Chapter 4

High-Temperatures isotope effect in the presence of a pseudogap

We wish to reexamine Eq.(3.31) from the framework of T. Dahm [Ref.38] to investigate E_g and T_c dependence of isotope exponent (α) , we rewrite Eq.(3.31)

$$L(\omega) = \frac{N(0)}{2\pi}\int_0^{2\pi} d\Theta\,\psi_\eta^2(\Theta)\int_0^{\omega} d\varepsilon\,\frac{\tanh(\sqrt{\varepsilon^2+(E_g(\Theta))^2}/2T_c)}{\sqrt{\varepsilon^2+(E_g(\Theta))^2}} \quad (4.1)$$

We will solve Eq.(4.1) exactly to find the expression of isotope exponent (α) in terms of pseudogap (E_g) and critical temperature (T_c) . In this work $E_g(\Theta)$ will be chosen to be either

$$\begin{aligned} E_g(\Theta) &= E_{go} = \text{constant} && \text{for an s - wave pseudogap} \\ E_g(\Theta) &= E_{go}\cos 2\Theta && \text{for a } d_{x^2-y^2} \text{ - wave pseudogap} \\ E_g(\Theta) &= E_{go}\sin 2\Theta && \text{for a } d_{xy} \text{ - wave pseudogap} \end{aligned} \quad (4.2)$$

And $\psi_\eta(\Theta)$ is the basis function for the pairing symmetry considered by

$$\begin{aligned} \psi_s(\Theta) &= 1 && \text{for s - wave pairing} \\ \psi_{d_{x^2-y^2}}(\Theta) &= \cos 2\Theta && \text{for } d_{x^2-y^2} \text{ - wave pairing} \\ \psi_{d_{xy}}(\Theta) &= \sin 2\Theta && \text{for } d_{xy} \text{ - wave pairing} \end{aligned} \quad (4.3)$$

For s-wave type we write Eq.(4.1) in the form

$$L_s(\omega) = \frac{N(0)}{2\pi}\int_0^{2\pi} d\Theta\int_0^{\omega} d\varepsilon\,\frac{\tanh(\sqrt{\varepsilon^2+E_{go}^2}/2T_c)}{\sqrt{\varepsilon^2+E_{go}^2}} \quad (4.4)$$

By using expansion of tanh(x) in series of simple fraction [81]

$$\tanh\left(\frac{\pi x}{2}\right) = \frac{4x}{\pi}\sum_{k=0}^{\infty}\frac{1}{(2k-1)^2+x^2} \quad (4.5)$$

Substituted Eq.(4.5) back into Eq.(4.4) , the integral can be performed directly and we obtain the following result

$$L_s(\omega) = 4N(0)T\sum_{n=0}^{\infty}\frac{\tan^{-1}\left(\omega/\sqrt{E_{go}^2+(\pi T(2n+1))^2}\right)}{\sqrt{E_{go}^2+(\pi T(2n+1))^2}} \quad (4.6)$$

From the previous chapter, the isotope exponent (α) is defined by:

$$\alpha = \frac{1}{2}\frac{d\ln T_c}{d\ln\omega_p} = -\frac{1}{2}\frac{\frac{\partial\lambda}{\partial L_p}\frac{\partial L_p}{\partial\omega_p}}{\frac{\partial\lambda}{\partial L_p}\frac{\partial L_p}{\partial T_c}+\frac{\partial\lambda}{\partial L_e}\frac{\partial L_e}{\partial T_c}} \quad (4.7)$$

λ is the eigenvalue according to Eq.(3.26) that given by:

$$\lambda(\omega_e,\omega_p,T) = \frac{V_{eo}L_e+V_{po}L_p}{2}+\frac{1}{2}\sqrt{(V_{eo}L_e-V_{po}L_p)^2+4V_{eo}V_{po}(L_e)^2} \quad (4.8)$$

$$\frac{\partial\lambda}{\partial L_p} = \frac{V_{po}}{2}-\frac{1}{2}\left[(V_{eo}L_e-V_{po}L_p)^2+4V_{eo}V_{po}L_e^2\right]^{-1/2}(V_{eo}L_e-V_{po}L_p)V_{po} \quad (4.9)$$

$$\frac{\partial\lambda}{\partial L_e} = \frac{V_{eo}}{2}+\left[(V_{eo}L_e-V_{po}L_p)^2+4V_{eo}V_{po}L_e^2\right]^{-1/2}\left[\frac{1}{2}V_{eo}(V_{eo}L_e-V_{po}L_p)+4V_{eo}V_{po}L_e\right] \quad (4.10)$$

From $\lambda(\omega_e,\omega_p,T_c) = 1$ so at $T = T_c$ we write Eq.(4.8) in the form

$$1 = \frac{V_{eo}L_e+V_{po}L_p}{2}+\frac{1}{2}\sqrt{(V_{eo}L_e-V_{po}L_p)^2+4V_{eo}V_{po}(L_e)^2}.$$

$$\left[(V_{eo}L_e-V_{po}L_p)^2+4V_{eo}V_{po}L_e^2\right]^{-1/2} = \frac{1}{2-V_{eo}L_e-V_{po}L_p}. \quad (4.11)$$

Substitute Eq.(4.11) back into Eq.(4.9) and Eq.(4.10) respectively, we obtain

$$\frac{\partial\lambda}{\partial L_p} = \frac{V_{po}-V_{po}V_{eo}L_e}{2-V_{eo}L_e-V_{po}L_p}. \quad (4.12)$$

$$\frac{\partial\lambda}{\partial L_e} = \frac{V_{po}-V_{po}V_{eo}L_p+2V_{po}V_{eo}L_e}{2-V_{eo}L_e-V_{po}L_p}. \quad (4.13)$$

Substitute Eq.(4.12) and (4.13) back into Eq.(4.7), so we get

$$\alpha = -\frac{1}{2}\frac{\omega_p}{T_c}\frac{V_{po}(1-V_{eo}L_e)\frac{\partial L_p}{\partial \omega_p}}{V_{po}(1-V_{eo}L_e)\frac{\partial L_p}{\partial T_c}+V_{eo}(1-V_{po}L_e-2V_{po}L_e)\frac{\partial L_e}{\partial T_c}}. \quad (4.14)$$

We re-consider Eq.(4.7) again

$$\alpha = \frac{1}{2}\frac{d\ln T_c}{d\ln \omega_p} = \frac{1}{2}\frac{\omega_p}{T_c}\frac{dT_c}{d\omega_p}.$$

$$\frac{dT_c}{d\omega_p} = \frac{2T_c\alpha}{\omega_p}. \quad (4.15)$$

Next, let us consider function L for s-wave pairing and s-wave pseudogap that already defined by Eq.(4.4)

$$L_s(\omega_p) = \frac{N(0)}{2\pi}\int_0^{2\pi} d\Theta \int_0^{\omega_p} d\varepsilon \frac{\tanh(\sqrt{\varepsilon^2+E_{go}{}^2}/2T_c)}{\sqrt{\varepsilon^2+E_{go}{}^2}}.$$

$$L_p = N(0)\int_0^{\omega_p} d\varepsilon \frac{\tanh(\sqrt{\varepsilon^2+E_{go}{}^2}/2T_c)}{\sqrt{\varepsilon^2+E_{go}{}^2}}. \quad (4.16)$$

where $L_s(\omega_p)$ denoted by L_p.

By using the formula [81]

$$\frac{d}{da}\int_{\psi(a)}^{\varphi(a)} f(x,a)dx = f(\varphi(a),a)\frac{d\varphi(a)}{da} - f(\psi(a),a)\frac{d\psi(a)}{da} + \int_{\psi(a)}^{\varphi(a)}\frac{d}{da}f(x,a)dx. \quad (4.17)$$

we then find

$$\frac{\partial L_p}{\partial \omega_p} = N(0)\frac{\tanh(\sqrt{\omega_p{}^2+E_{go}{}^2}/2T_c)}{\sqrt{\omega_p{}^2+E_{go}{}^2}} - N(0)\frac{\alpha}{\omega_p T_c}I_p. \quad (4.18)$$

$$\frac{\partial L_p}{\partial T_c} = N(0)\frac{\omega_p}{2T_c\alpha}\frac{\tanh(\sqrt{\omega_p{}^2+E_{go}{}^2}/2T_c)}{\sqrt{\omega_p{}^2+E_{go}{}^2}} - N(0)\frac{1}{2T_c^2}I_p. \quad (4.19)$$

$$\frac{\partial L_e}{\partial T_c} = -N(0)\frac{I_e}{2T_c^2}. \quad (4.20)$$

where $$I_{e,p} = \int_0^{\omega_{e,p}} \mathrm{sech}^2(\sqrt{\varepsilon^2 + E_{go}{}^2}/2T_c)d\varepsilon \qquad (4.21)$$

By using the relation

$$\tanh\frac{\pi x}{2} = \frac{4x}{\pi}\sum_{k=1}^{\infty}\frac{1}{(2k-1)^2 + x^2}$$

$$\tanh x = 8x\sum_{k=1}^{\infty}\frac{1}{(2k-1)^2\pi^2 + 4x^2} \qquad (4.23)$$

We differentiate Eq.(4.23) on the both sides

$$\mathrm{sech}^2 x = 8\sum_{k=1}^{\infty}\frac{1}{(2k-1)^2\pi^2 + 4x^2} - 64\sum_{k=1}^{\infty}\frac{x^2}{\left((2k-1)^2\pi^2 + 4x^2\right)^2} \qquad (4.24)$$

Substitute Eq.(4.24) back into Eq.(4.21) and then perform integration so we obtain

$$I_{e,p} = \sum_{k=0}^{\infty}\left(\frac{8\omega_{e,p}(2k+1)^2\pi^2}{\left((2k+1)^2\pi^2 + (E_{go}/T_c)^2\right)\left((2k+1)^2\pi^2 + (E_{go}/T_c)^2 + (\omega_{e,p}/T_c)^2\right)} - 8T_c(E_{go}/T_c)^2\frac{\tan^{-1}\left(\omega_{e,p}/\sqrt{((2k+1)\pi T_c)^2 + E_{go}^2}\right)}{\left((2k+1)^2\pi^2 + (E_{go}/T_c)^2\right)^{3/2}}\right) \qquad (4.25)$$

Now, we substitute Eq.(4.18) – (4.20) back into Eq.(4.14) and rearrange into the form

$$\alpha = \frac{2\omega_p T_c V_{po}(1 - V_{eo}L_e)\dfrac{\tanh\left(\sqrt{\omega_p^2 + E_{go}^2}/2T_c\right)}{\sqrt{\omega_p^2 + E_{go}^2}}}{2V_{po}(1 - V_{eo}L_e)I_p + V_{eo}(1 - V_{po}L_e - 2V_{po}L_e)I_e} \qquad (4.26)$$

where $$L_{e,p} = N(0)\int_0^{\omega_{e,p}} d\varepsilon\,\frac{\tanh(\sqrt{\varepsilon^2 + E_{go}{}^2}/2T_c)}{\sqrt{\varepsilon^2 + E_{go}{}^2}}$$

$$L_{e,p} = 4N(0)T_c\sum_{n=0}^{\infty}\frac{\tan^{-1}\left(\omega_{e,p}/\sqrt{E_{go}^2 + (\pi T_c(2n+1))^2}\right)}{\sqrt{E_{go}^2 + (\pi T_c(2n+1))^2}} \qquad (4.27)$$

We rearrange Eqs.(4.26) – (4.27) and rewrite them in terms of N_oV_{eo} , N_oV_{po} , ω_e/T_c , ω_p/T_c , and E_{go}/T_c , now we obtain the exact expression for α :

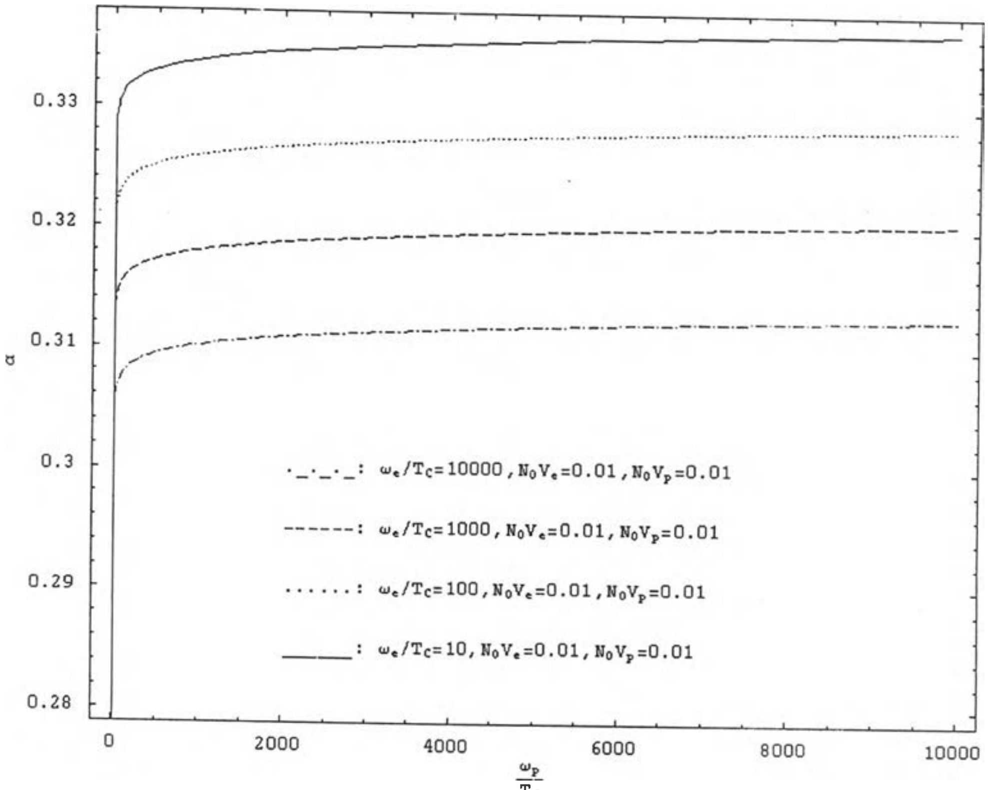
$$\alpha = \frac{2(\omega_p/T_c)(1 - N_oV_{eo}L_e)\tanh\left(\sqrt{(\omega_p/T_c)^2 + (E_{go}/T_c)^2}/2\right)}{\sqrt{(\omega_p/T_c)^2 + (E_{go}/T_c)^2}\left(2(1 - N_oV_{eo}L_e)I_p + \frac{V_{eo}}{V_{po}}(1 - N_oV_{po}L_e - 2N_oV_{po}L_e)I_e\right)} \qquad (4.28)$$

where

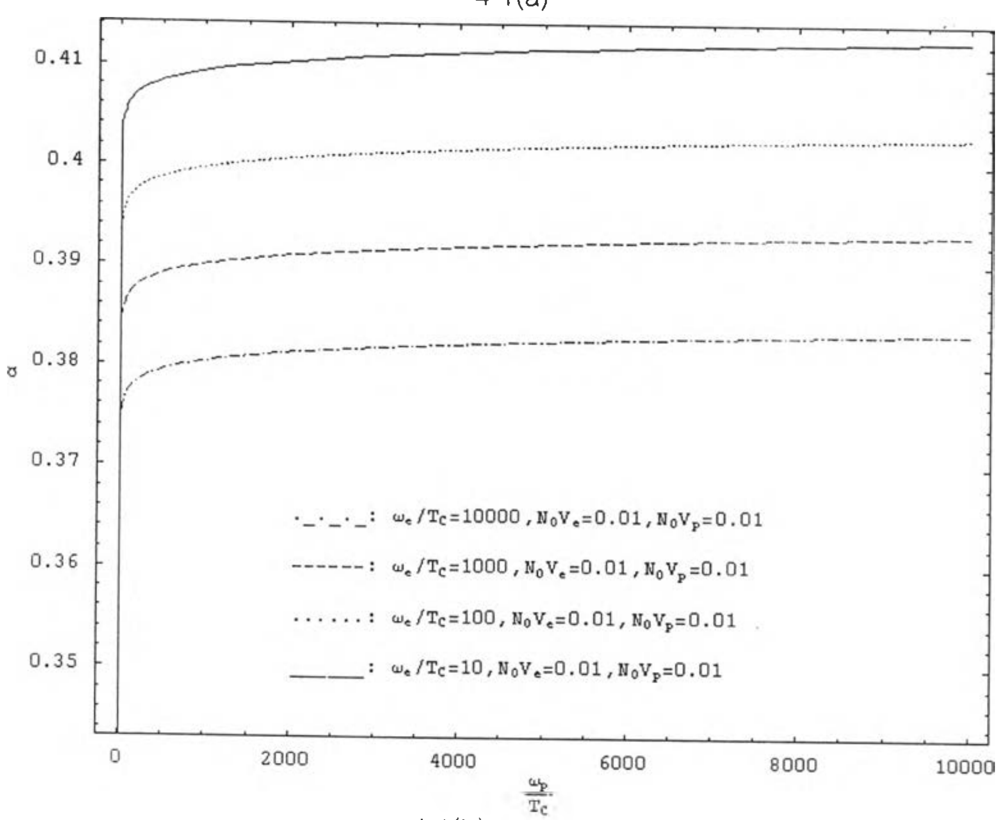
$$L_{e,p} = 4\sum_{n=0}^{\infty} \frac{\tan^{-1}\left((\omega_{e,p}/T_c)^2 / \sqrt{(E_{go}/T_c)^2 + (\pi(2n+1))^2}\right)}{\sqrt{(E_{go}/T_c)^2 + (\pi(2n+1))^2}} \qquad (4.29)$$

$$I_{e,p} = \sum_{k=0}^{\infty}\left(\frac{8(\omega_{e,p}/T_c)(2k+1)^2\pi^2}{\left((2k+1)^2\pi^2 + (E_{go}/T_c)^2\right)\left((2k+1)^2\pi^2 + (E_{go}/T_c)^2 + (\omega_{e,p}/T_c)^2\right)} - 8(E_{go}/T_c)^2 \frac{\tan^{-1}\left((\omega_{e,p}/T_c)/\sqrt{(2k+1)^2\pi^2 + (E_{go}/T_c)^2}\right)}{\left((2k+1)^2\pi^2 + (E_{go}/T_c)^2\right)^{3/2}} \right) \qquad (4.30)$$

By using these exact expressions for finding the isotope exponent (α) , we obtain α which depends on the values of N_oV_{eo} , N_oV_{po} , ω_e/T_c , ω_p/T_c , and E_{go}/T_c . First we wish to study the effect of the pseudogap (E_{go}/T_c) on the value of α , the results are shown in Figure 4-1(a) and Figure 4-1(b) for E_{go}/T_c=0.1 and 1, respectively.



4-1(a)



4-1(b)

Figure4-1:shows the value of α in the presence of the pseudogap for E_{go}/T_c=0.1 (a) and E_{go}/T_c=1 (b) with respect to ω_p/T_c.

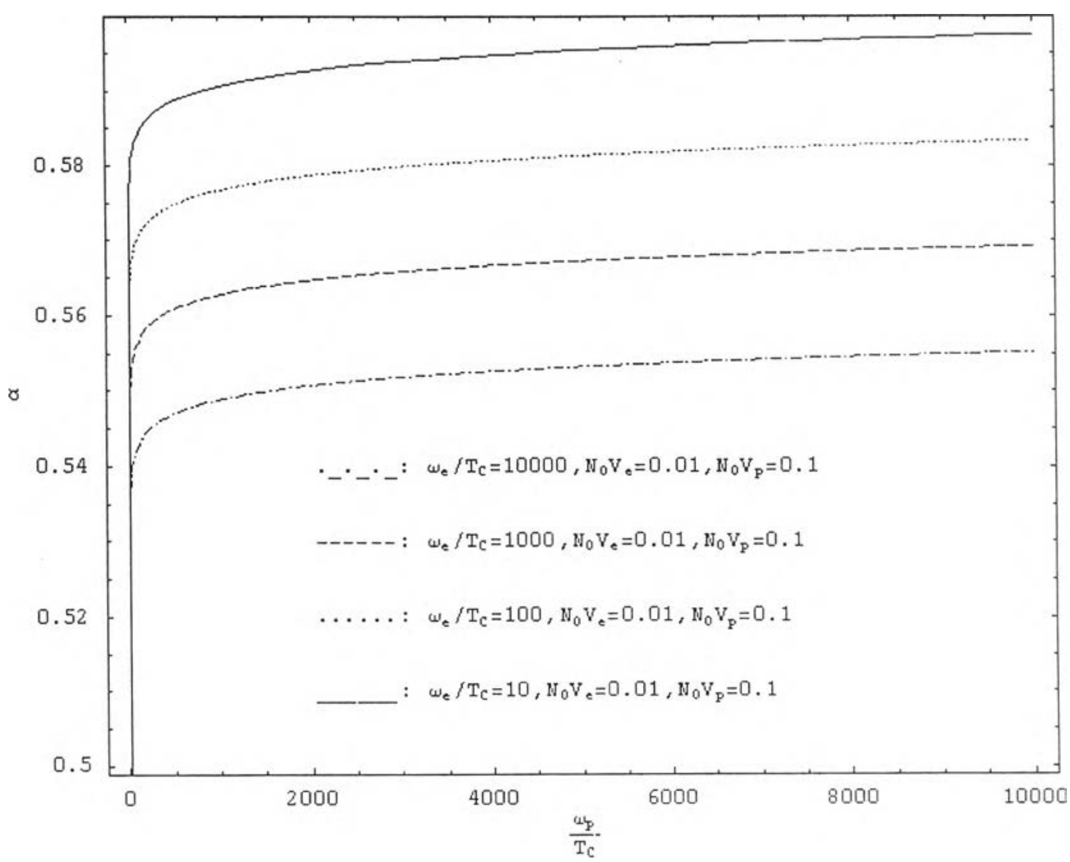
Results and Discussions for Figure 4-1(a) and 4-1 (b) (s-wave superconductors, simple metals and transition elements).

From both graphs we can see that the size of a pseudogap does not violate the BCS α (0.5). This is due to the fact that the pseudogap does not exists in the normal state of an s wave superconductor. From this result we can take the limit E_{go} approaches zero and consider for the following cases:

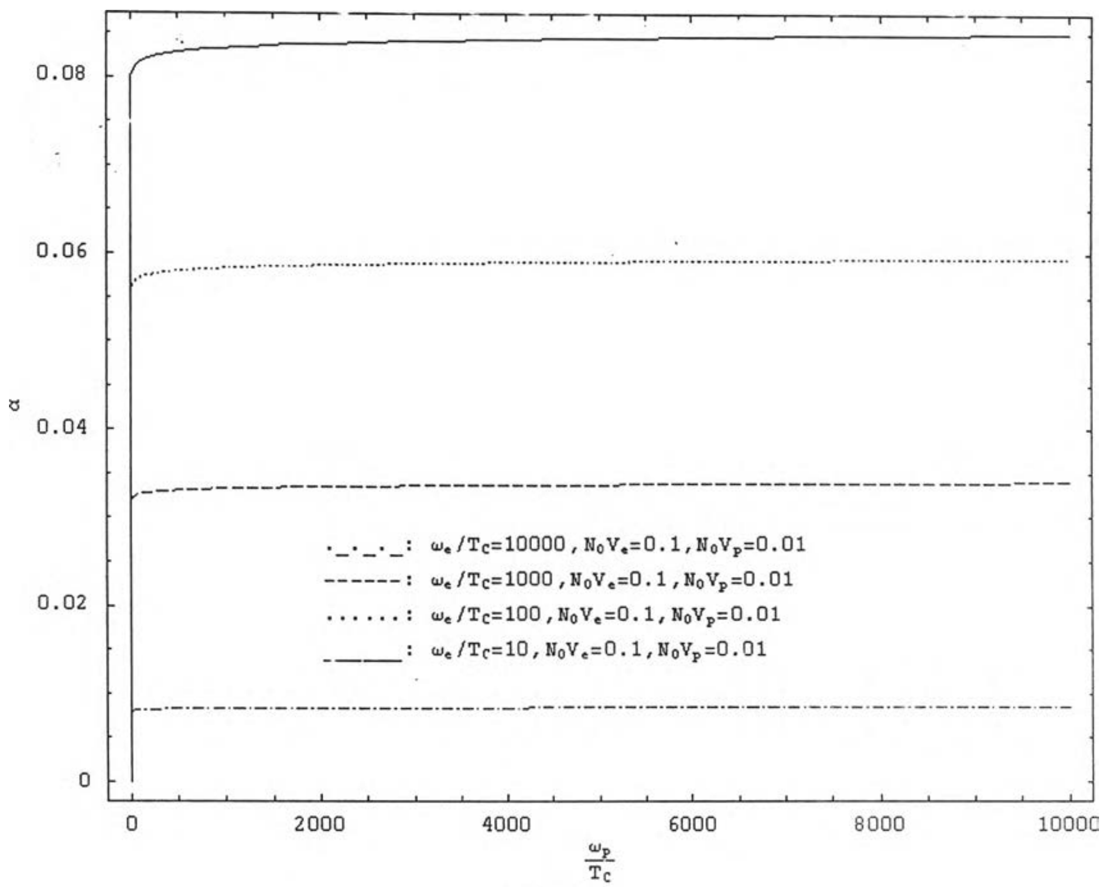
1) If $V_{eo} = 0$ we obtain $\alpha = 0.5 = \alpha_{BCS}$ as expected.

2) If $V_{po} = 0$ we obtain $\alpha = 0$ so T_c does not depend on the isotope mass anymore which is in contradiction to the experimental facts. We therefore conclude that an electron-phonon interaction is responsible for superconductivity in s-wave superconductors.

Next we wish to study the effect of the pairing interaction strength on the isotope exponent. This will be considered in two cases for (1) a dominant phononic part (N_oV_p) and (2) a dominant electronic part (N_oV_e) as shown in Figures 4-2(a) and 4-2(b), respectively.



4-2(a)



4-2(b)

Figure4-2: Value of α with respect to ω_p/T_c in the presence of a pseudogap (E_{go}/T_c=1) for the dominant phononic case (a) ,and for the dominant electronic case (b).

Results and Discussions for Figure 4-2(a) and 4-2 (b) (s-wave superconductors, simple metals and transition elements).

1) For a dominant phononic part (Figure 4-2(a)), α approaches α_{BCS} = 0.5 as we expect for a simple metal.
2) For a dominant electronic part (Figure 4-2(b)), α approaches zero as we expect for a transition element.

In the following section we will study the influence of a pseudogap on the isotope effect of the $d_{x^2-y^2}$ -wave type, we write Eq.(4.1) in the form

$$L_{d_{x^2-y^2}}(\omega) = \frac{N(0)}{2\pi}\int_0^{2\pi} d\Theta \cos^2 2\Theta \int_0^{\omega} d\varepsilon \frac{\tanh(\sqrt{\varepsilon^2 + E_{go}^2\cos^2 2\Theta}/2T_c)}{\sqrt{\varepsilon^2 + E_{go}^2\cos^2 2\Theta}} \quad (4.31)$$

By using the expression for tanh(x) in Eq.(4.5) and performing the angular integration , we obtain

$$L_{d_{x^2-y^2}}(\omega_{e,p}) = 4N(0)T_c \sum_{n=0}^{\infty}$$

$$\int_0^{\omega_{e,p}} d\varepsilon \frac{1}{\varepsilon^2 + E_{go}^2 + (\pi T_c(2n+1))^2 + \sqrt{\varepsilon^2 + E_{go}^2 + (\pi T_c(2n+1))^2}\sqrt{\varepsilon^2 + (\pi T_c(2n+1))^2}} \quad (4.32)$$

By substituting Eq.(4.32) back into Eq.(4.14) and doing the exact calculation ,after arrangement we finally find the isotope exponent expression for $d_{x^2-y^2}$ -wave type in terms of N_oV_{eo} , N_oV_{po} , ω_e/T_c , ω_p/T_c , and E_{go}/T_c in the following form :

$$\alpha = \frac{\left(\frac{\omega_p}{T_c}\right)(1 - 4N(0)V_{eo}l_e)a_p}{(1 - 4N(0)V_{eo}l_e)(-2l_e - 2b_p + 2e_p + 2d_p) + \frac{V_{eo}}{V_{po}}(1 - 4N(0)V_{po}l_p + 8N(0)V_{po}l_e)(l_e + b_e - e_e - d_e)} \quad (4.33)$$

where

$$a_p = \sum_{n=0}^{\infty} \frac{1}{(\omega_p/T_c)^2 + (E_{go}/T_c)^2 + (\pi(2n+1))^2 + \sqrt{(\omega_p/T_c)^2 + (E_{go}/T_c)^2 + (\pi(2n+1))^2}\sqrt{(\omega_p/T_c)^2 + (\pi(2n+1))^2}} \quad (4.34)$$

$$b_{e,p} = \sum_{n=0}^{\infty} \frac{(\pi(2n+1))^2 E\left(\arctan((\omega_{e,p}/T_c)/\pi(2n+1)), (E_{go}/T_c)/\sqrt{(E_{go}/T_c)^2 + (\pi(2n+1))^2}\right)}{(E_{go}/T_c)^2\sqrt{(E_{go}/T_c)^2 + (\pi(2n+1))^2}} \quad (4.35)$$

$$e_{e,p} = \sum_{n=0}^{\infty} \frac{(\omega_{e,p}/T_c)(\pi(2n+1))^2}{((E_{go}/T_c)^2 + (\pi(2n+1))^2)\sqrt{(\omega_{e,p}/T_c)^2 + (E_{go}/T_c)^2 + (\pi(2n+1))^2}\sqrt{(\omega_{e,p}/T_c)^2 + (\pi(2n+1))^2}} \quad (4.36)$$

$$d_{e,p} = \sum_{n=0}^{\infty} \frac{(\pi(2n+1))^2 F\left(\arctan((\omega_{e,p}/T_c)/\pi(2n+1)), (E_{go}/T_c)/\sqrt{(E_{go}/T_c)^2 + (\pi(2n+1))^2}\right)}{(E_{go}/T_c)^2\sqrt{(E_{go}/T_c)^2 + (\pi(2n+1))^2}} \quad (4.37)$$

and

$$l_{e,p} = \frac{1}{(E_{go}/T_c)^2}\sum_{n=0}^{\infty}\left((\omega_{e,p}/T_c)\left(1-\sqrt{1+\frac{(E_{go}/T_c)^2}{(\omega_{e,p}/T_c)^2+(\pi(2n+1))^2}}\right)\right) \tag{4.38}$$

$$-\frac{(\pi(2n+1))^2}{\sqrt{(E_{go}/T_c)^2+(\pi(2n+1))^2}}F\left(\arctan((\omega_{e,p}/T_c)/\pi(2n+1)),(E_{go}/T_c)/\sqrt{(E_{go}/T_c)^2+(\pi(2n+1))^2}\right)$$

$$+\sqrt{(E_{go}/T_c)^2+(\pi(2n+1))^2}\,E\left(\arctan((\omega_{e,p}/T_c)/\pi(2n+1)),(E_{go}/T_c)/\sqrt{(E_{go}/T_c)^2+(\pi(2n+1))^2}\right)$$

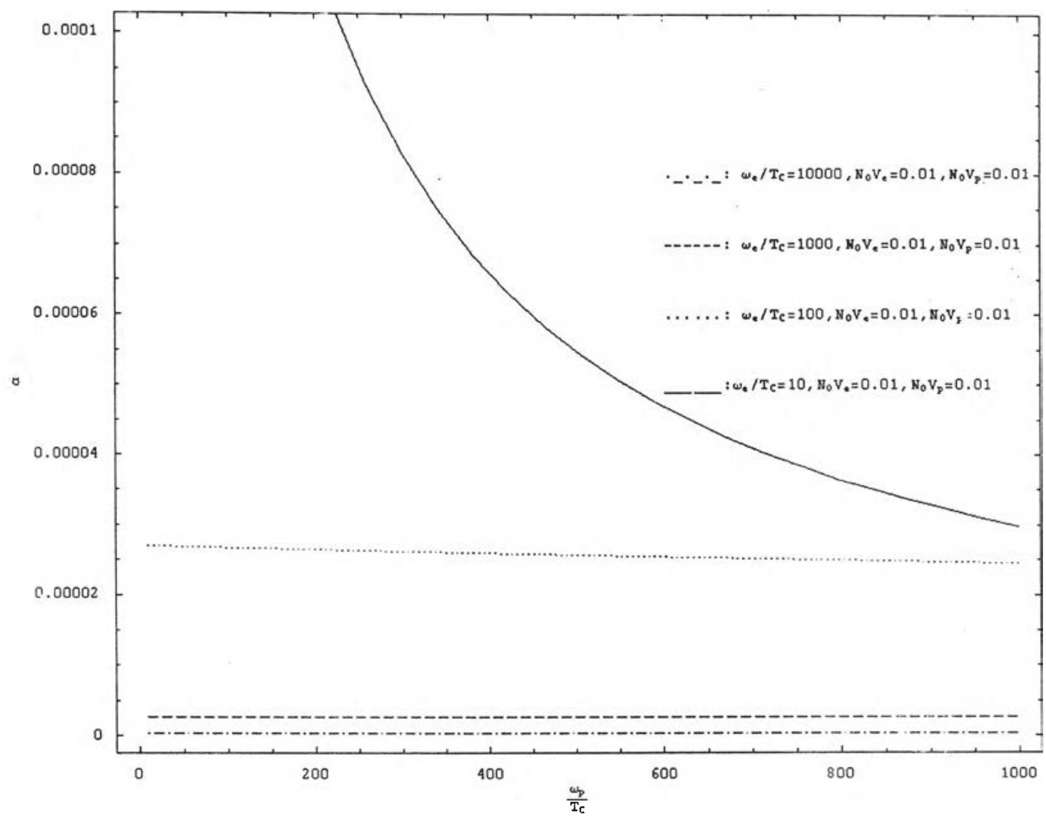
where $F(\varphi,k)$ is the elliptic integral of the first kind as defined by

$$F(\varphi,k) = \int_0^{\varphi}\frac{d\alpha}{\sqrt{1-k^2\sin^2\alpha}}. \tag{4.39}$$

and $E(\varphi,k)$ is the elliptic integral of the second kind as defined by

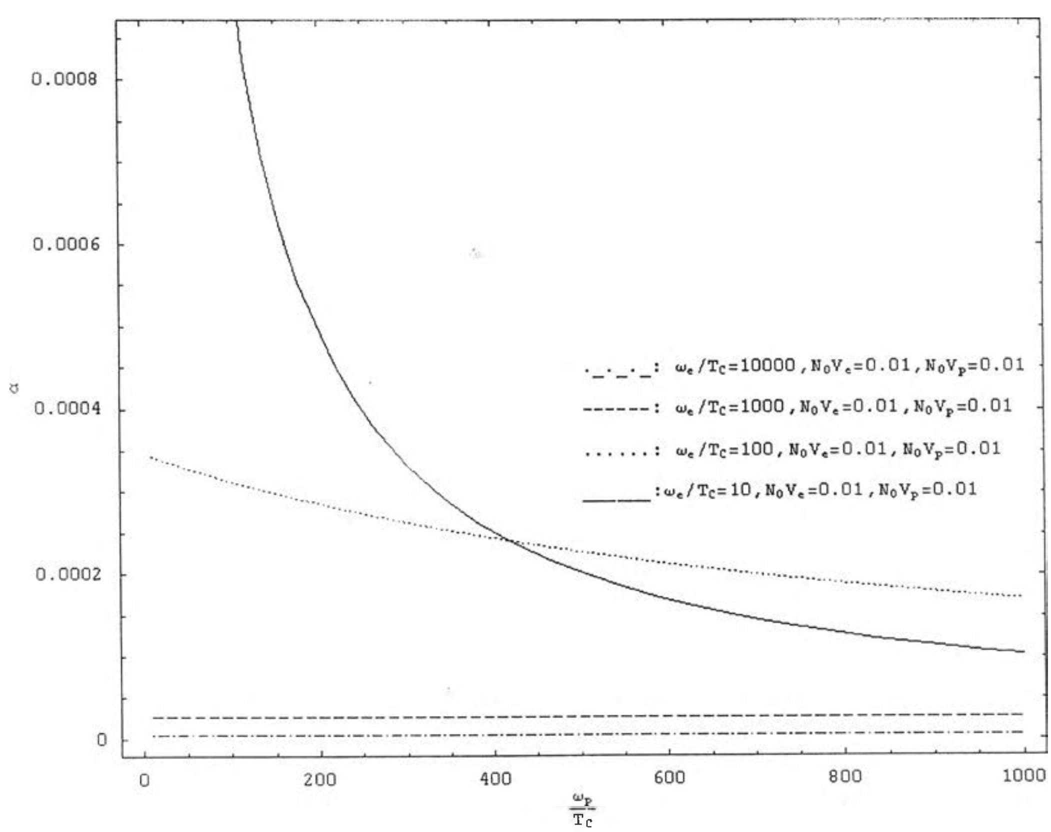
$$E(\varphi,k) = \int_0^{\varphi}\sqrt{1-k^2\sin^2\alpha}\,d\alpha. \tag{4.40}$$

By using these exact expressions (Eqs.(3.33) - (3.38)) for finding the isotope exponent (α) of a $d_{x^2-y^2}$ – wave superconductor , we obtain an expression for α which depends on the values of N_oV_{eo} , N_oV_{po} , ω_e/T_c , ω_p/T_c , and E_{go}/T_c . First we wish to study an effect of the pseudogap (E_{go}/T_c) on α, the results are shown in Figures 4-3(a) –(c).



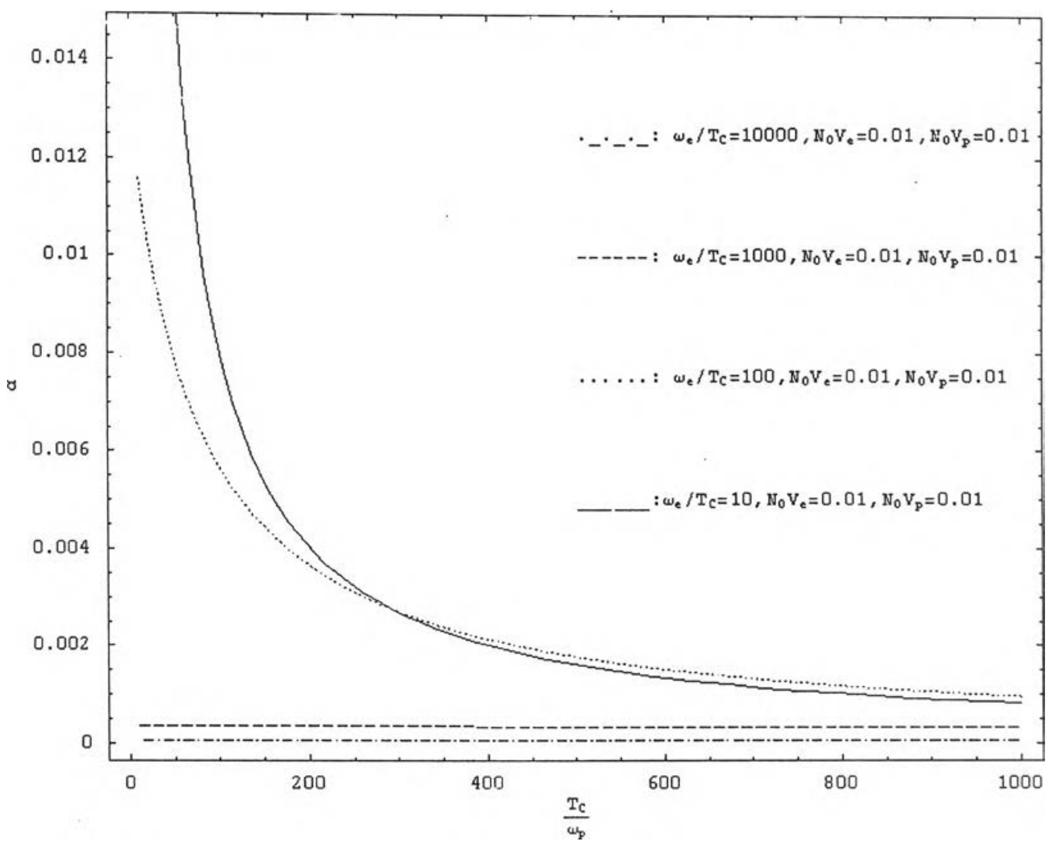
0.0001
0.00008
0.00006
0.00004
0.00002
0
α
0
200
400
600
800
1000
$\frac{\omega_p}{T_c}$
._._._: ω_e/T_C=10000, N_0V_e=0.01, N_0V_p=0.01
------: ω_e/T_C=1000, N_0V_e=0.01, N_0V_p=0.01
......: ω_e/T_C=100, N_0V_e=0.01, N_0V_p=0.01
______: ω_e/T_C=10, N_0V_e=0.01, N_0V_p=0.01

4-3(a)



0.0008
0.0006
0.0004
0.0002
0
α
0
200
400
600
800
1000
$\frac{\omega_p}{T_c}$
._._._: ω_e/T_C=10000, N_0V_e=0.01, N_0V_p=0.01
------: ω_e/T_C=1000, N_0V_e=0.01, N_0V_p=0.01
......: ω_e/T_C=100, N_0V_e=0.01, N_0V_p=0.01
______: ω_e/T_C=10, N_0V_e=0.01, N_0V_p=0.01

4-3(b)



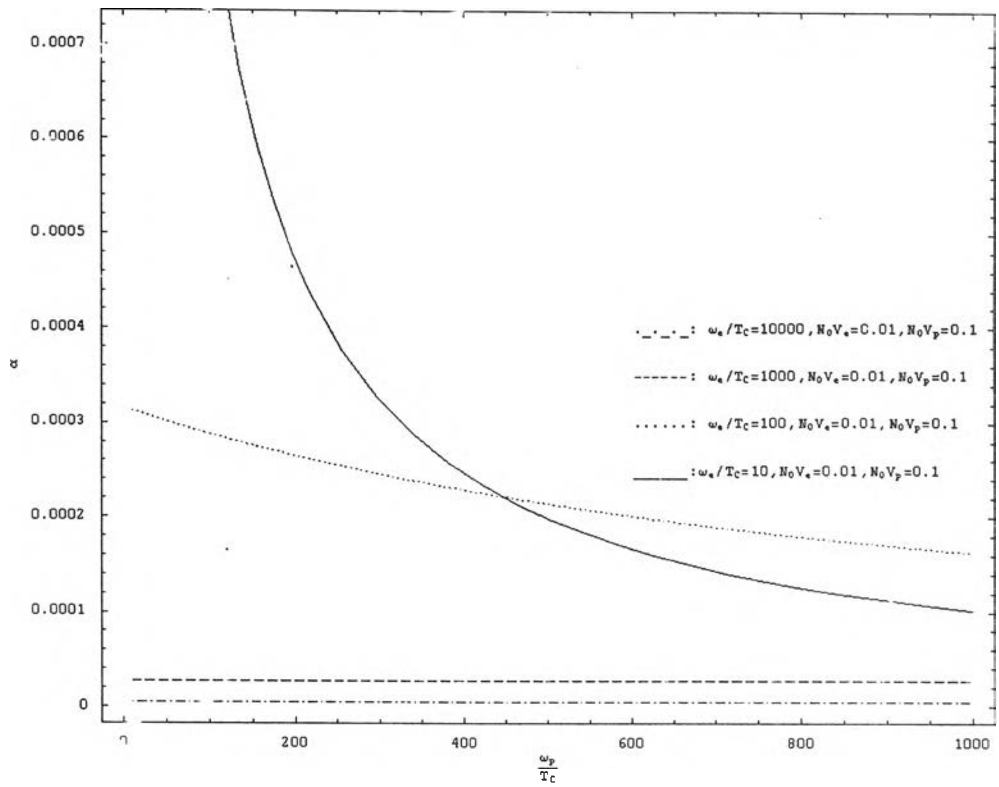
4-3(c)

Figures 4-3 (a)-(c): Value of α with respect to ω_p/T_c for $d_{x^2-y^2}$ -wave superconductor in the presence of a pseudogap for E_{go}/T_c=0.01 (a) , E_{go}/T_c=0.1 (b) and E_{go}/T_c=1 (c) .

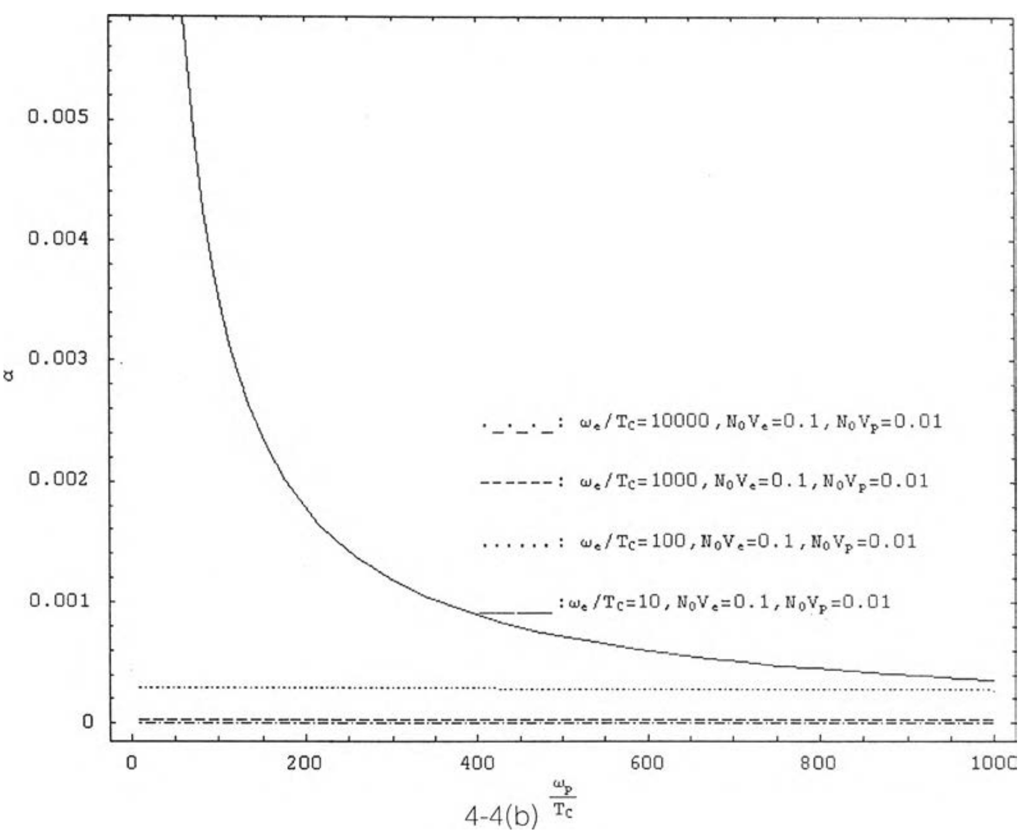
Results and Discussions for Figure 4-3(a)-4-3(c) (d-wave superconductor ,high T_c superconductors).

From the above graphs, we find that the α value depends on the size of the pseudogap so we can conclude that the pseudogap is generally strongly increases the α value corresponds to the experimental facts.

Next we wish to study the effect of the pairing interaction strength on the isotope exponent which we classify into two cases, (1) for a dominant phononic part (N_oV_p) and (2) a dominant electronic part (N_oV_p) as shown in Figures 4-4(a) and 4-4(b), respectively.



4-4(a)



4-4(b)

Figured4-4(a) - 4-4(b) : Value of α with respect to ω_p/T_c for a $d_{x^2-y^2}$ -wave type in the presence of the pseudogap (E_{go}/T_c=0.1) for dominant phononic part (a) and for the dominant electronic part (b) .

Results and Discussions for Figure 4-4(a) and 4-4 (b) (d-wave superconductors, high T_c superconductors).

For optimal doping (small pseudogap) maximum in T_c is obtained which give α value tends to zero as we expect and α value at optimal doping may not involves to the strength of the coupling interaction.