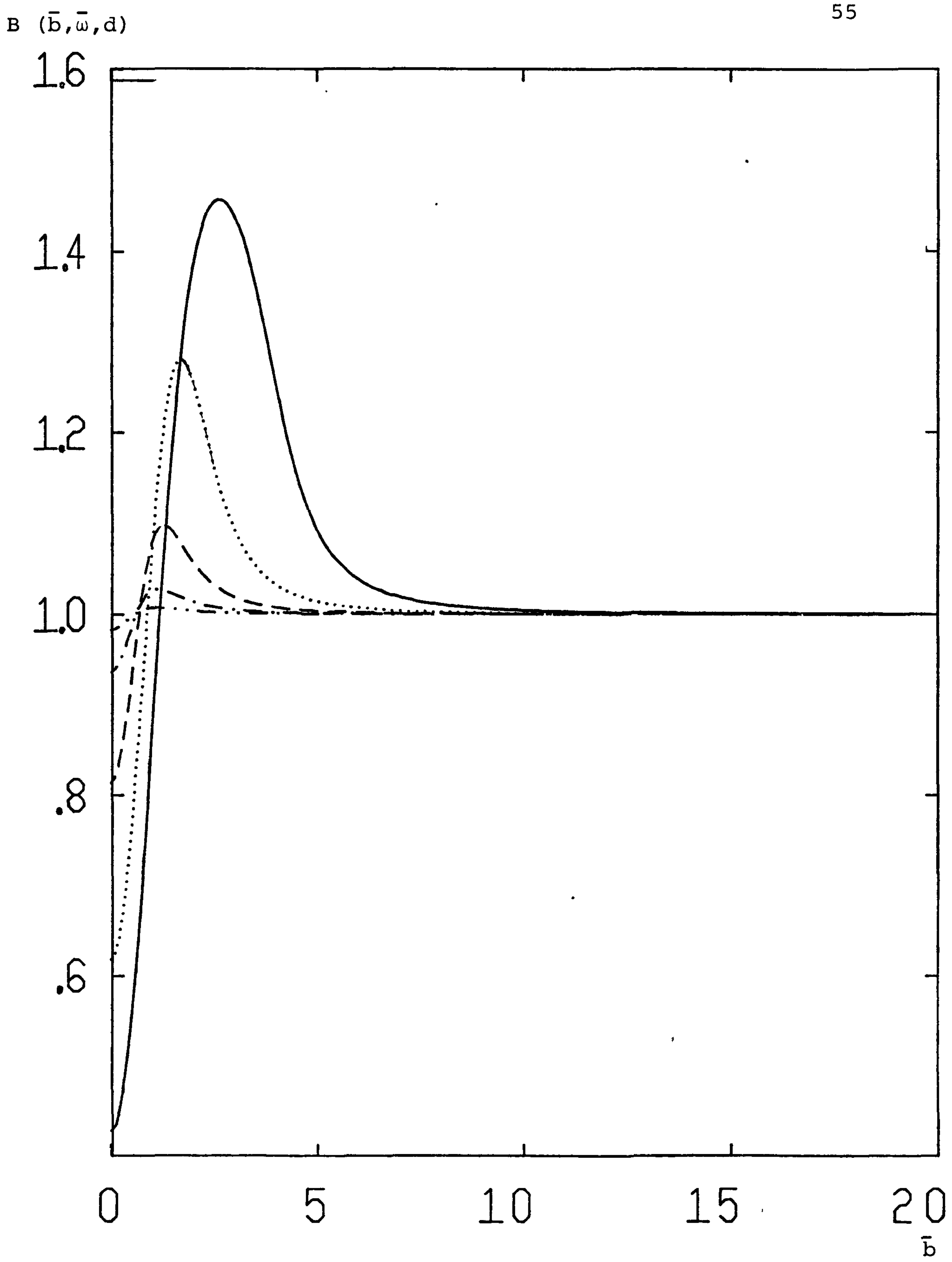

B ($\bar{b}$,$\bar{\omega}$,d)
1.6
1.4
1.2
1.0
.8
.6
0
5
10
15
20
$\bar{b}$

Fig. (3.11)

A plot of B ($\bar{b},\bar{\omega}$,d) versus $\bar{b}$ for d = 1 and for $\bar{\omega}$ = 4 (———), 2(•••••), 1(-----), .5(-•-•-•-) and .25 (-••-••-••-).

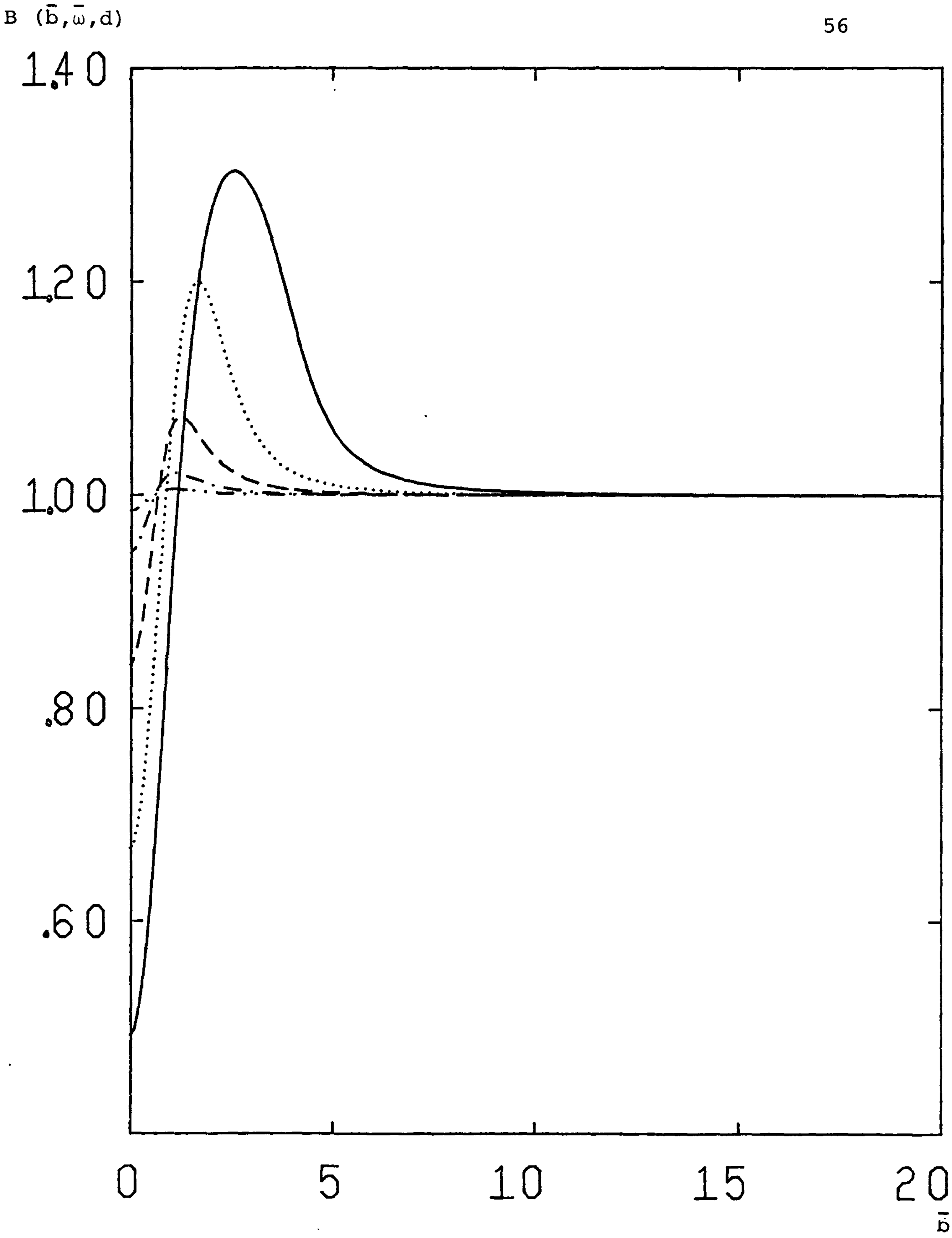

B ($\bar{b}$,$\bar{\omega}$,d)
1.40
1.20
1.00
.80
.60
0
5
10
15
20
$\bar{b}$

Fig. (3.12)

A plot of B $(\bar{b},\bar{\omega},d)$ versus $\bar{b}$ for $d = .75$ and for $\bar{\omega} = 4$ (———), 2(•••••), 1(-----), .5(-•-•-•-) and .25 (-••-••-••-).

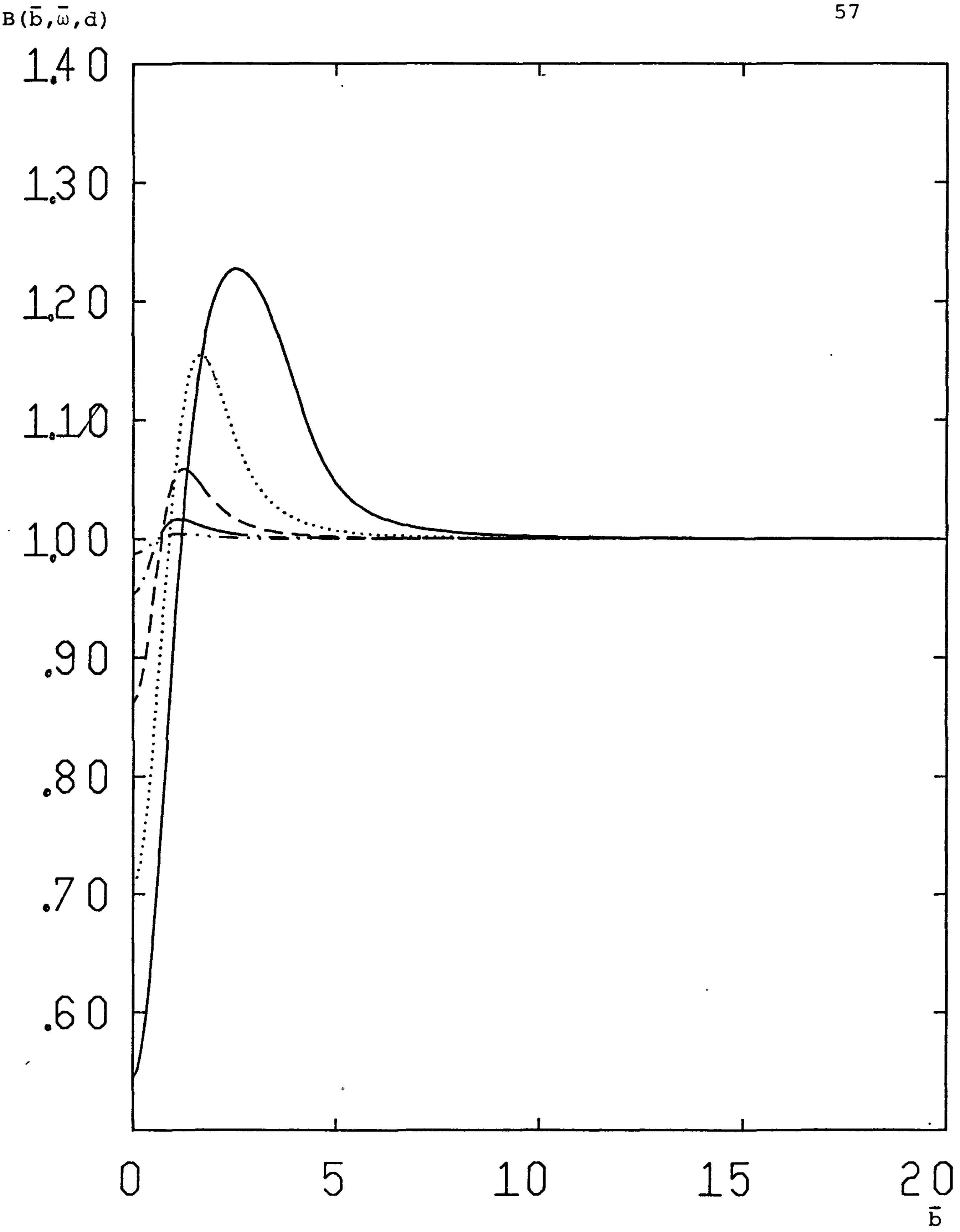
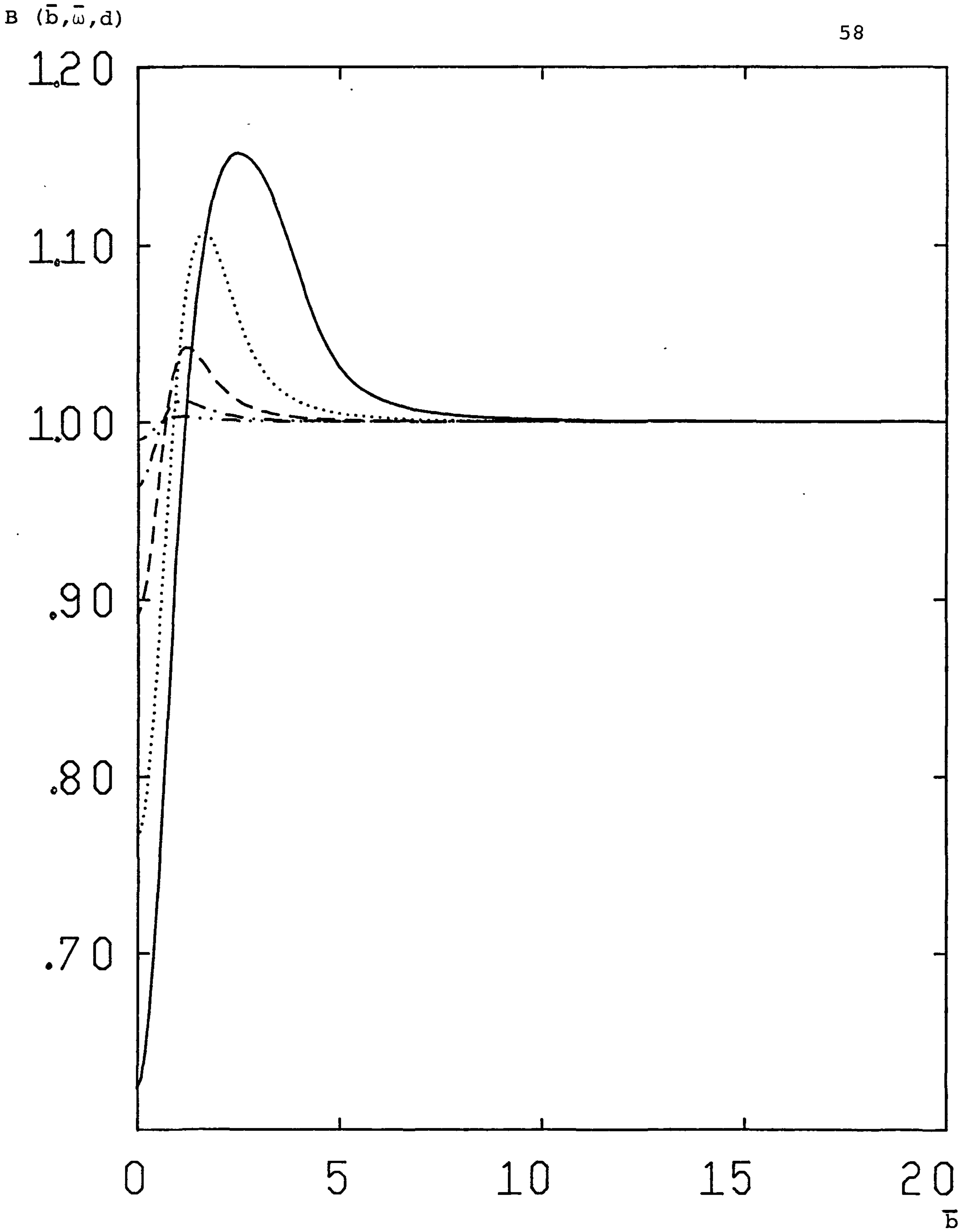

B(b̄,ω̄,d)
1.40
1.30
1.20
1.10
1.00
.90
.80
.70
.60
0
5
10
15
20
b̄

Fig. (3.13)

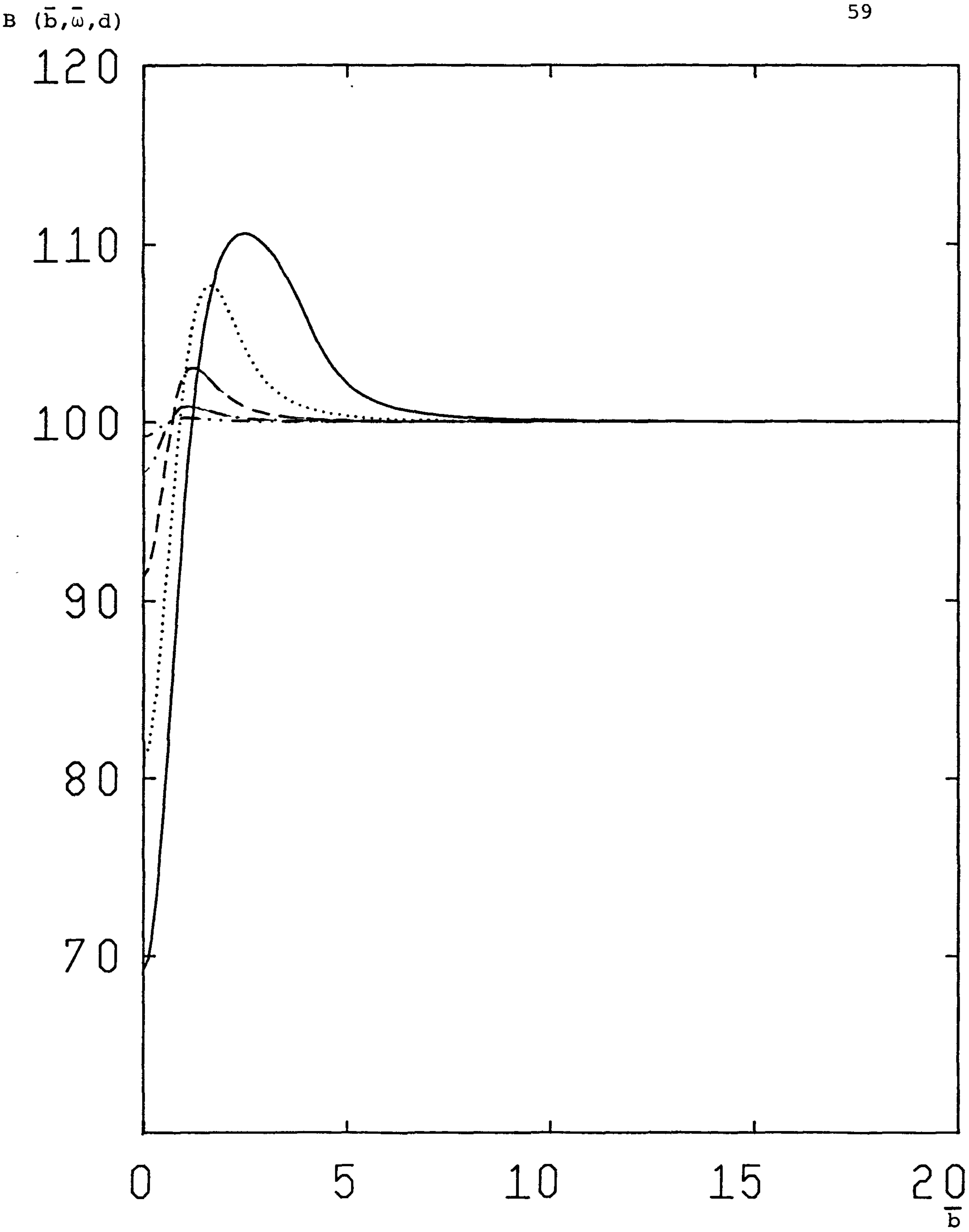
A plot of B $(\bar{b},\bar{\omega},d)$ versus $\bar{b}$ for $d = .5$ and for $\bar{\omega} = 4$ (———), 2(•••••), 1(-----), .5(-•-•-•-) and .25 (-••-••-••-).



B ($\bar{b}$,$\bar{\omega}$,d)
1.20
1.10
1.00
.90
.80
.70
0
5
10
15
20
$\bar{b}$

Fig. (3.14)

A plot of B $(\bar{b},\bar{\omega},d)$ versus $\bar{b}$ for $d = .35$ and for $\bar{\omega} = 4$ (———), 2(•••••), 1(-----), .5(-•--•--•-) and .25 (-••-••-••-).


B (b̄,ω̄,d)
120
110
100
90
80
70
0
5
10
15
20
b̄

peak in N(ε), B is always less than one and consequently T_c is reduced below $T_c°$ but for $-1 < D < 0$ B will be greater than one and T_c will be increased above $T_c°$. Basically this situation has been observed$^{(13)}$. In the calculation of T_c, some values of the electronic density of states are sampled which for $D > 0$ are smaller than the value at the peak, namely N(0)(1+D), but, which, for $-1 < D < 0$ are greater than the minimum value N(0)(1+D) when we are at the bottom of the valley in N(ε).

3.3 Chemical potential for Lorentzian form

Before giving a discussion of the thermodynamic properties of A15 compounds - specifically the specific heats - for our model for the energy dependence of the electronic density of states, it is necessary to study mathematically the shift in b - the center of a Lorentzian - as a function of temperature. We proceed mathematically in the following manner.

The total number of Fermions in a bulk superconductor is given by

$$N = \int_{-\varepsilon_1}^{\infty} N(\varepsilon) f(\beta\varepsilon) d\varepsilon \qquad (3.34)$$

where ε_1 is the end point energy of a the energy band we are dealing with and f(ε) is the Fermi-Dirac distribution function - $f(\beta\varepsilon) = \frac{1}{(e^{\varepsilon\beta}+1}$ - which gives the probability that a state with energy ε is occupied.

With reference to equation (3.2), equation (3.34) can be written as

$$N = N(0) \int_{-\varepsilon_1}^{\infty} f(\beta\varepsilon)d\varepsilon + N(0)\,\frac{ga}{\pi} \int_{-\varepsilon_1}^{\infty} \frac{f(\beta\varepsilon)}{[a^2+(\varepsilon-b)^2]}\,d\varepsilon \qquad (3.35)$$

The first term in the integral can be done by parts to give

$$\int_{-\varepsilon_1}^{\infty} f(\beta\varepsilon)d\varepsilon = \varepsilon f(\varepsilon)\Big|_{-\varepsilon_1}^{\infty} - \int_{-\varepsilon_1}^{\infty} \varepsilon\, f'(\beta\varepsilon)d\varepsilon \qquad (3.36)$$

$$= \varepsilon_1 [\frac{1}{e^{-\varepsilon_1/kT}+1}] + \frac{1}{kT} \int_{-\varepsilon_1}^{\infty} \frac{\varepsilon\, e^{\varepsilon/kT}}{[e^{\varepsilon/kT}+1]^2}\, d\varepsilon \qquad (3.37)$$

Since $\varepsilon_1 >> kT$, $e^{-\varepsilon_1/kT} << 1$ and $\{1/e^{-\varepsilon_1/kT} + 1\} = 1$ (to a very good approximation), so that

$$\int_{-\varepsilon_1}^{\infty} f(\beta\varepsilon)d\varepsilon = \varepsilon_1 + \int_{-\infty}^{\infty} (\frac{1}{kT})^{-1} \frac{xe^x}{(e^x+1)^2}dx \qquad (3.38)$$

where the substitution $(x = \varepsilon/kT)$ has been made and the lower limit of integration is taken as $-\infty$ with sufficient accuracy. The integrand on the right of this equation is an odd function of x since

$$\frac{xe^x}{(e^x+1)^2} = - [\frac{(-x)e^{-x}}{(e^{-x}+1)^2}]$$

and the integral is therefore identically zero. It follows that the second term in equation (3.37) is zero, i.e.

$$N(0)\int_{-\varepsilon_1}^{\infty} f(\beta\varepsilon)d\varepsilon = N(0)\varepsilon_1 \ .$$

The evaluation of the second term in equation (3.35) can also be done by parts as follows:

$$N(0)da^2\int_{-\varepsilon_1}^{\infty} \frac{1}{[a^2+(\varepsilon-b)^2]} f(\beta\varepsilon)d\varepsilon = I$$

with

$$I = N(0)da^2[\frac{1}{a}\tan^{-1}(\frac{\varepsilon-b}{a})] f(\beta\varepsilon)\Big|_{-\varepsilon_1}^{\infty} - \int_{-\varepsilon_1}^{\infty} \frac{1}{a}\tan^{-1}(\frac{\varepsilon-b}{a}) f'(\beta\varepsilon)d\varepsilon] \qquad (3.39)$$

and hence

$$I = N(0)da^2[-\frac{1}{a}\tan^{-1}(\frac{-\varepsilon_1-b}{a})] - \int_{-\varepsilon_1}^{\infty} \frac{1}{a}\tan^{-1}(\frac{\varepsilon-b}{a}) f'(\beta\varepsilon)d\varepsilon] \qquad (3.40)$$

Because $\frac{\varepsilon_1+b}{a} >> 1$, then $\tan^{-1}\frac{-(\varepsilon+b)}{a} \cong -\frac{\pi}{2}$ (taking only the first term to be sufficient in expanding $\tan^{-1}x$ for $x >> 1$). In addition since $f'(\beta\varepsilon)$ at zero temperature is different from zero only for $\varepsilon = 0$ we get

$$I = N(0)da^2[\frac{\pi}{2a} - \frac{1}{a}\tan^{-1}(\frac{-b_0}{a}) \int_{-\varepsilon_1}^{\infty} f'(\beta\varepsilon)d\varepsilon] \qquad (3.41)$$

since

$$\int_{-\varepsilon_1}^{\infty} f'(\beta\varepsilon)d\varepsilon \equiv [f(\beta\varepsilon)]_{-\infty}^{\infty} = -1 \ .$$

Therefore

$$I = N(0)da^2[\frac{\pi}{2a} - \tan^{-1}(\frac{b_0}{a})] \qquad (3.42)$$

in which we picked up only the zero temperature term. Combination of equations (3.38) and (3.42) gives us the total number of electrons in the system at zero temperature

$$N = N(0)[\varepsilon_1 + da^2[\frac{\pi}{2a} - \frac{1}{a}\tan^{-1}(\frac{b_0}{a})]] \qquad (3.43)$$

where b_0 is the zero temperature b, while the total number of electrons in the system at finite temperature is given by

$$N=N(0)[\varepsilon_1+da^2[\frac{\pi}{2a}-\frac{1}{a}\tan^{-1}(\frac{b}{a})+\text{corrections from higher expansion in } \tan^{-1}(\frac{\varepsilon-b}{a})]] \qquad (3.44)$$

or

$$N=N(0)[\varepsilon_1+da^2[\frac{\pi}{2a}-\int_{-\varepsilon_1}^{\infty}\frac{1}{a}\{[\tan^{-1}\frac{\varepsilon-b}{a}-\tan^{-1}\frac{-b}{a}]+\tan^{-1}\frac{-b}{a}\}\times f'(\beta\varepsilon)d\varepsilon] \qquad (3.45)$$

From equations (3.44) and (3.45), it is clear that the correction term at finite temperature can be written as

$$-da\int_{-\varepsilon_1}^{\infty}[\tan^{-1}\frac{\varepsilon-b}{a} - \tan^{-1}\frac{-b}{a}]f'(\beta\varepsilon)d\varepsilon \qquad (3.46)$$

$$\cong -da\int_{-\varepsilon_1}^{\infty}[\frac{\varepsilon a}{(a^2+b^2)} + \frac{ba}{(a^2+b^2)^2}\varepsilon^2]f'(\beta\varepsilon)d\varepsilon \qquad (3.47)$$

in which we have used the identity $\tan^{-1} x \pm \tan^{-1} y = \tan^{-1} \frac{x \pm y}{1 \mp xy}$ for $|\tan^{-1} x + \tan^{-1} y| \leq \frac{\pi}{2}$ and $\tan^{-1} x = x - \frac{x^3}{3} + \frac{x^5}{5} \cdots$ for x<1. We have taken only the first term of this expansion to the second order in ε. Equation (3.37) can be written as

$$\text{correction} = -da\left[\int_{-\varepsilon_1}^{\infty} \frac{a}{a^2+b^2}\, \varepsilon f'(\beta\varepsilon)d\varepsilon + \int_{-\varepsilon_1}^{\infty} \frac{ba}{(a^2+b^2)^2}\, \varepsilon^2 f'(\beta\varepsilon)d\varepsilon\right] \tag{3.48}$$

$$\equiv -da\left[(-kT)\frac{a}{a^2+b^2}\int_{-\infty}^{\infty} \frac{xe^x}{(e^x+1)^2}\,dx - (kT)^2 \frac{ba}{(a^2+b^2)^2} \times \int_{-\infty}^{\infty} \frac{x^2e^x}{(e^x+1)^2}\,dx\right] \tag{3.49}$$

when the change of variable to $x = \varepsilon/kT$ is made. The first integrand on the right of this equation is an odd function of x and it is therefore identically zero. The second integrand in equation (3.49) is an even function of x so that

$$\int_{-\infty}^{\infty} \frac{x^2e^x}{(e^x+1)^2}\,dx = 2\int_{0}^{\infty} \frac{x^2e^x}{(e^x+1)^2}\,dx = 2\int_{0}^{\infty} \frac{x^2e^{-x}}{(e^{-x}+1)^2}\,dx \tag{3.50}$$

This latter integral may be expanded as an infinite series in e^{-x} by writing

$$(1+e^{-x})^{-2} = \sum_{n=1}^{\infty} (-1)^{n-1} ne^{-(n-1)x} \tag{3.51}$$

where n is an integer, so that

$$\int_0^{\infty} \frac{x^2e^{-x}}{(e^{-x}+1)^2}\, dx = \sum_{n=1}^{\infty} (-1)^{n-1} n \int_0^{\infty} e^{-nx} x^2 dx \tag{3.52}$$

using the form of Γ-integral which is given by

$$\int_0^{\infty} e^{-nx} x^2 dx = \frac{1}{n^3}\, \Gamma(3) = 2/n^3 \tag{3.53}$$

so that equation (3.52) becomes

$$\int_0^{\infty} \frac{x^2e^{-x}}{(e^{-x}+1)^2}\, dx = 2 \sum_{n=1}^{\infty} (-1)^{n-1} \frac{1}{n^2} = \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6} \tag{3.54}$$

Substituting from equation (3.54) into equation (3.49) gives

$$\text{Correction} = d\, \frac{a^4 b}{(a^2+b^2)^2} \left[\frac{kT}{a}\right]^2 \frac{2\pi^2}{6} \tag{3.55}$$

From equations (3.43) and (3.44) it is clear that

$$-da \tan^{-1}\left(\frac{b_0}{a}\right) = -da \tan^{-1}\left(\frac{b}{a}\right) + \text{correction from higher order expansion in } \tan^{-1}\left(\frac{\varepsilon-b}{a}\right) \tag{3.56}$$

or

$$\tan^{-1}\left(\frac{b}{a}\right) - \tan^{-1}\left(\frac{b_0}{a}\right) = \frac{a^3 b}{(a^2+b^2)^2}\, \frac{2\pi^2}{6} \left[\frac{kT}{a}\right]^2 \tag{3.57}$$

where b_0 and b are respectively the absolute zero and finite temperature b. Equation (3.57) can be reduced to

$$\tan^{-1} \frac{(b-b_0)a}{a^2+bb_0} = \frac{a^3b}{(a^2+b^2)^2} \frac{2\pi^2}{6} [\frac{kT}{a}]^2$$

$$\tan^{-1} [\frac{\Delta ba}{a^2+b^2+b_0\Delta b}] = \frac{a^3b}{(a^2+b^2)^2} \frac{2\pi^2}{6} [\frac{kT}{a}]^2$$

$$\tan^{-1} \frac{a\Delta b}{(a^2+b_0^2)} [1 - \frac{b_0\Delta b}{(a^2+b_0^2)} + \cdots] = \frac{a^3b}{(a^2+b^2)^2} \frac{2\pi^2}{6} (\frac{kT}{a})^2 \qquad (3.58)$$

where the identity $\tan^{-1}x \pm \tan^{-1}y = \tan^{-1} \frac{x\pm y}{1\mp xy}$ has again been used and we have put $b = b_0 + \Delta b$. Taking only the first term of the expansion to be sufficient, equation (3.58) can be reduced to

$$\tan^{-1} \frac{a\Delta b}{(a^2+b_0^2)} \cong \frac{a\Delta b}{a^2+b_0^2} \cong \frac{a^3b_0}{(a^2+b_0^2)^2} \frac{2\pi^2}{6} (\frac{kT}{a})^2 \qquad (3.59)$$

so that

$$\Delta b = \frac{a^2}{(a^2+b_0^2)} \frac{2\pi^2}{6} (\frac{kT}{a})^2 b_0 \qquad (3.60)$$

since

$$b = b_0 + \Delta b .$$

Therefore

$$b = b_0[1 + \frac{a^2}{(a^2+b_0^2)} \frac{2\pi^2}{6} (\frac{kT}{a})^2] \qquad (3.61)$$

It is the fact that the correction term $\frac{a^2}{(a^2+b_0^2)} \frac{2\pi^2}{6} (\frac{kT}{a})^2$ is negligible compared with unity which generally allows the substitution of b_0 for b to be made without the introduction of any measurable error. Quantitatively the correction term $\simeq$ 1/60.

3.4 Condensation energy per unit volume

In this section we present the steps carried out in evaluating the condensation energy per unit volume; the energy difference between the normal and superconducting state. This calculation based on our model for the energy dependent electronic density of states but with the Fermi energy taken to be at the center of the Lorentzian so as to simplify the mathematics which we are about to carry out.

We start by writing down the equation for the condensation energy in its final form

$$\Delta W = 2\int_0^{\omega_D} d\varepsilon N(\varepsilon)\{\varepsilon[1 - \frac{\varepsilon}{\sqrt{\varepsilon^2+\Delta^2(0)}}] - \frac{\Delta^2(0)}{2\sqrt{\varepsilon^2+\Delta^2(0)}}\} \qquad (3.62)$$

with $N(\varepsilon)$ given by

$$N(\varepsilon) = N(0)\{1 + \frac{g}{\pi}\frac{a}{a^2+\varepsilon^2}\} \qquad (3.63)$$

With reference to equation (3.63) equation (3.62) can be written as

$$\Delta W = 2N(0)\{\int_0^{\omega_D} d\varepsilon\{\varepsilon - \frac{\varepsilon^2}{\sqrt{\varepsilon^2+\Delta^2(0)}} - \frac{\Delta^2(0)}{2\sqrt{\varepsilon^2+\Delta^2(0)}}\} +$$

$$\frac{ga}{\pi}\int_0^{\omega_D} d\varepsilon \frac{1}{(a^2+\varepsilon^2)}\{\varepsilon - \sqrt{\varepsilon^2+\Delta^2(0)} + \frac{1}{2}\frac{\Delta^2(0)}{\sqrt{\varepsilon^2+\Delta^2(0)}}\}\} \qquad (3.64)$$

To evaluate the first integral in equation (3.64) we make the change of variable $\varepsilon = \Delta(0)\sinh\theta$. Therefore the first term can be written in terms of the new variable as

$$I_1 = 2N(0)\int_0^{\omega_D} d\varepsilon\{\varepsilon - \frac{\varepsilon^2}{\sqrt{\varepsilon^2+\Delta^2(0)}} - \frac{\Delta^2(0)}{2\sqrt{\varepsilon^2+\Delta^2(0)}}\}$$

$$= 2N(0)\int_0^{\sinh^{-1}\{\frac{\omega_D}{\Delta(0)}\}} \Delta(0)\cosh\theta\{\Delta(0)\sinh\theta - \frac{\Delta^2(0)\sinh^2\theta}{\Delta(0)\cosh\theta} - \frac{\Delta^2(0)}{2\Delta(0)\cosh}\}\, d\theta$$

$$= 2N(0)\Delta^2(0)\int_0^{\sinh^{-1}\{\frac{\omega_D}{\Delta(0)}} \{\sinh\theta(\cosh\theta-\sinh\theta) - \frac{1}{2}\}d\theta$$

$$= 2N(0)\Delta^2(0)\int_0^{\sinh^{-1}(\frac{\omega_D}{\Delta(0)}} [e^{-\theta}\sinh\theta - \frac{1}{2}]d\theta$$

$$= N(0)\Delta^2(0)\int_0^{\sinh^{-1}(\omega_D/\Delta(0))} - e^{-2\theta}d\theta$$

$$= \frac{1}{2}N(0)\Delta^2(0)\{e^{-2\sinh^{-1}(\omega_D/\Delta(0))} -1\} \simeq -\frac{1}{2}N(0)\Delta^2(0) \qquad (3.65)$$

The second term of Eq. (3.64) can be evaluated as follows

$$I_2 = 2N(0)\,\frac{ga}{\pi}\int_0^{\omega_D} d\varepsilon\,\frac{1}{(a^2+\varepsilon^2)}\,\{\varepsilon - \sqrt{\varepsilon^2+\Delta^2(0)} + \frac{1}{2}\,\frac{\Delta(0)}{\sqrt{\varepsilon^2+\Delta^2(0)}}\}$$

$$= 2N(0)\,\frac{ga}{\pi}\,\{\frac{1}{2}\,\ell n(\frac{a^2+\omega_D^2}{a^2}) - \int_0^{\omega_D}\frac{\sqrt{\varepsilon^2+\Delta^2(0)}}{(a^2+\varepsilon^2)}\,d\varepsilon +$$

$$\frac{1}{2}\,\Delta^2(0)\int_0^{\omega_D}\frac{1}{(a^2+\varepsilon^2)}\,\frac{1}{\sqrt{\varepsilon^2+\Delta^2(0)}}\,d\varepsilon\} \qquad (3.66)$$

To integrate the last two parts of Eq. (3.66) the substitution $v = \frac{\varepsilon}{\sqrt{\varepsilon^2+\Delta^2(0)}}$ is suggested, which by differentiation gives $dv = \{\frac{v}{\varepsilon}\}^3\,\Delta^2(0)d\varepsilon$. So that the first part can be written in terms of the new variable as

$$\int_0^{\omega}\frac{\sqrt{\varepsilon^2+\Delta^2(0)}}{a^2+\varepsilon^2} = -\,\frac{\Delta^2(0)}{(a^2-\Delta^2(0))}\int_0^{\omega_D\sqrt{\omega_D^2+\Delta^2(0)}} dv\{\frac{1}{1-v^2}\cdot\frac{1}{A^2-v^2}\}$$

$$= -\,\frac{\Delta^2(0)}{(a^2-\Delta^2(0))}\int_0^{\omega_D/\sqrt{\omega_D^2+\Delta^2(0)}} dv\{\frac{1}{1-v^2}-\frac{1}{A^2-v^2}\}\frac{1}{A^2-1}$$

$$= \frac{-\Delta^2(0)}{2(a^2-\Delta^2(0))}\,\frac{1}{(A^2-1)}\int_0^{\omega_D/\sqrt{\omega_D^2+\Delta^2(0)}} dv\{(\frac{1}{1-v}+\frac{1}{1+v}) - \frac{1}{A}\,(\frac{1}{A-v}+\frac{1}{A+v})\}$$

with $A = a^2/a^2-\Delta^2(0)$.

Simple integration of this equation gives

$$\int_0^{\omega_D} \frac{\sqrt{\varepsilon^2+\Delta^2(0)}}{a^2+\varepsilon^2} = \frac{1}{2}\ \{\ell n(\frac{1-v}{1+v}) - \frac{1}{A}\ \ell n(\frac{A-v}{A+v})\Big|_0^{\omega_D/\sqrt{\omega_D^2+\Delta^2(0)}}\ \}$$

$$= \frac{1}{2}\{\ell n\{\frac{\sqrt{\omega_D^2+\Delta^2(0)}-\omega_D}{\sqrt{\omega_D^2+\Delta^2(0)}+\omega_D}\{\ -$$

$$\{\frac{a^2-\Delta^2(0)}{a^2}\}^{1/2}\ \ell n\{\frac{a\sqrt{\omega_D^2+\Delta^2(0)}-\omega_D\sqrt{a^2+\Delta^2(0)}}{a\sqrt{\omega_D^2+\Delta^2(0)}+\omega_D\sqrt{a^2-\Delta^2(0)}}\ \}\} \qquad (3.67)$$

The second part can be written in terms of the new variable as

$$\frac{1}{2}\ \Delta^2(0)\int_0^{\omega_D} \frac{1}{(a^2+\varepsilon^2)}\ \frac{1}{\sqrt{\varepsilon^2+\Delta^2(0)}}\ d\varepsilon \equiv \frac{1}{2}\ \Delta^2(0)\ \frac{1}{a^2-\Delta^2(0)} \times \int_0^{\omega_D/\sqrt{\omega_D^2+\Delta^2(0)}} \frac{1}{A^2-v^2}\ dv$$

$$= \frac{1}{2}\ \frac{\Delta^2(0)}{a^2-\Delta^2(0)}\int_0^{\omega_D/\sqrt{\omega_D^2+\Delta^2(0)}} \frac{1}{2A}\{\frac{1}{A-v} + \frac{1}{A+v}\}dv$$

$$= \frac{1}{2}\ \frac{\Delta^2(0)}{a^2-\Delta^2(0)}\ \frac{1}{2A}\ \ell n\{\frac{A+v}{A-v}\}\Big|_0^{\omega_D/\sqrt{\omega_D^2+\Delta^2(0)}}$$

$$= \frac{1}{2}\ \frac{\Delta^2(0)}{a^2+\Delta^2(0)}\ \frac{\sqrt{a^2-\Delta^2(0)}}{a}\ \ell n\{\frac{a\sqrt{\omega_D^2+\Delta^2(0)}+\omega_D\sqrt{a^2-\Delta^2(0)}}{a\sqrt{\omega_D^2+\Delta^2(0)}-\omega_D\sqrt{a^2-\Delta^2(0)}} \qquad (3.68)$$

Substituting from Eq. (3.67) and Eq. (3.68) into Eq. (3.66) and from Eq. (3.65) and then into Eq. (3.64) gives

$$\Delta W = -\frac{1}{2}\, N(0)\Delta^2(0) + dN(0)a^2\{\ell n(\frac{a^2+\omega_D^2}{a^2}) + \ell n\{\frac{\sqrt{\omega_D^2+\Delta^2(0)}-\omega_D}{\sqrt{\omega_D^2+\Delta^2(0)}+\omega_D}\}$$

$$-\frac{\sqrt{a^2-\Delta^2}}{a}\,\ell n\{\frac{a\sqrt{\omega_D^2+\Delta^2(0)}-\omega_D\sqrt{a^2-\Delta^2(0)}}{a\sqrt{\omega_D^2+\Delta^2(0)}+\omega_D\sqrt{a^2-\Delta^2(0)}} -$$

$$\frac{1}{2}\,\frac{\Delta^2(0)}{a\sqrt{a^2-\Delta^2(0)}}\,\ell n\{\frac{a\sqrt{\omega_D^2+\Delta^2(0)}-\omega_D\sqrt{a^2-\Delta^2(0)}}{a\sqrt{\omega_D^2+\Delta^2(0)}+\omega_D\sqrt{a^2-\Delta^2(0)}}\}$$

$$= -\frac{1}{2}\, N(0)\Delta^2(0) + dN(0)a^2\{\ell n(\frac{a^2+\omega_D^2}{a^2}) + \ell n\{\frac{\sqrt{\omega_D^2+\Delta^2(0)}-\omega_D}{\sqrt{\omega_D^2+\Delta^2(0)}+\omega_D}\}$$

$$-\frac{a^2-\Delta^2(0)+\frac{1}{2}\Delta^2(0)}{a\sqrt{a^2-\Delta^2(0)}}\,\ell n\{\frac{a\sqrt{\omega_D^2+\Delta^2(0)}-\omega_D\sqrt{a^2-\Delta^2(0)}}{a\sqrt{\omega_D^2+\Delta^2(0)}+\omega_D\sqrt{a^2-\Delta^2(0)}}$$

$$= -\frac{1}{2}\, N(0)\Delta^2(0) + dN(0)a^2\{\ell n(\frac{a^2+\omega_D^2}{a^2}) + \ell n\{\frac{\sqrt{1+\Delta^2(0)/\omega_D^2}-1}{\sqrt{1+\Delta^2(0)/\omega_D^2}+1}$$

$$-\frac{2a^2-\Delta^2(0)}{2a\sqrt{a^2-\Delta^2(0)}}\,\ell n\{\frac{\sqrt{1+(\Delta(0)/\omega_D)^2}-\sqrt{1-(\Delta(0)/a)^2}}{\sqrt{1+(\Delta(0)/\omega_D)^2}+\sqrt{1-(\Delta(0)/a)^2}}\}\}$$

This equation simplifies considerably if we take under consideration the fact that $a >> \Delta$ and $\omega_D >> \Delta$. The expression for ΔW can be approximated as follows:

$$\Delta W \cong -\frac{1}{2}N(0)\Delta^2(0) + dN(0)a^2\{\ln(\frac{a^2+\omega_D^2}{a^2} +$$

$$\ln\{\frac{\sqrt{1+(\Delta(0)/\omega_D)^2}-1}{\sqrt{1+(\Delta(0)/\omega_D)^2}+1}\} + \ln\{\frac{\sqrt{1+(\Delta(0)/\omega_D)^2}-\sqrt{1-(\Delta(0)/a)^2}}{\sqrt{1+(\Delta(0)/\omega_D)^2}+\sqrt{1-(\Delta(0)/a)^2}}\}\}$$

$$\cong -\frac{1}{2}N(0)\Delta^2(0) + dN(0)a^2\{\ln(\frac{a^2+\omega_D^2}{a^2}) +$$

$$\ln\{\frac{(\Delta(0)/\omega_D)^2 - \frac{1}{4}(\Delta(0)/\omega_D)^4}{(\Delta(0)/\omega_D)^2+(\Delta(0)/a)^2 - \frac{1}{4}(\Delta(0)/\omega_D)^4 + \frac{1}{4}(\Delta(0)/a)^4}\} +$$

$$\ln\{1 + \frac{1}{4}(\Delta(0)/\omega_D)^2 - \frac{1}{4}(\Delta(0)/a)^2 - \frac{1}{4}(\Delta(0)/\omega_D)^2\}\}$$

$$\cong -\frac{1}{2}N(0)\Delta^2(0) + dN(0)a^2\{\ln(\frac{a^2+\omega_D^2}{a^2}) - \frac{1}{4}(\frac{\Delta(0)}{a})^2 +$$

$$\ln\{\frac{1 - \frac{1}{4}(\Delta(0)/\omega_D)^2}{1 + (\omega_D/a)^2 - \frac{1}{4}\{(\Delta(0)/\omega_D)^2 - (\Delta(0)/a)^2(\omega_D/a)^2\}}\}\}$$

$$\cong -\frac{1}{2}N(0)\Delta^2(0)+dN(0)a^2\{\ln(\frac{a^2+\omega_D^2}{a^2}) - \frac{1}{4}(\frac{\Delta(0)}{a})^2 -$$

$$\ln\{1 + (\frac{\omega_D}{a})^2 - \frac{1}{4}\{(\frac{\Delta(0)}{\omega_D})^2 - (\frac{\Delta(0)}{a})^2(\frac{\omega_D}{a})^2\} + \frac{1}{4}(\frac{\Delta(0)}{\omega_D})^2(1+(\frac{\omega_D}{a})^2)\}\}$$

$$\cong -\frac{1}{2}N(0)\Delta^2(0)+dN(0)a^2\{\ln(\frac{a^2+\omega_D^2}{a^2}) - \frac{1}{4}(\frac{\Delta(0)}{a})^2 - \ln(1+(\frac{\omega_D}{a})^2)$$

$$- \{\frac{1}{4}(\frac{\Delta(0)}{\omega_D})^2 - \frac{1}{4}\{(\Delta(0)/\omega_D)^2-(\Delta(0)/a)^2(\omega_D/a)^2/(1+(\omega_D/a)^2)\}\}\}$$

which after rearrangement gives:

$$\Delta W \cong -\frac{1}{2} N(0)(1+d)\Delta^2(0) \qquad (3.67)$$

with

$$d = \frac{g}{\pi a} \quad \text{and} \quad \Delta(0) = 2\omega_D\left[\frac{1}{\sqrt{1+(\omega_D/a)^2}}\right]^{\left(\frac{d}{1+d}\right)} e^{-\frac{1}{N(0)V(1+d)}} \qquad (14)$$

Equation (3.67) is the final equation for the condensation energy at absolute zero temperature in the weak coupling limit with N(0)(1+d) the electronic density of states right at the Fermi energy. There is no other change in this formula due to the energy dependence for a >> k_BT_c.

CHAPTER IV

EVALUATION OF SPECIFIC HEAT NEAR T_c AND NEAR $T = 0$

The theoretical study of this chapter includes the mathematical developments needed to obtain the gap parameter at temperatures just below the critical temperature ($T \to T_c$) and at temperatures just above zero ($T \to 0$). The results obtained for the gap are used in evaluating the discontinuity in the specific heat at the transition and of its behaviour at very low temperature.

4.1.a Determination of the gap function $\Delta(T)$

To find the gap parameter at any temperature between the absolute zero and T_c, it is necessary to solve the finite BCS gap equation in the weak coupling limit ($\Delta(0) << \hbar\omega_D$). Since its solution requires numerical methods, we shall not attempt a detailed analysis and instead merely treat the limiting behaviour as mentioned above.

For temperatures just below the critical temperature the gap parameter as a function of temperature can be determined analytically by solving the BCS finite-temperature gap equation which is given by

$$1 = \frac{V}{2} \int_{-\omega_D}^{\omega_D} \frac{N(\varepsilon)}{[\varepsilon^2+\Delta^2(T)]^{1/2}} \tanh \frac{[\varepsilon^2+\Delta^2(T)]^{1/2}}{2kT} \, d\varepsilon \qquad (4.1)$$

It is evident that Eq. (4.1) reduces to Eq. (3.10) as T → 0 and gives the same solution for $\Delta(0)$ as before. In the opposite limit ($T \to T_c$) the gap vanishes identically and we find

$$1 = \frac{V}{2} \int_{-\omega_D}^{\omega_D} \frac{N(\varepsilon)}{\varepsilon} \tanh \frac{\varepsilon}{2k_B T_c} \, d\varepsilon$$

which has the approximate solution for T_c given by Eq. (3.9).

The integral equation for $\Delta(T)$ may be expanded as an infinite series by writing

$$\tanh \frac{x}{2} = 4x \sum_{n=0}^{\infty} \frac{1}{\pi^2 (2n+1)^2 + x^2} \tag{4.2}$$

where n is an integer, so that

$$1 = \frac{2V}{\beta} \int_{-\omega_D}^{\omega_D} d\varepsilon \sum_n \frac{N(\varepsilon)}{[\varepsilon^2 + \Delta^2(T) + \omega_n^2]} \tag{4.3}$$

with $\beta = \frac{1}{kT}$; $\omega_n = \pi k_B T_c (2n+1)$

where ω_n is the n'th Matsubara frequency. The gap equation (4.3) can be expanded in powers of Δ:

$$1 = \frac{2V}{\beta} \left[\int_{-\omega_D}^{\omega_D} d\varepsilon \sum_n N(\varepsilon) \frac{1}{\varepsilon^2 + \omega_n^2} + \int_{-\omega_D}^{\omega_D} d\varepsilon \sum_n \frac{\Delta^2(T)}{(\varepsilon^2 + \omega_n^2)^2} + \cdots \right] \tag{4.4}$$

The derivative with respect to Δ is easily evaluated. Since

$\omega_D >> k_B T_c$ the second integral may be extended to infinity. The first integral on the right of equation (4.4) has been done previously and its approximate solution has been given by equation (3.9). Therefore equation (4.4) can be written as

$$N(0)V(1+D)\ln(\frac{T}{T_c}) = -\frac{2VN(0)\Delta^2(T)}{\beta}\int_{-\infty}^{\infty} d\varepsilon \sum_n \frac{N(\varepsilon)}{N(0)(\varepsilon^2+\omega_n^2)^2} \qquad (4.5)$$

The latter integral may be done by applying the residue theorem; to see this we proceed as follows.

$$I = \int_{-\infty}^{\infty} d\varepsilon \sum_n \frac{N(\varepsilon)}{N(0)(\varepsilon^2+\omega_n^2)^2} =$$

$$\int_{-\infty}^{\infty} d\varepsilon \sum_n \frac{1}{(\varepsilon^2+\omega_n^2)^2} + \frac{ga}{\pi}\int_{-\infty}^{\infty} d\varepsilon \sum_n \frac{1}{\{a^2+(\varepsilon-b)^2\}\{\varepsilon^2+\omega_n^2\}^2} \qquad (4.6)$$

The first term in the integral I can be done as follows

$$\int_{-\infty}^{\infty} d\varepsilon \sum_n \frac{1}{(\varepsilon^2+\omega_n^2)^2} = \sum_n \frac{-1}{2\omega_n}\frac{d}{d\omega_n}\int_{-\infty}^{\infty}\frac{d\varepsilon}{(\varepsilon^2+\omega_n^2)}$$

$$= \sum_n \frac{-1}{2\omega_n}\frac{d}{d\omega_n}\int_{-\infty}^{\infty}\frac{d\varepsilon}{(\varepsilon+i\omega_n)(\varepsilon-i\omega_n)}$$

By applying the residue theorem this term becomes:

$$= 2\pi i \sum_n \frac{-1}{2\omega_n} \frac{d}{d\omega_n} \lim_{\varepsilon\to i\omega_n} (\varepsilon-i\omega_n) \frac{1}{(\varepsilon+i\omega_n)(\varepsilon-i\omega_n)}$$

$$= \frac{\pi}{2} \sum_n \frac{1}{\omega_n^3} = \frac{\pi}{2} (k\pi T)^{-3} \sum_n \frac{1}{(2n+1)^3}$$

$$= \frac{\pi}{2} (k\pi T)^{-3} \frac{7}{8} \xi(3) \qquad (4.7)$$

where $\xi(3)$ is the Riemann zeta-function.

The evaluation of the second term in equation (4.6) follows a way similar to that used for the first term. Thus

$$\int_{-\infty}^{\infty} \frac{d\varepsilon}{\{a^2+(\varepsilon-b)^2\}(\varepsilon^2+\omega_n^2)^2} = \frac{-1}{2\omega_n} \frac{d}{d\omega_n} \int_{-\infty}^{\infty} \frac{d\varepsilon}{\{a^2+(\varepsilon-b)^2\}(\varepsilon^2+\omega_n^2)} \qquad (4.8)$$

Rewriting the integrand as

$$\frac{1}{\{a^2+(\varepsilon-b)^2\}(\varepsilon^2+\omega_n^2)} = \frac{1}{(\varepsilon-b+ia)(\varepsilon-b-ia)(\varepsilon+i\omega_n)(\varepsilon-i\omega_n)}$$

we see that there are simple poles at

$$\varepsilon = b-ia \;,\; \varepsilon = -i\omega_n \;,\; \varepsilon = b+ia \text{ and } \varepsilon = i\omega_n \;.$$

The contour of integration can be extended by a semicircle in either the upper or lower half planes. Choosing the upper semicircle and applying the residue theorem we get

$$\int_{-\infty}^{\infty} \frac{d\varepsilon}{\{a^2+(\varepsilon-b)^2\}(\varepsilon^2+\omega_n^2)^2} = \frac{-1}{2\omega_n}\frac{d}{d\omega_n} 2\pi i\{ \lim_{\varepsilon\to b+ia} (\varepsilon-b-ia) \times$$

$$\frac{1}{(\varepsilon-b+ia)(\varepsilon-b-ia)} \cdot \frac{1}{(\varepsilon^2+\omega_n^2)} + \lim_{\varepsilon\to i\omega_n} (\varepsilon-i\omega_n) \times$$

$$\frac{1}{\{a^2+(\varepsilon-b)^2\}} \cdot \frac{1}{(\varepsilon-i\omega_n)(\varepsilon+i\omega_n)}\}$$

$$= \frac{-\pi}{2\omega_n}\frac{d}{d\omega_n}\{\frac{1}{a\{(b+ia)^2+\omega_n^2\}} + \frac{1}{\omega_n\{a^2+(i\omega_n-b)^2\}}\}$$

The two denominators can be rewritten as

$$\{(b+ia)^2+\omega_n^2)\} = \{b+i(a+\omega_n)\}\{b+i(a-\omega_n)\} ;$$

$$\{(i\omega_n-b)^2+a^2\} = \{b-i(a+\omega_n)\}\{b+i(a-\omega_n)\}$$

After simple mathematical manipulations the integral given by equation (4.8) can be reduced to the following form

$$\int_{-\infty}^{\infty} \frac{d\varepsilon}{\{a^2+(\varepsilon-b)^2\}(\varepsilon^2+\omega_n^2)^2} = \frac{-\pi}{2\omega_n}\frac{d}{d\omega_n}\{\frac{(\omega_n+a)}{a\omega_n\{b^2+(a+\omega_n)^2\}}\}$$

$$= \frac{\pi\{ab^2+a(a+\omega_n)^2+2\omega_n(a+\omega_n)^2\}}{2a\omega_n^3\{b^2+(a+\omega_n)^2\}^2} \qquad (4.9)$$

It is possible to use the lower semicircle but this choice will lead to the same result that we obtained by choosing the upper semicircle.

Substituting equations (4.7) and (4.9) in equation (4.5) gives

$$N(0)V(1+D)\ln\frac{T}{T_c} = -\frac{2VN(0)}{\beta}\Delta^2(T)\{\frac{\pi}{2}(kT\pi)^{-3}\frac{7}{8}\xi(3) + g\sum_n\frac{\{ab^2+a(a+\omega_n)^2+2\omega_n(a+\omega_n)^2\}}{2\omega_n^3\{b^2+(a+\omega_n)^2\}^2}\} \tag{4.10}$$

which after rearrangement gives:

$$\Delta^2(T) = (kT_c\pi)^2(\frac{8}{7\xi(3)})(1+D)(1-\frac{T}{T_c})\{1 + (kT_c)^3\frac{8}{7\xi(3)}2\pi^2 g\sum_n\frac{\{ab^2+a(a+\omega_n)^2+2\omega_n(a+\omega_n)^2\}}{2\omega_n^3\{b^2+(a+\omega_n)^2\}^2}\}^{-1} \tag{4.11}$$

Therefore the gap parameter at temperature just below the critical temperature is given by

$$\Delta(T) = K_B T_c\pi\{8/7\xi(3)\}^{1/2}(1+D)^{1/2}\{1-\frac{T}{T_c}\}^{1/2}\{1+(kT_c)^3(7/8\xi(3))\pi^2 g \times \sum_n\frac{ab^2+a(a+\omega_n)^2+2\omega_n(a+\omega_n)^2}{2\omega_n^3\{b^2+(a+\omega_n)^2\}^2}\}^{-1/2} \tag{4.12}$$

This is the expression for $\Delta(T)$ at temperatures just below the critical temperature ($T \to T_c$).

4.1.b Entropy and Specific heat

Discontinuity in the electronic specific heat

Experiment shows that the transition from normal to superconducting state is of second order; the entropy is continuous at the critical temperature T_c - no latent heat evolved at the transition - but there is a discontinuity in the specific heat.

Based on our model for the energy dependent electronic density of state, the specific heat jump according to the BCS theory can be calculated in the following way.

The entropy of a superconductor is given by

$$S = -\ 2k_B \sum_k \{\{1-f(\beta E_k)\}\ell n\{1-f(\beta E_k)\}+f(\beta E_k)\ell n f(\beta E_k)\} \qquad (4.13)$$

The specific heat per unit volume of the electrons can be calculated from the formula

$$C_s = \frac{T}{\Omega}\ \{\frac{\partial S}{\partial T}\} = \frac{-\beta}{\Omega}\ \{\frac{\partial S}{\partial \beta}\}_{V,b} \qquad (4.14)$$

In order to evaluate the electronic specific heat (C_s) equation (4.13) has to be differentiated with respect to β.

$$S = -2k_B \sum_k\{\frac{-\ell n(1+e^{-\beta E_k})}{1+e^{\beta E_k}} - \frac{\ell n(1+e^{\beta E_k})}{1+e^{\beta E_k}}\}$$

$$= 2k_B \sum_k \{\frac{\beta E_k}{1+e^{\beta E_k}} + \ell n(1+e^{-\beta E_k})\}$$

$$= 2k_B \int N(\varepsilon)d\varepsilon\{\beta E_k f(\beta E_k) + \ell n(1+e^{-\beta E_k})\} \qquad (4.15)$$

in which we have replaced $\{1-f(\beta E_k)\}$ by $1/1+e^{\beta E_k}$ and the substitution $\ell n\{1+e^{\beta E_k}\} = \beta E_k + \ell n(1+e^{-\beta E_k})$ has been made. Straightforward differential of equation (4.15) gives

$$C_s = -2k_B\beta \int N(\varepsilon)d\varepsilon \quad \frac{-\beta E_k e^{\beta E_k}}{(1+e^{\beta E_k})^2} \frac{\partial}{\partial\beta} (\beta E_k) \qquad (4.16)$$

Since $E_k = \{\varepsilon_k^2+\Delta^2(T)\}^{1/2}$ and in the limit when $T \to T_c$, it is permissible to set $\Delta \simeq 0$ and $E_k \simeq \varepsilon_k$, then equation (4.16) can be written as, putting $\varepsilon_k = \varepsilon$

$$\begin{aligned} C_s &= -2 \int N(\varepsilon)d\varepsilon\{\varepsilon^2 + \frac{\beta}{2} \frac{\partial\Delta^2(T)}{\partial\beta}\}\frac{\partial f(\beta\varepsilon)}{\partial\varepsilon} \\ &= -2 \int N(\varepsilon)d\varepsilon \ \varepsilon^2 \frac{\partial f(\beta\varepsilon)}{\partial\varepsilon} - \frac{1}{k_B T^2} \int d\varepsilon \ N(\varepsilon) \left.\frac{\partial\Delta^2(T)}{\partial\beta}\right|_{T_c} \frac{\partial f(\beta\varepsilon)}{\partial\varepsilon} \\ &= \frac{2}{3} \pi^2 N(0)(1+D)k_B^2 T - \frac{1}{k_B T^2} \int d\varepsilon \ N(\varepsilon) \left.\frac{\partial\Delta^2(T)}{\partial\beta}\right|_{T_c} \frac{\partial f(\beta\varepsilon)}{\partial\varepsilon} \end{aligned}$$

The first term on the right of this equation gives the electronic specific heat in the normal state with $N(\varepsilon)$ replaced in the integral by $N(0)(1+D)$; the electronic density of state right at the Fermi energy which is valid for small temperature. Equation (4.16) can be written as

$$\begin{aligned} C_s - C_n &= (-1) \frac{1}{k_B T^2} \int_{\omega_D} d\varepsilon \ N(\varepsilon) \left.\frac{\partial\Delta^2(T)}{\partial\beta}\right|_{T_c} \frac{\partial f(\beta\varepsilon)}{\partial\varepsilon} \\ &= -\frac{N(0)}{kT^2} \left.\frac{\partial\Delta^2(T)}{\partial\beta}\right|_{T_c} [\int_{-\omega_D}^{\omega_D} d\varepsilon f'(\beta\varepsilon) + \frac{ga}{\pi} \int_{-\omega_D}^{\omega_D} \frac{1}{\{a^2+(\varepsilon-b)^2\}} f'(\beta\varepsilon)d\varepsilon] \\ &= \frac{N(0)}{kT^2} \left.\frac{\partial\Delta^2(T)}{\partial\beta}\right|_{T_c} [1 - \frac{ga}{\pi} \int_{-\omega_D}^{\omega_D} \frac{1}{\{a^2+(\varepsilon-b)^2\}} f'(\beta\varepsilon)d\varepsilon] \qquad (4.17) \end{aligned}$$

where we have used the fact that $\int_{-\omega_D}^{\omega_D} d\varepsilon f'(\beta\varepsilon) = -1$ (to a very good approximation). Since $f'(\beta\varepsilon)$ is only significantly different from zero in the neighbourhood of $\varepsilon = 0$, so that it is sufficient for the present purposes if $\frac{1}{\{a^2+(\varepsilon-b)^2\}}$ is expanded as a Taylor series about $\varepsilon = 0$. Taking only the first three terms of the expansion to be significant because of the small range of energies, the expansion is

$$\frac{1}{\{a^2+(\varepsilon-b)^2\}} = \frac{1}{(a^2+b^2)} + \frac{2b}{(a^2+b^2)^2}\,\varepsilon + \frac{3b^2-a^2}{(a^2+b^2)^3}\,\varepsilon^2 + \cdots$$

then equation (4.17) becomes

$$C_s-C_n = \frac{N(0)}{kT^2}\,\frac{\partial\Delta^2(T)}{\partial\beta}\bigg|_{T_c}\left[1 - \frac{ga}{\pi}\left\{\frac{1}{(a^2+b^2)}\int_{-\omega_D}^{\omega_D} f'(\beta\varepsilon)d\varepsilon + \frac{2b}{(a^2+b^2)^2}\int_{-\omega_D}^{\omega_D} \varepsilon f'(\beta\varepsilon)d\varepsilon + \frac{3b^2-a^2}{(a^2+b^2)^3}\int_{-\omega_D}^{\omega_D} \varepsilon^2 f'(\beta\varepsilon)d\varepsilon\right\}\right]. \quad (4.18)$$

Now

$$\int_{-\omega_D}^{\omega_D} f'(\beta\varepsilon)d\varepsilon = -1 \quad ; \quad \int_{-\omega_D}^{\omega_D} \varepsilon f'(\beta\varepsilon)d\varepsilon = 0$$

(since the integrand is an odd function of (ε)) and the last integral $\int_{-\omega_D}^{\omega_D} \varepsilon^2 f'(\beta\varepsilon)d\varepsilon = \frac{\pi^2}{3}(k_BT)^2$. In fact these three integrals have been evaluated in detail in the mathematical treatment of the chemical potential, so that equation (4.18) becomes

$$C_s-C_n = \frac{N(0)}{k_BT^2}\left.\frac{\partial\Delta^2(T)}{\partial\beta}\right|_{T_c}[(1+D)+D\,\frac{3b^2-a^2}{3(a^2+b^2)^2}\,\pi^2(kT_c)^2 \tag{4.19}$$

where $\frac{\partial\Delta^2(T)}{\partial\beta}$ can be written as

$$\left.\frac{\partial\Delta^2(T)}{\partial\beta}\right|_{T_c} = \left.\frac{\partial\Delta^2(T)}{\partial T}\,\frac{\partial T}{\partial\beta}\right|_{T_c} = -\left.\frac{T_c}{\beta_c}\,\frac{\partial\Delta^2(T)}{\partial T}\right|_{T_c} \tag{4.20}$$

By differentiating equation (4.11) and using the fact that

$$C_n = \frac{2}{3}\pi^2 k_B^2\,N(0)(1+D)T_c = \gamma T_c \tag{4.21}$$

we find

$$\frac{C_s-C_n}{C_n} = \frac{3}{2}\,\frac{8}{7\xi(3)}\,C \tag{4.22}$$

with C given by

$$C = [(1+D)+D\,\frac{3b^2-a^2}{3(a^2+b^2)^2}\,\pi^2(kT_c)] \times$$

$$[1+\frac{8\pi^2}{7\xi(3)}\,(kT_c)^3 g\sum_{n=0}^{\infty}\frac{ab^2+a(a+\omega_n)^2+2\omega_n(a+\omega_n)^2}{\omega_n^3\{b^2+(a+\omega_n)^2\}^2}\,]^{-1}$$

Eq. (4.22) is our final equation for the specific heat jump based on our model for the energy dependent electronic density of state. We see that it is modified from the BCS formula for the jump by the quantity C which is new and reflects the energy dependent electronic density of state.

Figures (4.1) and (4.2) illustrate the jump in specific heat against b for two values of ω_D (20 and 35 mev). We note from these graphs that as b increases from zero to 50 mev the jump in the specific heat stays constant and equal to the BCS value of 1.426 except for small values of a and b in which the deviation ranges from .35 to 11%. Since this deviation from the BCS value is due to the new parameter C which contains all the information about the energy dependence of the electronic density of states, it is instructive to look at this parameter in more detail and try to investigate the behaviour of C as a function of the various parameters. To do so it was found that it is more convenient to rewrite C in terms of three variables instead of four just to make our task easier. The parameter C is given by

$$C \simeq \{1+D\}\{1+\frac{8\pi^2}{7\xi(3)}(k_BT_c)^2 g \sum_{n=0}^{\infty} \frac{ab^2+a(a+\omega_n)^2+2\omega_n(a+\omega_n)^2}{\omega_n^3\{b^2+(a+\omega_n)^2\}^2}\}^{-1}$$

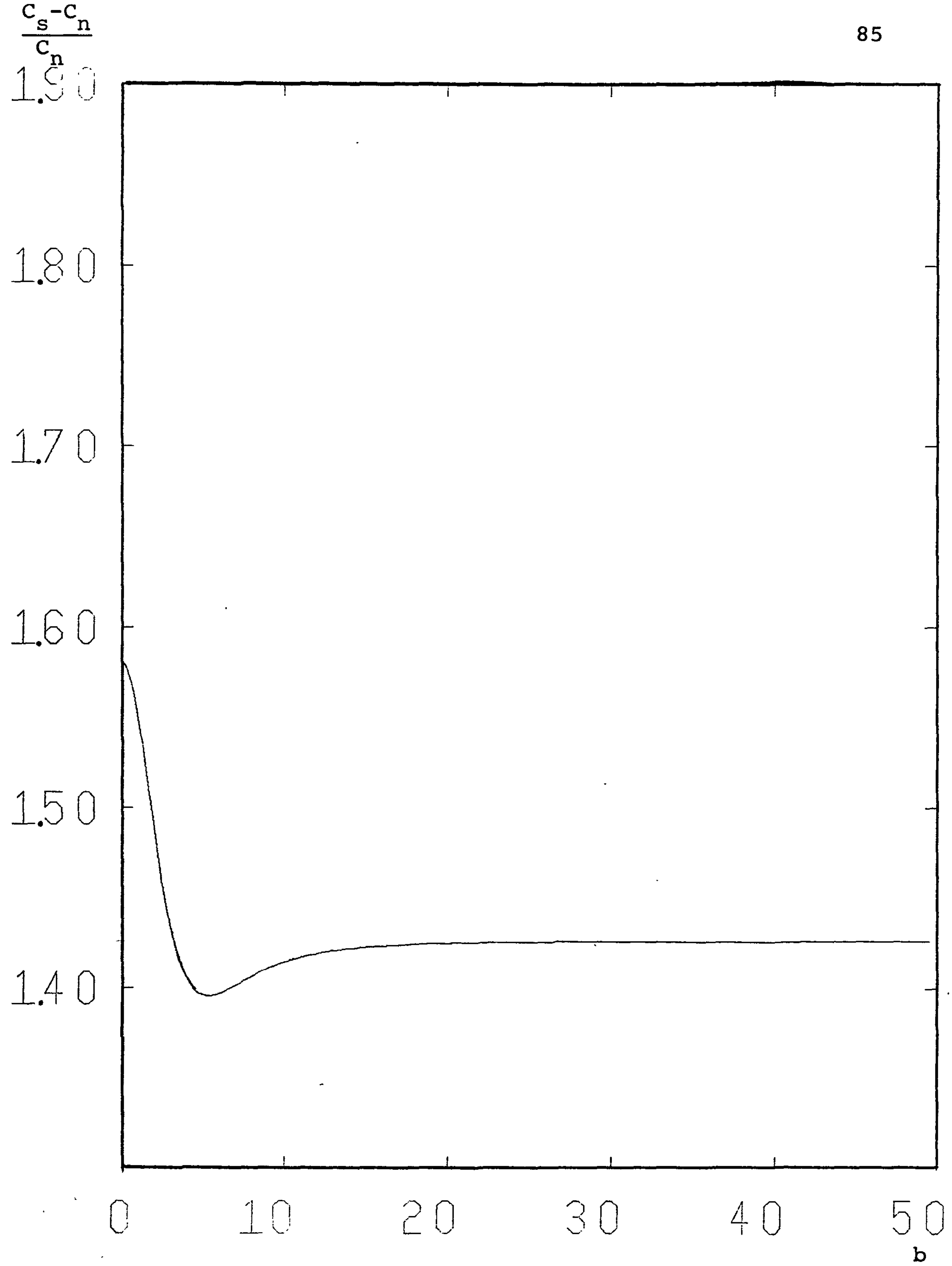
$$= \{1+d\frac{a^2}{a^2+d^2}\}\{1+\frac{8\pi^2}{7\xi(3)}(\frac{a}{\pi k_BT_c})\sum_{n=0}^{\infty}(\frac{a}{\pi k_BT_c})(\frac{b}{\pi k_BT_c})^2+(\frac{a}{\pi k_BT_c}+(2n-1))^2 \times$$

$$(\frac{a}{\pi k_BT_c}+2(2n+1))/(2n+1)^3\{(\frac{b}{\pi k_BT_c})^2+(\frac{a}{\pi k_BT_c}+(2n+1))^2\}^2\}$$

$$\equiv \{1+d(\frac{1}{1+\bar{b}^2})\}\{1+\frac{8d}{7\xi(3)}\tilde{\bar{a}}\sum_{n=0}^{\infty}\frac{\tilde{\bar{a}}^3\bar{b}^2+\{\tilde{\bar{a}}(2n+1)\}^2(\tilde{\bar{a}}+2(2n+1))}{(2n+1)^3\{\tilde{\bar{a}}^2\bar{b}^2+(\tilde{\bar{a}}+(2n+1))^2\}^2}\}^{-1}$$

Fig. (4.1.a)

A plot of the jump in specific heat versus b(mev) for $a = 5$ mev and $\omega_D = 20$ mev.



$\frac{c_s-c_n}{c_n}$
1.90
1.80
1.70
1.60
1.50
1.40
0
10
20
30
40
50
b

Fig. (4.1.b)

A plot of the jump in specific heat versus b (mev) for $a = 15$ mev and $\omega_D = 20$ mev.

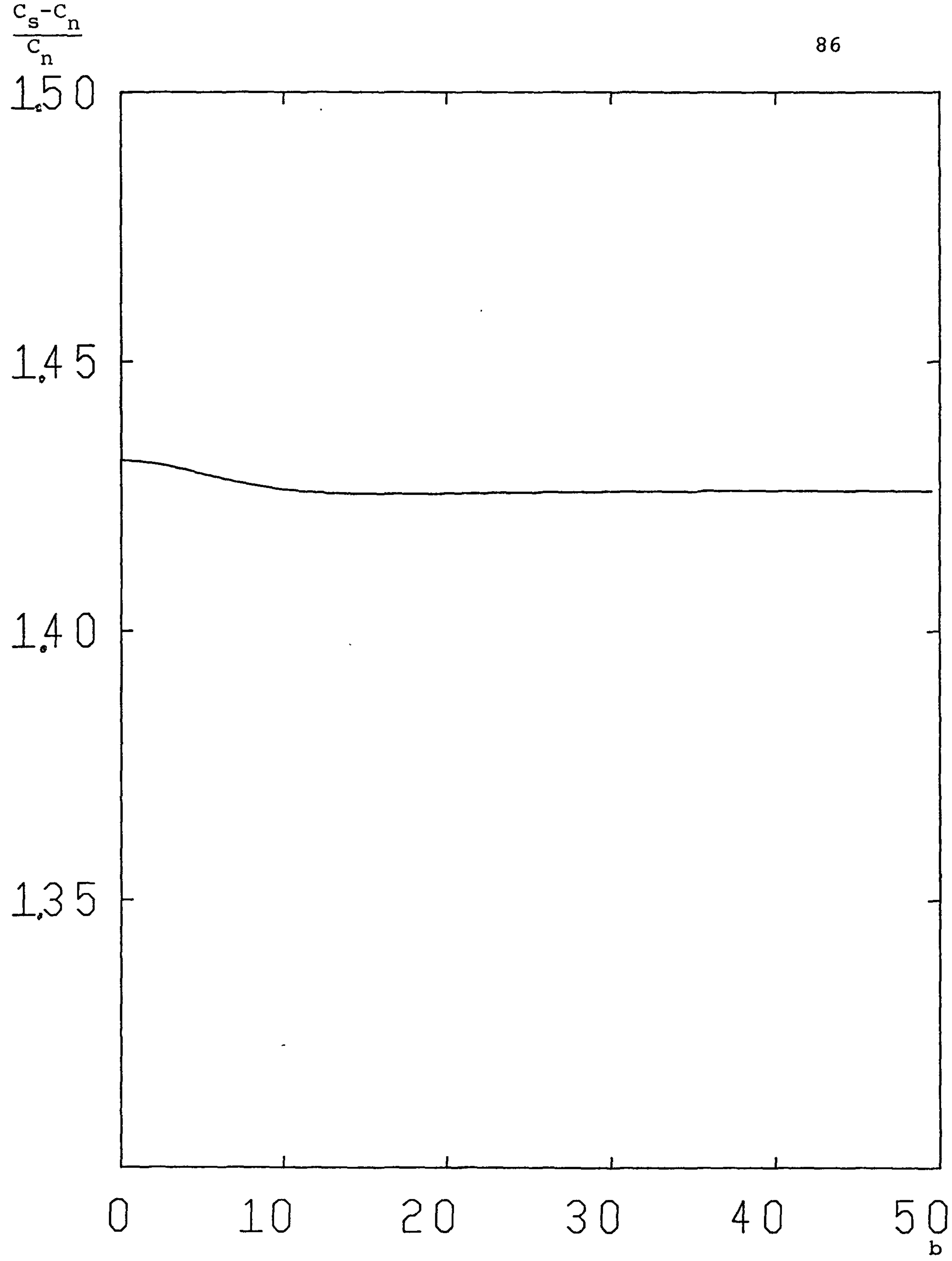

$\frac{C_s - C_n}{C_n}$
1,50
1,45
1,40
1,35
0
10
20
30
40
50
b

Fig. (4.1.c)

A plot of the jump in specific heat versus b (mev) for $a = 25$ mev and $\omega_D = 20$ mev.

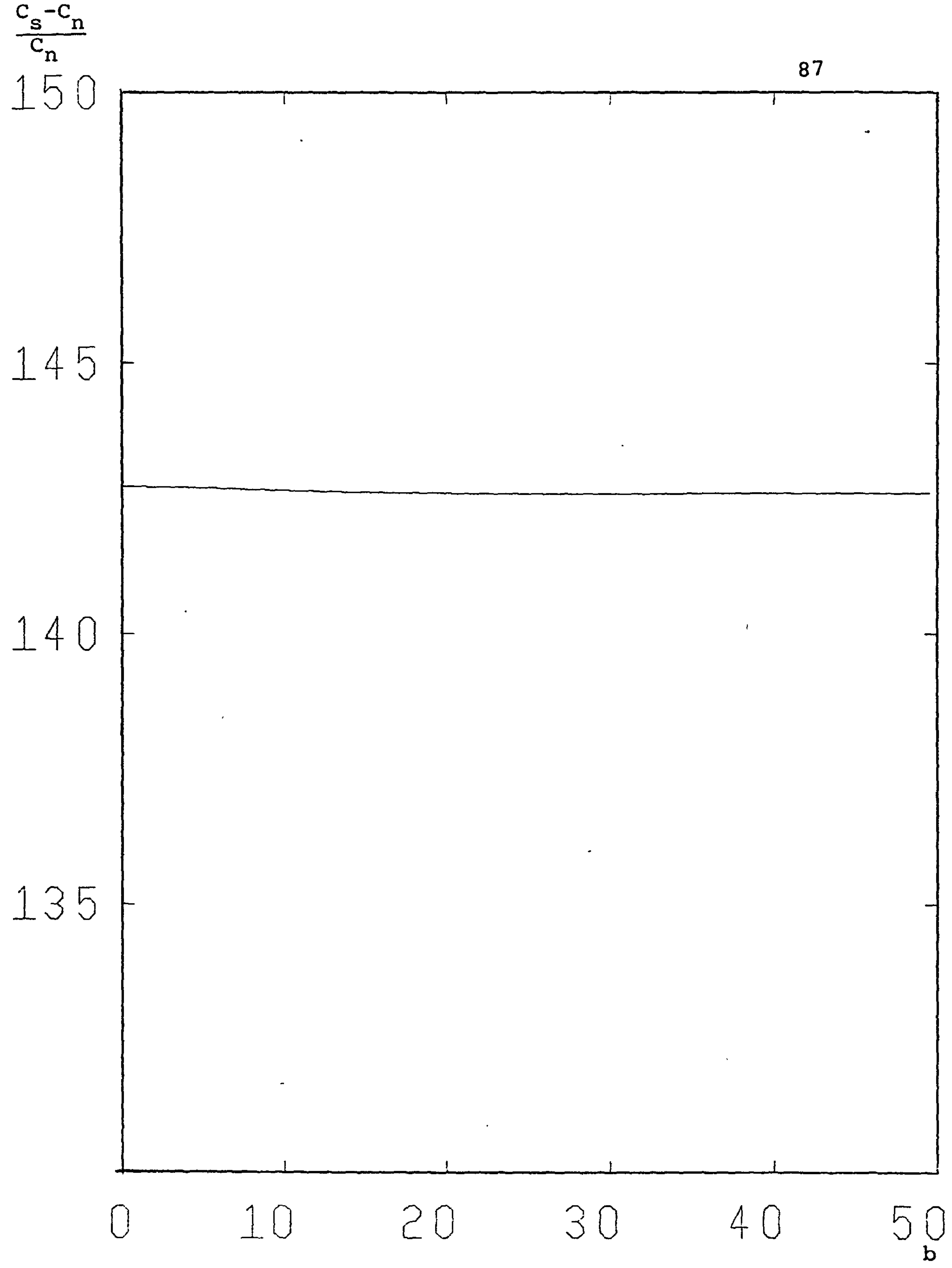

$\frac{c_s - c_n}{c_n}$
150
145
140
135
0
10
20
30
40
50
b

Fig. (4.2.a)

A plot of the jump in specific heat versus b (mev) for a = 5 mev and ω_D = 35 mev.

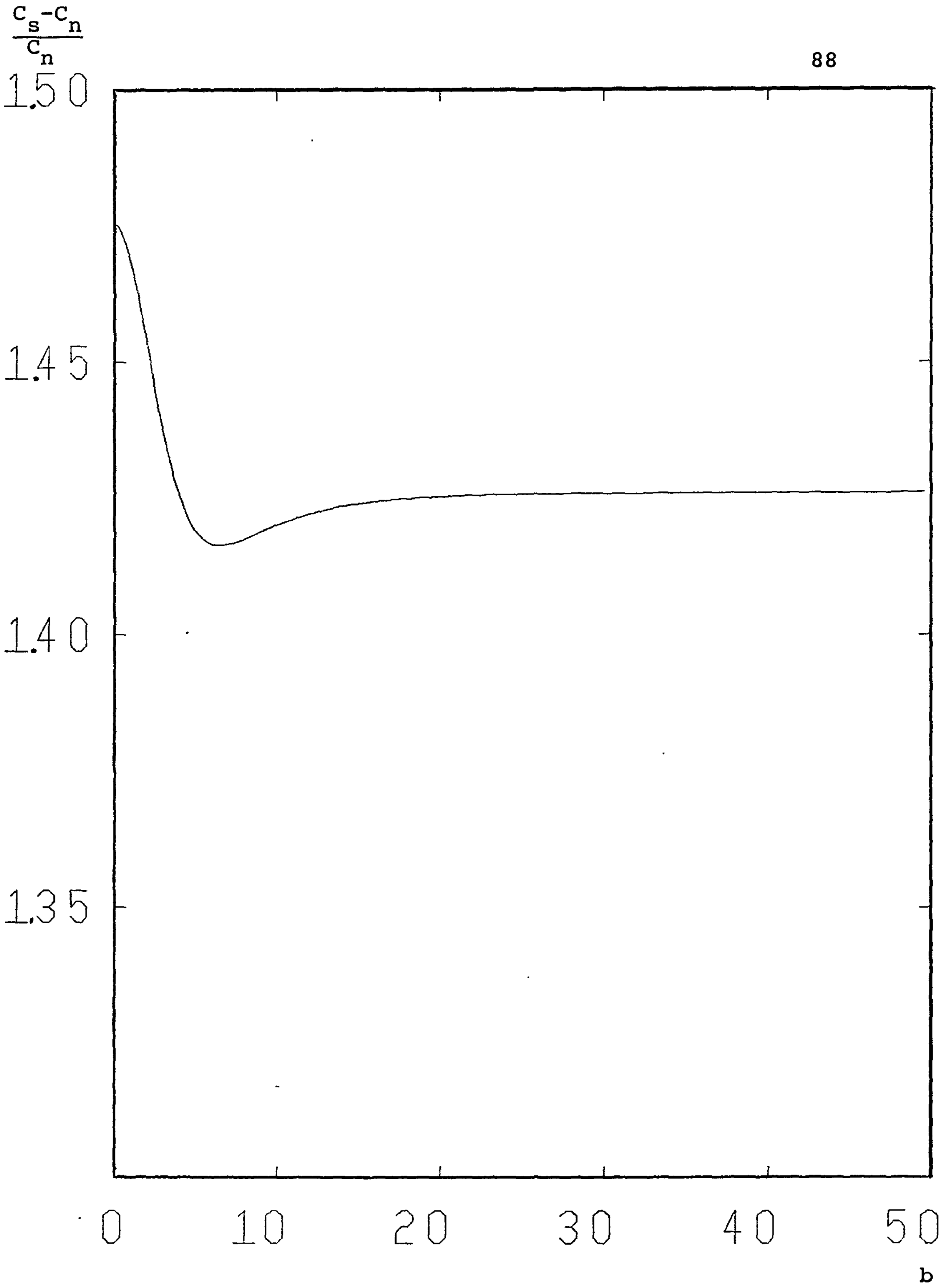

$\frac{c_s - c_n}{c_n}$
1.50
1.45
1.40
1.35
0
10
20
30
40
50
b

Fig. (4.2.b)

A plot of the jump in specific heat versus b (mev) for $a = 15$ mev and $\omega_D = 35$ mev.

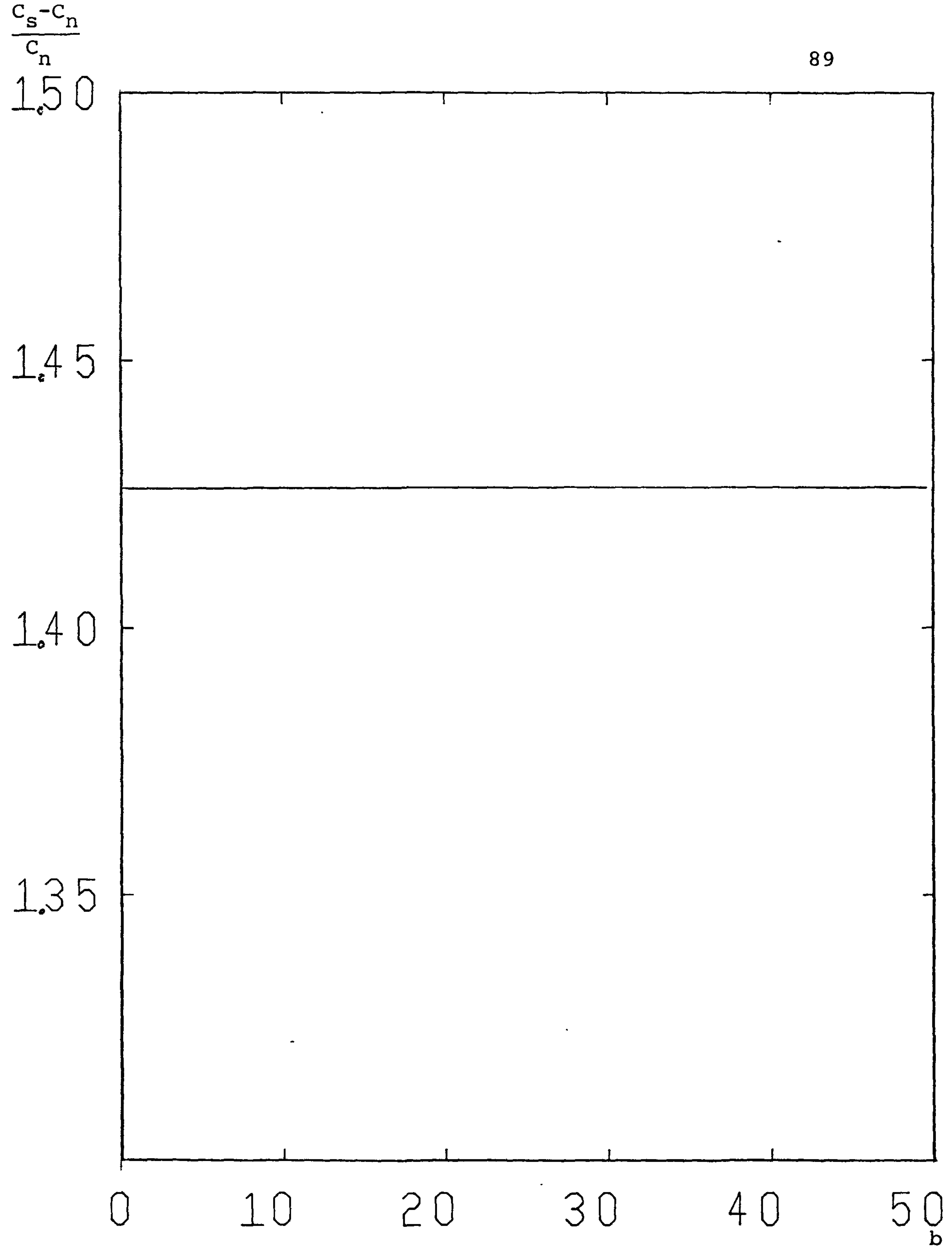
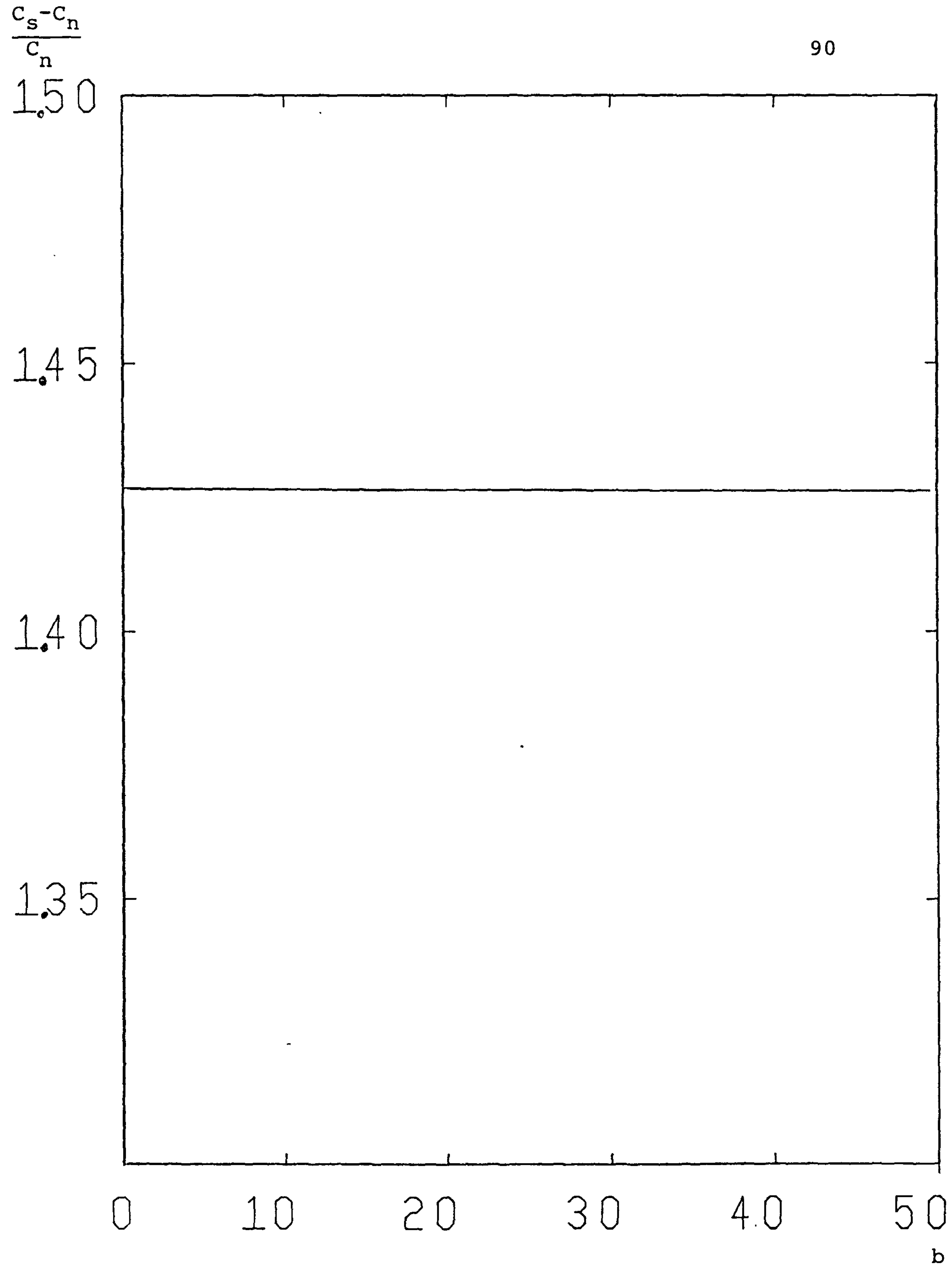

$\frac{c_s-c_n}{c_n}$
1.50
1.45
1.40
1.35
0
10
20
30
40
50
b

Fig. (4.2.c)

A plot of the jump in specific heat versus b (mev) for $a = 25$ mev and $\omega_D = 35$ mev.


$\frac{c_s - c_n}{c_n}$
1.50
1.45
1.40
1.35
0
10
20
30
40
50
b

in which $\tilde{\tilde{a}}$, $\bar{b}$ and d are defined as

$$\tilde{\tilde{a}} = \frac{a}{\pi k_B T_c} \quad ; \quad \tilde{b} \equiv \frac{b}{\pi k_B T_c} \quad \text{and} \quad d = \frac{g}{\pi a}$$

The variation of $C(\tilde{\tilde{a}},\bar{b},d)$ has been studied for various values of $\tilde{\tilde{a}}$, $\bar{b}$ and d covering the region required for the most practical cases of interest. In Figs. 4.3, 4.4, 4.5 and 4.6 we plot $C(\tilde{\tilde{a}},\bar{b},d)$ versus $\bar{b}$ for various values of d (2, 1, .5 and .35) while each graph has been taken for eight values of $\tilde{\tilde{a}}$ (1.5, 2, 3, 4, 5, 10, 15 and 20) since we are interested only in $\tilde{\tilde{a}} >> 1$. It can be seen from these graphs especially for small values of $\tilde{\tilde{a}}$, that C deviates from 1 for small values of $\bar{b}$ and then saturates to 1 to give the BCS limit for the jump as expected. In fact the behaviour of $C(\tilde{\tilde{a}},\bar{b},d)$ as a function of these three variables accounts quantitatively for the deviation in the jump at small values of a and b.

Dependence of electronic specific heat on temperature

The dependence of the specific heat in a superconducting state on temperature has to be evaluated numerically. Basically in this section we present the mathematical steps developed in evaluating the electronic specific heat as a function of temperature in the low temperature limit. In this limit it is permissible to evaluate the integral equation of the electronic specific heat by setting $\omega_D \to \infty$ and $\Delta(T) \simeq \Delta(0)$. Having done that the integral equation for

Fig. (4.3)

A plot of $C(\tilde{\bar{a}},\bar{b},d)$ versus $\bar{b}$ for $d = 2$ and for $\tilde{\bar{a}} = 1.5$ (———), 2(•••••), 3(-----), 4(-•--•--•-), 5(-••-••-), 10(-•••-•••-), 15(•••••) and 20(-----).

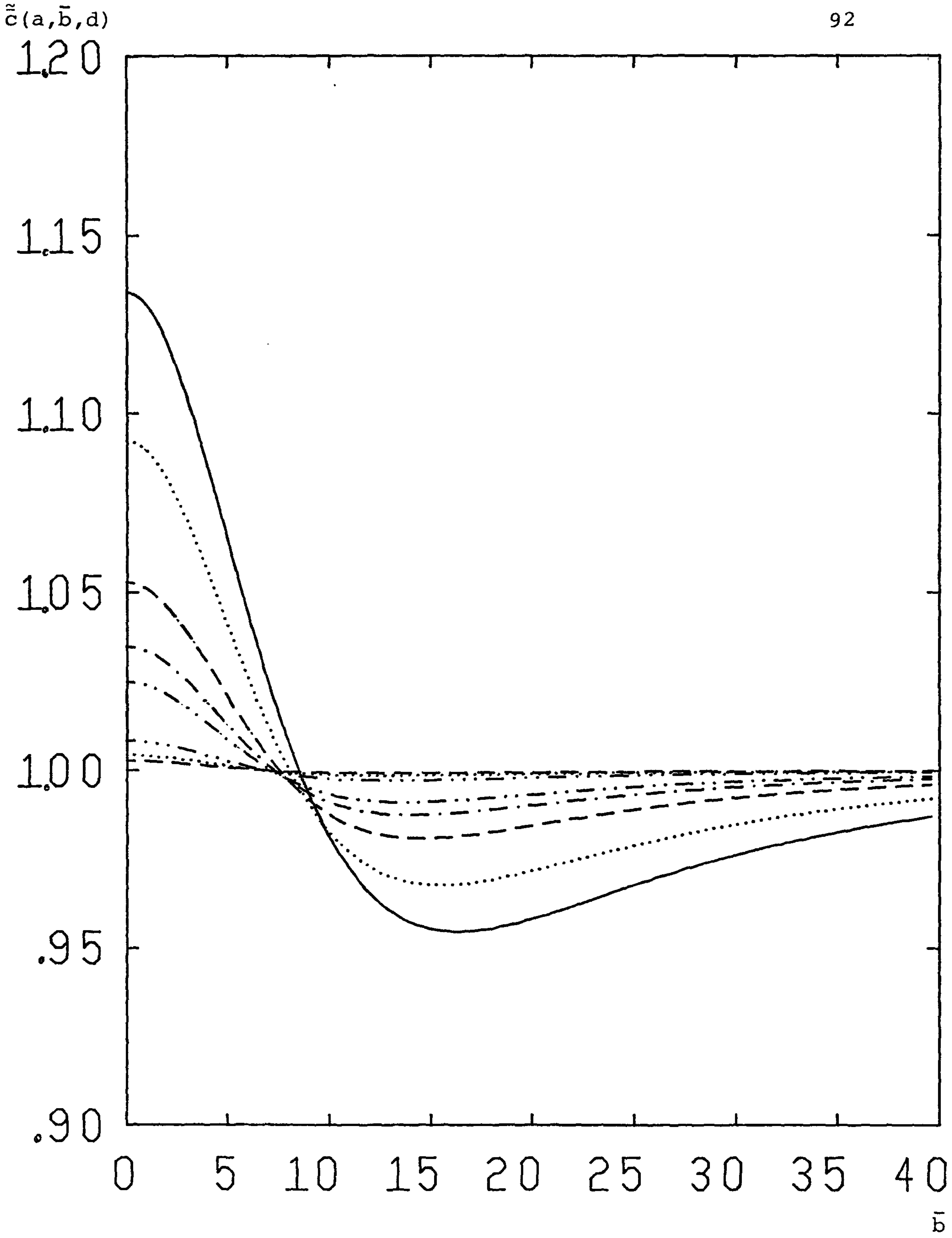

$\tilde{\tilde{c}}(a,\bar{b},d)$
1.20
1.15
1.10
1.05
1.00
.95
.90
0
5
10
15
20
25
30
35
40
$\bar{b}$

Fig. (4.4)

A plot of $C(\tilde{\tilde{a}},\bar{b},d)$ versus $\bar{b}$ for $d = 1$ and for $\tilde{\tilde{a}} = 1.5$ (———), 2(•••••), 3(-----), 4(-•-•-•-•), 5(-••-••-), 10(-•••-•••-), 15(•••••) and 20(-----).

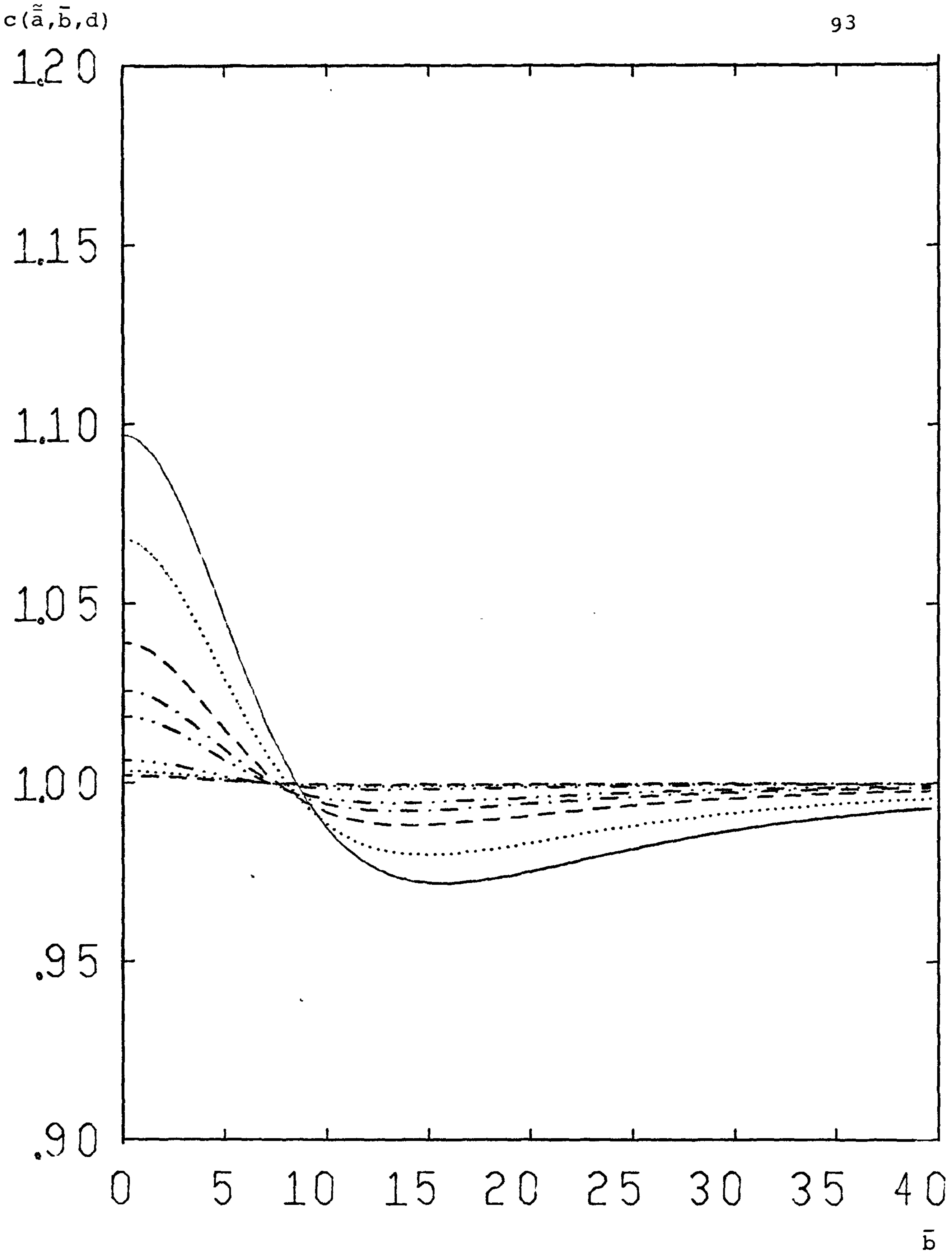

$c(\tilde{\tilde{a}},\bar{b},d)$
1.20
1.15
1.10
1.05
1.00
.95
.90
0
5
10
15
20
25
30
35
40
$\bar{b}$

Fig. (4.5)

A plot of $C(\tilde{\tilde{a}},\bar{b},d)$ versus $\bar{b}$ for $d = .5$ and for $\tilde{\tilde{a}} =$ 1.5 (———), 2(•••••), 3(-----), 4(-•-•-•-•-•), 5 (-••-••-••-), 10(-•••-•••-), 15(•••••) and 20(-----).

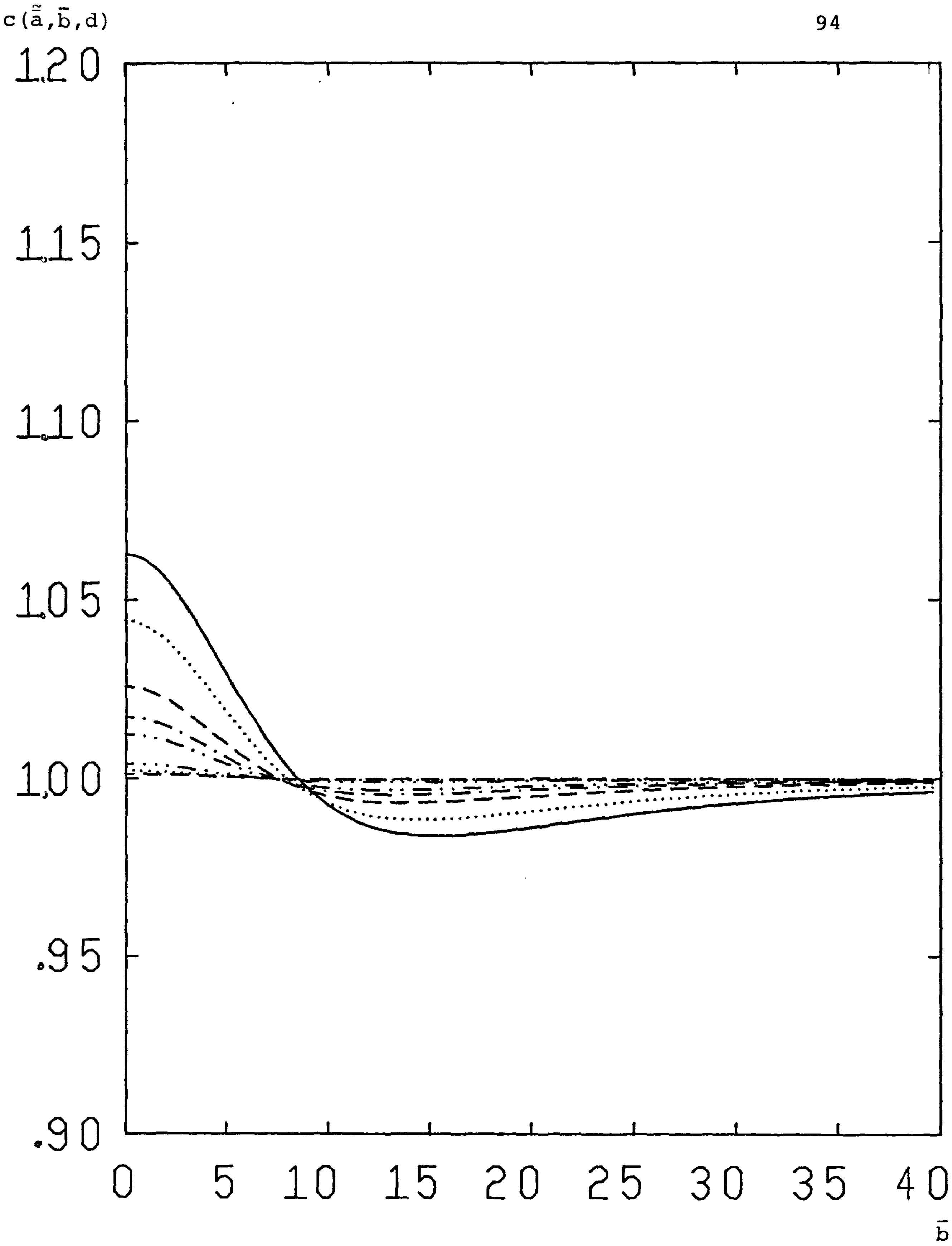
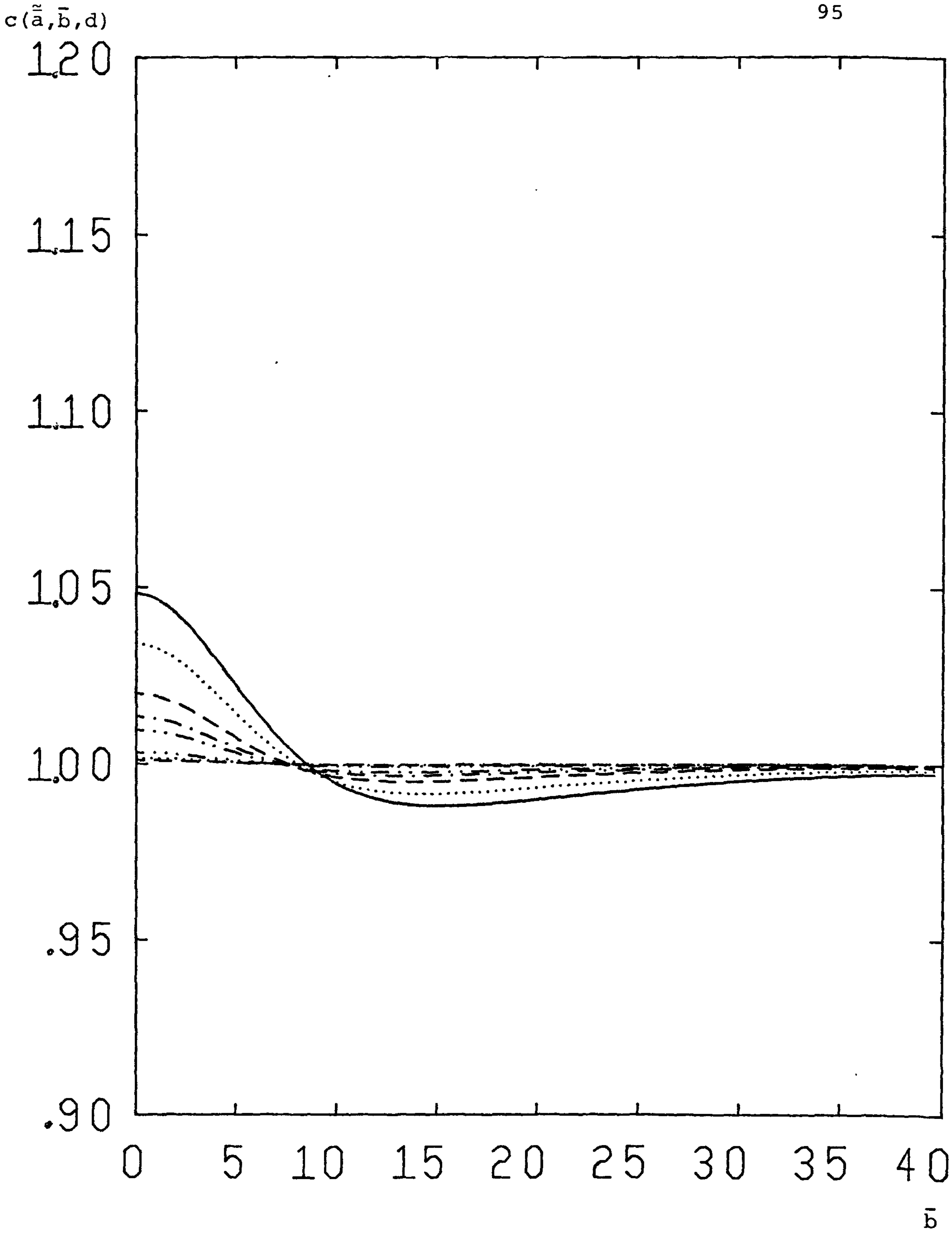

c($\tilde{\tilde{a}}$,$\bar{b}$,d)
1.20
1.15
1.10
1.05
1.00
.95
.90
0
5
10
15
20
25
30
35
40
$\bar{b}$

Fig. (4.6)

A plot of $C(\tilde{\bar{a}},\bar{b},d)$ versus $\bar{b}$ for $d = .35$ and for $\tilde{\bar{a}} = 1.5$ (———), 2(•••••), 3(-----), 4(-•--•--•--•), 5(-••-••-••-), 10(-•••-•••-), 15(•••••) and 20 (-----)


c($\tilde{\tilde{a}}$,$\bar{b}$,d)
1.20
1.15
1.10
1.05
1.00
.95
.90
0
5
10
15
20
25
30
35
40
$\bar{b}$

evaluating the electronic specific heat in the low-temperature limit (4.16) can be written as

$$C_s(T\rightarrow 0) = \frac{2k_B}{\Omega}\,\beta^2 \int_{-\omega_D}^{\omega} N(\varepsilon_k)\,d\varepsilon_k E_k^2\,\frac{e^{\beta E_k}}{(1+e^{\beta E_k})^2} \tag{4.23}$$

with $E_k = \{\varepsilon_k^2+\Delta^2(0)\}^{1/2}$.

Since $E_k >> kT$; $e^{\beta E_k} >$ in this limit, equation (4.23) can be reduced to

$$C_s(T\rightarrow 0) = \frac{2k_B}{\Omega}\,\beta^2\Delta^2(0)\int_{-\omega_D}^{\omega_D} N(\varepsilon_k)\,d\varepsilon_k\{1+\frac{\varepsilon^2}{\Delta^2(0)}\}e^{-\beta\Delta(0)\{1+(\frac{\varepsilon}{\Delta(0)})^2\}^{1/2}} \tag{4.24}$$

$$= \frac{2k_B}{\Omega}\,\beta^2\Delta^3(0)N(0)\{\int_{-\omega_D/\Delta}^{\omega_D/\Delta} dx\{1+x^2\}e^{-\beta\Delta(0)(1+x^2)^{1/2}} +$$

$$\frac{ga}{\pi}\int_{-\omega_D/\Delta}^{\omega_D/\Delta}\frac{1}{\{a^2+(x\Delta(0)-b)^2\}}(1+x^2)e^{-\beta\Delta(0)(1+x^2)^{1/2}}\,dx\} \tag{4.25}$$

where a substitution from equation (3.2) into equation (4.24) and a change of variable to $x = (\varepsilon/\Delta(0))$ have been made. Since $e^{-\beta\Delta(0)(1+x^2)^{1/2}}$ is extremely sharp and significantly different from zero only in the neighbourhood of $x=0$, it will therefore introduce no detectable error if $(1+x^2)$ in the first integrand and $\frac{(1+x^2)}{a^2+(\Delta(0)x-b)^2}$ in the second integrand in the last equation are expanded as a Taylor series about $x = 0$ and take only the first term of the expansion to be significant because of the small range of interest. In addition because of the sharpness of $e^{-\beta\Delta(0)(1+x^2)^{1/2}}$, it is permissible to expand $(1+x^2)^{1/2}$ as a power series and take only the first two terms of the expansion to be sufficient. Having done that equation (4.25) can be written as

$$C_v(T\to 0) = \frac{4k_B}{\Omega}\,\beta^2\Delta^3(0)N(0)e^{-\Delta(0)/kT}\{\int_0^\infty e^{-\frac{\beta\Delta(0)}{2}x^2}\,dx + \frac{g}{\pi a}\,\frac{a^2}{(a^2+b^2)}\int_0^\infty e^{-\frac{\beta\Delta(0)}{2}x^2}\,dx\} \qquad (4.26)$$

Using $\int_0^\infty e^{-ax^2}dx = \frac{1}{2}\{\frac{\pi}{a}\}^{1/2}$, equation (4.26) becomes

$$C_s(T\to 0) = \frac{2\Delta(0)k_B}{\Omega}\{\frac{\Delta(0)}{k_BT}\}^{3/2}\sqrt{2\pi}\,N(0)(1+D)e^{-\Delta(0)/k_BT} \qquad (4.27)$$

This is the final approximate expression for the electronic specific heat in the low-temperature limit. Strictly speaking this expression is valid only at temperatures below about $T_c/10$. We note that it is the electronic density of states $N(0)(1+D)$ right at the Fermi energy that enters the expression. As in the BCS theory it can be seen from equation (4.27) $C_s(T\to 0)$ is proportional to $e^{-\Delta(0)/k_BT}$.

CHAPTER V

CONCLUSION

A modified BCS gap equation has been solved both analytically and numerically taking into account the sharp variation in the electronic density of states close to which the Fermi level is situated. This rapid variation has been represented approximately by a Lorentzian peak of width a and strength g superimposed on a constant background. An approximate analytic solution has been found for the critical temperature and the gap parameter at absolute zero. The analytic expressions obtained for both are valid for a and b $>> k_BT_c$ and $\omega_D >> \Delta(0)$. The solutions we have obtained for T_c and $\Delta(0)$ reflect the energy dependence of the electronic density of states through a pre exponential factor B in the equations for T_c and $\Delta(0)$. Basically this factor B is completely responsible for the small changes from an exponential of the behaviour of T_c and $\Delta(0)$ as a function of b. Further it was found that in the limit where a and b $>> k_BT_c$ and $\omega_D >> \Delta(0)$ the universal ratio $2\Delta(0)/k_BT_c$ remains unchanged and equal to the BCS value of 3.54.

For the purpose of studying the thermodynamic properties of A-15 compounds, the effect on the chemical potential due to raising the temperature above the absolute zero has been studied. It was found that the correction term is almost negligible compared to unity which generally allows the substitution b_0 for b to be made without introducing any measurable error. In addition we have obtained a simple analytic expression for the condensation energy ΔW valid for the case when the Fermi energy is situated right at the centre of the Lorentzian and for $a >> k_B T_c$.

We have applied the same model for the energy dependent electronic density of states in a solution of the finite-temperature BCS gap equation and have obtained an approximate analytic expression for the gap parameter as a function of temperature at temperatures just below the critical one. Based on this equation for $\Delta(T)$, we have obtained an analytic formula for the specific heat jump. Numerical calculation for the specific heat jump as a function of b reveals that at small values of a and b the numerical value for the jump deviates from the BCS value but at large values of b even when a is small it saturates and gives the BCS value of 1.426. Finally, in the low-temperature limit the specific heat is evaluated approximately and found to be proportional to $e^{-\Delta(0)/k_B T}$ as in the BCS theory.

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