APPENDIX I

(A) Second and third order corrections to energy: alternate derivation of Halemane's result.

The corrections to the ground state energy as given by equation (12), chapter 2 are

$$S_p(E_o) = \frac{1}{p!}\frac{\partial^p E_\alpha}{(\partial\alpha)^p}\Big|_{\alpha=0}$$

For convenience, we introduce α-dependent terms $S_1(E_\alpha)$, $S_2(E_\alpha)$ $S_3(E_\alpha)$ etc, so that the coefficients of pertubation series can be obtained as :

$$S_i(E_o) = \lim_{\alpha \to 0} S_i(E_\alpha).$$

In that case, we can also write

$$S_2(E_\alpha) = \frac{1}{2}\frac{\partial}{\partial\alpha} S_1(E_\alpha), \quad S_3(E_\alpha) = \frac{1}{3}\frac{\partial}{\partial\alpha} S_2(E_\alpha)$$

and so on.

We already have an expression for $S_1(E_\alpha)$ from eqn.5, chapter 2):

$$S_1(E_\alpha) = \frac{\partial E_\alpha}{\partial\alpha} = \frac{-1}{\rho_\alpha(E_\alpha)} \int_{-\infty}^{E_\alpha} \frac{\partial\rho_\alpha(x)}{\partial\alpha}\, dx \qquad (1)$$

$$\text{or } - S_1(E_\alpha)\,\rho_\alpha(E_\alpha) = \int_{-\infty}^{E_\alpha} \frac{\partial\rho_\alpha(x)}{\partial\alpha}\, dx . \qquad (2)$$

Differentiating (2) with respect to α yields

$$-\rho_\alpha(E_\alpha)\frac{\partial}{\partial\alpha} S_1(E_\alpha) - S_1(E_\alpha)\frac{\partial}{d\alpha}\rho_\alpha(E_\alpha)$$

$$= \frac{\partial E_\alpha}{\partial\alpha}\, \frac{\partial\rho_\alpha(x)}{\partial\alpha}\Big|_{x=E_\alpha} + \int_{-\infty}^{E_\alpha} \frac{\partial^2\rho_\alpha(x)}{\partial\alpha^2}\, dx. \qquad (3)$$

Certain terms can be further simplified ;

$$\frac{\partial \rho_\alpha(E_\alpha)}{\partial \alpha} = \frac{\partial}{\partial \alpha}\left[\rho_\alpha(E_0) + (E_\alpha - E_0)\frac{\partial \rho_\alpha}{\partial x}(x)\Big|_{x=E_0} + \frac{(E_\alpha-E_0)^2}{2}\frac{\partial^2 \rho_\alpha(x)}{\partial x^2}\Big|_{x=E_0} + \cdots\right]$$

$$= \frac{\partial \rho_\alpha(E_0)}{\partial \alpha} + \frac{\partial E_\alpha}{\partial \alpha}\frac{\partial \rho_\alpha(x)}{\partial x}\Big|_{x=E_0} + (E_\alpha - E_0)\frac{\partial^2 \rho_\alpha(x)}{\partial \alpha \partial x}\Big|_{x=E_0} + \ldots \quad (4)$$

from equation (2), we have

$$-\frac{\partial}{\partial E_0}(S_1(E_\alpha)\,\rho_\alpha(E_\alpha)) = \frac{\partial \rho_\alpha(x)}{\partial \alpha}\Big|_{x=E_\alpha} \quad (5)$$

Substituting equations (4) and (5) in equation (3) yields

$$-2S_2(E_\alpha)\,\rho_\alpha(E_\alpha) = S_1(E_\alpha)\left\{\frac{-\partial}{\partial E_0}(S_1(E_\alpha)\,\rho_\alpha(E_\alpha))\right\} + S_1^2(E_\alpha)\frac{\partial \rho_\alpha(E_\alpha)}{\partial E_0}$$

$$- S_1(E_\alpha)\frac{\partial}{\partial E_0}(S_1(E_\alpha)\,\rho_\alpha(E_\alpha)) + \int_{-\infty}^{E_\alpha}\frac{\partial^2 \rho_\alpha(x)}{(\partial \alpha)^2}\,dx$$

Adjusting all terms yields

$$-2S_2(E_\alpha)\,\rho_\alpha(E_\alpha) = \int_{-\infty}^{E_\alpha}\frac{\partial^2 \rho_\alpha(x)}{\partial \alpha^2}\,dx \quad \frac{-\partial}{\partial E_0}(S_1^2(E_\alpha)\,\rho_\alpha(E_\alpha)) \quad (6)$$

Taking limit $\alpha \to 0$, one has for the first inverse energy weighted sum

$$S_2(E_0) = -\frac{1}{2\rho_0(E_0)}\left[\int_{-\infty}^{E_0}\frac{\partial^2}{\partial \alpha^2}\rho_\alpha(x)\,dx\Big|_{\alpha=0} - \frac{\partial}{\partial E_0}(S_1^2(E_0)\,\rho_0(E_0))\right] \quad (7)$$

For obtaining the third order correction term, we simply differentiate eqn.(6) once again with respect to α, so that

$$- 2\, S_2(E_\alpha)\left(\frac{\partial \rho_\alpha}{\partial\alpha}(E_\alpha)\right) - 2\, \rho_\alpha(E_\alpha)\left(\frac{\partial}{\partial\alpha} S_2(E_\alpha)\right)$$

$$= \left(\frac{\partial}{\partial\alpha} E_\alpha\right)\frac{\partial^2 \rho_\alpha(x)}{\partial\alpha^2}\Big|_{x=E_\alpha} + \int_{-\infty}^{E_\alpha} \frac{\partial^3 \rho_\alpha(x)\,dx}{\partial\alpha^3} - \frac{\partial}{\partial E_0}\left\{\frac{\partial}{\partial\alpha}(S_1^2(E_\alpha)\ \rho_\alpha(E_\alpha))\right\}$$

$$\therefore - 6S_3(E_\alpha)\rho_\alpha(E_\alpha) = 2S_2(E_\alpha)\left\{\frac{\partial}{\partial\alpha}\rho_\alpha(E_o) + S_1(E_\alpha)\frac{\partial\rho_\alpha(x)}{\partial x}\Big|_{x=E_0}\right\}$$

$$+ S_1(E_\alpha)\frac{\partial^2}{\partial\alpha^2}\rho_\alpha(x)\Big|_{x=E_\alpha} + \int_{-\infty}^{E_\alpha}\frac{\partial^3\rho_\alpha(x)dx}{\partial\alpha^3}$$

$$-\frac{\partial}{\partial E_0}\left\{2S_1(E_\alpha)\left[\frac{\partial}{\partial\alpha}S_1(E_\alpha)\right]\rho_\alpha(E_\alpha) + S_1^2(E_\alpha)\frac{\partial\rho_\alpha}{\partial\alpha}(E_\alpha)\right\}$$

$$= -2S_2(E_\alpha)\frac{\partial}{\partial E_0}\left\{S_1(E_\alpha)\rho_\alpha(E_\alpha)\right\} + 2S_1(E_\alpha)\ S_2(E_\alpha)\frac{\partial}{\partial x}\rho_\alpha(x)\Big|_{x=E_0}$$

$$+ S_1(E_\alpha)\frac{\partial^2}{(\partial E_0)^2}\{S_1^2(E_\alpha)\ \rho_\alpha(E_\alpha)\} + S_1(E_\alpha)\frac{\partial}{\partial E_0}\{S_2(E_\alpha)\ \rho_\alpha(E_\alpha)\}$$

$$- \frac{4\partial}{\partial E_0} S_1(E_\alpha)S_2(E_\alpha)\rho_\alpha(E_\alpha) + \frac{\partial}{\partial E_0}\left\{S_1^2(E_\alpha)*\frac{\partial}{\partial E_0}(S_1(E_\alpha)\ \rho_\alpha(E_\alpha))\right\}$$

$$- \frac{\partial}{\partial E_o} S_1^3(E_\alpha)\frac{\partial}{\partial E_0}\rho_\alpha(E_\alpha) + \int_{-\infty}^{E_\alpha}\frac{\partial^3\rho_\alpha(x)\,dx}{\partial\alpha^3}.$$

Expanding once again, and then collecting all terms yields :

$$-6S_3(E_\alpha)\rho_\alpha(E_\alpha) = - 6\frac{\partial}{\partial E_0}\{S_1(E_\alpha)S_2(E_\alpha)\rho_\alpha(E_\alpha)\}$$

$$+ \frac{\partial^2}{\partial E_o^2} (S_1^3 (E_\alpha) \rho_\alpha(E_\alpha) + \int_{-\infty}^{E_\alpha} \frac{\partial^3}{(\partial\alpha)^3} \rho_\alpha (x) \, dx \tag{8}$$

Once again, taking limit $\alpha \to 0$, the second inverse energy weighted sum is

$$S_3(E_o) = -\frac{1}{\rho_o(E_o)} \int_{-\infty}^{E_o} \frac{\partial^3}{\partial\alpha^3} \rho_\alpha (x) \, dx \Big|_{\alpha=0} - \frac{6\partial}{\partial E_o}(S_1(E_o) S_2(E_o) \rho_o(E_o))$$

$$+ \frac{d^2}{\partial E_o^2} (S_1^3(E_o) \rho_o (E_o)). \tag{9}$$

Fourth and higher terms can be obtained by further differen- tiation of eqn.(8), with respect to α.

(B) Configuration space corrections to ground state energy- extension to Halemane's result :

From equation (1) ,

the first order correction term is given by

$$S_1(E_\alpha) = -\frac{1}{\rho(E_\alpha)} \frac{\partial F_\alpha(E)}{\partial\alpha} \Big|_{\alpha=0} \tag{1}$$

Recalling that the perturbed hamiltonian can be written as $H \to H + \alpha K$, the centroid changes as:

$$\epsilon(c) \to \epsilon_\alpha(c) = \langle H \rangle^c + \alpha \langle K \rangle^c$$

$$= \epsilon_o(c) + \alpha \langle K \rangle^c$$

$$\therefore \frac{\partial \epsilon_\alpha(c)}{\partial\alpha} = \langle K \rangle^c \tag{2}$$

Change in width also takes place similarly :

$$\sigma^2(c) \to \sigma_\alpha^2(c) = \sigma_o^2(c) + 2\zeta_c \alpha \sigma_k(c)\,\sigma_o(c) + \alpha^2 \sigma_k^2(c)$$

$$\therefore \frac{\partial \sigma^2}{\partial \alpha}(c) = 2\zeta_c \sigma_o(c)\,\sigma_k(c) + 2\alpha \sigma_k^2(c) \tag{3}$$

We have also used the symbols σ_o and σ_k for $\sigma_o(c)$ and $\sigma_k(c)$ below. In the limit $\alpha \to o$, the integration limits do not depend upon α. The integration over x can be interchanged with differentiation with respect to α,

$$\therefore \frac{\partial F_\alpha(E)}{\partial \alpha} = \frac{\partial}{\partial \alpha} \int_{-\infty}^{E_o} \rho_\alpha(x)\,dx = \int_{-\infty}^{E_o} \frac{\partial \rho_\alpha(x)}{\partial \alpha}\,dx$$

Since the space is decomposed into configurations, we have :

$$\frac{\partial F_\alpha(E)}{\partial \alpha} = \int_{-\infty}^{E} \sum_c \frac{d_c}{D} \frac{\partial}{\partial \alpha} \rho_\alpha^c(x)\,dx \tag{4}$$

Now $\rho_\alpha^c(x) = \frac{1}{\sqrt{2\pi}\sigma_\alpha(c)} \exp\left\{-\frac{1}{2}\left(\frac{x-\epsilon_\alpha(c)}{\sigma_\alpha(c)}\right)^2\right\}$

$$\therefore \frac{\partial}{\partial \alpha}\rho_\alpha^c(x) = \frac{\partial \rho_\alpha^c(x)}{\partial \sigma^2(c)} \frac{\partial \sigma_\alpha^2(c)}{\partial \alpha} + \frac{\partial \rho_\alpha^c(x)}{\partial \epsilon_\alpha(c)} \frac{\partial \epsilon_\alpha(c)}{\partial \alpha}$$

$$= \left(2\zeta_c \sigma_k \sigma_o + 2\alpha \sigma_k^2\right) \rho_\alpha^c(x) \left\{-\frac{1}{2} \frac{(x-\epsilon_\alpha(c))^2\,(-1)}{\sigma_\alpha^4(c)} + (-1/2)\,\sigma_\alpha^2(c)\right\}$$

$$+ \langle K \rangle^c \rho_\alpha^c(x) * \frac{(+2)\,(x-\epsilon_\alpha(c))}{2\sigma_\alpha^2(c)}$$

For convenience, let $\tilde{x}_c = (x - \epsilon_\alpha(c))/\sigma_\alpha(c)$.

$$\therefore \quad \frac{\partial \rho^c_\alpha(x)}{\partial \alpha} = \rho^c_\alpha(x)\left[\frac{\tilde{x}_c}{\sigma_\alpha(c)}\langle K\rangle^c + \frac{[\zeta_c\sigma_K(c)\sigma_o(c)+\alpha\sigma_k^2(c)]}{(\sigma_\alpha(c))^2}(\tilde{x}_c^{\,2} - 1)\right]$$

Hence
$$\left.\frac{\partial \rho^c_\alpha(x)}{\partial \alpha}\right|_{\alpha\to o} = \rho^c_o(x)\left[\frac{\tilde{x}_c\langle K\rangle^c}{\sigma_o(c)} + \frac{\zeta_c\sigma_K(c)}{\sigma_o(c)}(\tilde{x}_c^{\,2} - 1)\right] \tag{5}$$

In terms of Hermite Polynomials $He_i(\tilde{x}_c)$, the above expression can be written as :

$$\left.\frac{\partial \rho^c_\alpha(x)}{\partial \alpha}\right|_{\alpha=o} = \frac{\rho_o(x)}{\sigma_o(c)}\left(\tilde{x}_c\langle K\rangle^c + \zeta_c\sigma_K(c)\, He_2(\tilde{x}_c)\right) \tag{6}$$

To carry out the integration,we make use of the identity

$$\int_{-\infty}^{x} He_\nu\, e^{-x^2/2}\, dx = He_{\nu-1}\, e^{-x^2/2}$$

Also since $\tilde{x}_c = (x - \epsilon_o(c))/\sigma_o(c)$,

$$d\tilde{x}_c = dx/\sigma_o(c) \text{ or } dx = \sigma_o(c)\, d\tilde{x}_c \tag{7}$$

$$\therefore \quad \frac{\partial F_\alpha(E)}{\partial \alpha} = \sum_c \frac{dc}{D}\int_{-\infty}^{E} \frac{\rho^c_\alpha(\tilde{x}_c)}{\sigma_o(c)}\left\{\tilde{x}_c\langle K\rangle^c + \zeta_c\sigma_K(c)He_2(\tilde{x}_c)\right\} dx$$

$$= \sum_c \frac{dc}{D}\int_{-\infty}^{E_c} \rho^c_\alpha(\tilde{x}_c)\quad \tilde{x}_c\langle K\rangle^c + \sigma_K(c)He_2(\tilde{x}_c)\,\zeta_c\, d\tilde{x}_c$$

$$= - \sum_c \frac{d_c}{D} \quad \rho_\alpha^c(E_c) \quad \langle K \rangle^c + \sigma_K(c) He_1 \; (E_c) \zeta_c \tag{8}$$

$$\therefore \quad \frac{1}{\rho(E)} \quad \frac{\partial F_\alpha(E)}{\partial \alpha}\Big|_{\alpha=0} = \frac{1}{\rho(E)} \quad \sum_c \frac{dc}{D} \; \rho_\alpha^c(E_c) \quad \langle K \rangle^c + \sigma_k(c) E_c \zeta_c \tag{9}$$

Where $E_c = (E - \epsilon_o(c)) / \sigma_o(c)$.

Finally, one has

$$S_1(E) = \sum_c \frac{I^c(E)}{I\,(E)} \left\{ \langle K \rangle^c + \sigma_K(c) E_c \zeta_c \right\} \tag{10}$$

The second order correction

$$S_2(E) = \frac{-1}{2\rho(E)} \left[\frac{\partial^2 F_\alpha(E)}{(\partial\alpha)^2}\Big|_{\alpha=0} - \frac{\partial}{\partial E} \left[\frac{1}{\rho(E)} \left\{ \frac{\partial F_\alpha(E)}{\partial \alpha}\Big|_{\alpha=0} \right\}^2 \right] \right] \tag{11}$$

We already have expression for $\frac{\partial F_\alpha(E)}{\partial\alpha}\Big|_{\alpha=0}$ from $S_1(E)$.

We need to evaluate $\frac{\partial^2 F_\alpha(E)}{\partial\alpha^2}\Big|_{\alpha=0}$.

$$\therefore \quad \frac{\partial^2 F_\alpha(E)}{\partial\alpha^2} = \int_{-\infty}^{E} \frac{\partial^2}{\partial\alpha^2} \rho_\alpha \; (x) \; dx = \int_{-\infty}^{E} \sum_c \frac{dc}{D} \frac{\partial^2}{(\partial\alpha)^2} \rho_\alpha^c(x) \; dx \tag{12}$$

$$\frac{\partial^2}{\partial\alpha^2} \; \rho_\alpha^c(x) = \frac{\partial}{\partial\alpha} \left[\frac{1}{\sqrt{2\pi}\sigma_\alpha(c)} \exp\left[-\frac{1}{2} \left(\frac{x - \epsilon_\alpha(c)}{\sigma_\alpha(c)} \right)^2 \right] * \left\{ \langle K \rangle^c \frac{(x - \epsilon_\alpha(c))}{\sigma_\alpha^2(c)} \right.\right.$$

$$\left.\left. + \frac{1}{\sigma_\alpha^2(c)} (\zeta_c \sigma_K \sigma_0 + \alpha\sigma_k^2) \left(\frac{(x - \epsilon_\alpha(c))^2}{\sigma_\alpha^2(c)} - 1 \right) \right\} \right] \tag{13}$$

For convenience, let us split up the expression into three terms.

$$T_1 = \rho_\alpha^c(x) = \frac{1}{\sqrt{2\pi}\sigma_\alpha(c)} \quad \exp\left\{ -\frac{1}{2} \left(\frac{x - \epsilon_\alpha(c)}{\sigma_\alpha(c)} \right)^2 \right\}$$

$$T_2 = \langle K \rangle^c \, (x - \epsilon_\alpha(c) \, / \, \sigma_\alpha^2(c) \tag{14}$$

and $T_3 = \frac{1}{\sigma_\alpha^2(c)} \left(\zeta_c \sigma_o(c) \sigma_k(c) + \alpha \sigma_k^2(c) \right) \left\{ \left(\frac{x - \epsilon_\alpha(c)}{\sigma_\alpha(c)} \right)^2 - 1 \right\}$

$$\therefore \quad \frac{\partial^2 \rho_\alpha^c(x)}{\partial \alpha^2} = \frac{\partial}{\partial \alpha} \left[T_1 (T_2 + T_3) \right]$$

$$= \frac{\partial T_1}{\partial \alpha} (T_2 + T_3) + T_1 \left(\frac{\partial T_2}{\partial \alpha} + \frac{\partial T_3}{\partial \alpha} \right)$$

$$\frac{\partial T_1}{\partial \alpha} = \rho_\alpha(x) \left[\langle K \rangle^c \frac{(x - \epsilon_\alpha(c))}{\sigma_\alpha^2(c)} + \frac{1}{\sigma_\alpha^2(c)} \left(\zeta_c \sigma_o(c) \sigma_k(c) + \alpha \sigma_k^2(c) \right) \left\{ \frac{(x - \epsilon_\alpha(c))^2}{\sigma_\alpha^2(c)} - 1 \right\} \right.$$

$$\therefore \quad \left. \frac{\partial T_1}{\partial \alpha} \right|_{\alpha=0} = \rho_o^c(x) \left[\frac{\langle K \rangle^c \, \tilde{x}_c}{\sigma_o(c)} + \frac{\zeta_c \sigma_k(c)}{\sigma_o(c)} (\tilde{x}_c^2 - 1) \right] \tag{15}$$

$$\frac{\partial T_2}{\partial \alpha} = \langle K \rangle^c \left[\frac{(x - \epsilon_\alpha(c))(-1)}{\sigma_\alpha^4(c)} \frac{\partial \sigma_\alpha^2(c)}{\partial \alpha} + \frac{1}{\sigma_\alpha^2(c)} (-1) \frac{\partial \epsilon_\alpha(c)}{\partial \alpha} \right]$$

$$= \langle K \rangle^c \left[\frac{-(x - \epsilon_\alpha(c))}{\sigma_\alpha^4(c)} \left(2 \zeta_c \sigma_o(c) \, \sigma_k(c) + 2 \alpha \sigma_k^2(c) \right) - \frac{\langle K \rangle^c}{\sigma_\alpha^2(c)} \right]$$

$$= - \langle K \rangle^c \left(\frac{x - \epsilon_\alpha(c)}{\sigma_\alpha^4(c)} \right) \left(2 \zeta_c \sigma_o(c) \, \sigma_k(c) + 2 \alpha \sigma_k^2(c) - \frac{\left(\langle K \rangle^c \right)^2}{\sigma_\alpha^2(c)} \right.$$

$$\therefore \quad \left. \frac{\partial T_2}{\partial \alpha} \right|_{\alpha=0} = - \frac{\langle K \rangle^c \, \tilde{x}_c}{\sigma_o^2(c)} \left(2 \zeta_c \sigma_k(c) \right) - \frac{\left(\langle K \rangle^c \right)^2}{\sigma_o^2(c)} \tag{16}$$

$$T_3 = \frac{1}{\sigma_\alpha^2(c)}(\zeta_c\,\sigma_o\sigma_k + \alpha\sigma_k^2)\left\{\left(\frac{x-\epsilon_\alpha(c)}{\sigma_\alpha(c)}\right)^2 - 1\right\}$$

$$\therefore\ \frac{\partial T_3}{\partial\alpha} = \left\{(\zeta_c\sigma_o\sigma_k + \alpha\sigma_k^2)\frac{(-1)}{\sigma_\alpha^4(c)}\frac{\partial\sigma_\alpha^2(c)}{\partial\alpha} + \frac{\sigma_k^2(c)}{\sigma_\alpha^2(c)}\right\} * \left\{\left(\frac{x-\epsilon_\alpha(c)}{\sigma_\alpha(c)}\right)^2 - 1\right\}$$

$$+ \frac{1}{\sigma_\alpha^2(c)}(\zeta_c\sigma_o\sigma_k + \alpha\sigma_k^2) * \left\{2\frac{(x-\epsilon_\alpha(c))}{\sigma_\alpha^2(c)}(-1) * \frac{\partial\,\epsilon_\alpha(c)}{\partial\alpha}\right.$$

$$\left. - \frac{(x-\epsilon_\alpha(c))^2}{\sigma_\alpha^4(c)}\frac{\partial\sigma_\alpha^2(c)}{\partial\alpha}\right\}$$

$$= \left\{-2\left(\frac{\zeta_c\sigma_o\sigma_k + \alpha\sigma_k^2}{\sigma_\alpha^4(c)}\right)^2 + \frac{\sigma_k^2(c)}{\sigma_\alpha^2(c)}\right\}\left\{\frac{(x-\epsilon_\alpha(c))^2}{\sigma_\alpha^2(c)} - 1\right\}$$

$$+\left\{\frac{\zeta_c\sigma_o\sigma_k + \alpha\sigma_k^2}{\sigma_\alpha^2(c)}\right\}\left\{-2\langle K\rangle^c\frac{(x-\epsilon_\alpha(c))}{\sigma_\alpha^2(c)} - 2(\zeta_c\sigma_o\sigma_k + \alpha\sigma_k^2)\frac{(x-\epsilon_\alpha(c))^2}{\sigma_\alpha^4(c)}\right\}$$

$$\therefore \left.\frac{\partial T_3}{\partial\alpha}\right|_{\alpha=0} = -2\frac{(\zeta_c\sigma_o\sigma_k)^2}{\sigma_o^4(c)} + \frac{\sigma_k^2(c)}{\sigma_o^2(c)}(\tilde{x}_c^2 - 1) + \frac{1}{\sigma_o^2(c)}\zeta_c\sigma_o\sigma_k\left\{\frac{-2\langle K\rangle^c\tilde{x}_c}{\sigma_o(c)}\right.$$

$$\left. - 2\frac{\zeta_c\sigma_o\sigma_k\,\tilde{x}_c^2}{\sigma_o^2(c)}\right\}$$

$$= \frac{1}{\sigma_o^2(c)} \left\{ \left(\sigma_k^2(c) - 2\zeta_c^2 \sigma_k^2(c) \right) (\tilde{x}_c^2 - 1) - 2\zeta_c \sigma_k(c) \langle K \rangle^c \tilde{x}_c - 2\zeta_c^2 \sigma_k^2(c)\, \tilde{x}_c^2 \right\} .$$

$$= \frac{1}{\sigma_o^2(c)} \left\{ \sigma_k^2(c)\, (\tilde{x}_c^2 - 1) - 4\zeta_c^2 \sigma_k^2(c)\, \tilde{x}_c^2 + 2\zeta_c^2 \sigma_k^2(c) - 2\zeta_c \sigma_k(c) \tilde{x}_c \langle K \rangle^c \right\} \tag{17}$$

$$\therefore \frac{\partial^2 \rho_\alpha^c(x)}{\partial \alpha^2}\Big|_{\alpha=0} = (T_2+T_3) \frac{\partial T_1}{\partial \alpha}\Big|_{\alpha=0} + T_1 \left(\frac{\partial T_2}{\partial \alpha}\Big|_{\alpha=0} + \frac{\partial T_3}{\partial \alpha}\Big|_{\alpha=0} \right)$$

Substituting from equations 14-17, we get

$$(T_2+T_3) \frac{\partial T_1}{\partial \alpha}\Big|_{\alpha=0} = \left[\langle K \rangle^c \frac{\tilde{x}_c}{\sigma_o(c)} + \frac{\zeta_c \sigma_k(c)}{\sigma_o(c)} (\tilde{x}_c^2 - 1) \right] * \frac{\rho_o^c(x)}{\sigma_o(c)} \left[\tilde{x}_c \langle K \rangle^c + \zeta_c \sigma_k(c) (\tilde{x}_c^2 - 1) \right]$$

$$= \frac{\rho_o^c(x)}{\sigma_o^2(c)} \left[\langle K \rangle^c \tilde{x}_c + \zeta_c \sigma_k(c)\, (\tilde{x}_c^2 - 1) \right]^2$$

$$T_1 \left[\frac{\partial T_2}{\partial \alpha}\Big|_{\alpha=0} + \frac{\partial T_3}{\partial \alpha}\Big|_{\alpha=0} \right] = \rho_o^c(x) \left(\frac{\partial T_2}{\partial \alpha}\Big|_{\alpha=0} + \frac{\partial T_3}{\partial \alpha}\Big|_{\alpha=0} \right)$$

$$= \frac{\rho_o^c(x)}{\sigma_o^2(c)} \left(-2\langle K\rangle^c \tilde{x}_c \zeta_c \sigma_k(c) + \sigma_k^2(c)(x_c^2-1) - 4\zeta_c^2 \sigma_k^2(c)\tilde{x}_c^2\right.$$

$$\left. + 2\zeta_c^2 \sigma_k^2(c) - 2\zeta_c \sigma_k(c)\tilde{x}_c \langle K\rangle^c - (\langle K\rangle^c)^2 \right)$$

$$\therefore \left.\frac{\partial^2 \rho_\alpha^2(x)}{\partial\alpha}\right|_{\alpha=0} = \frac{\rho_o^c(x)}{\sigma_o^2(c)} \left[(\langle K\rangle^c)^2 \tilde{x}_c^2 + \sigma_k^2(c)(\tilde{x}_c^2-1)\right.$$

$$+ \zeta_c \sigma_k^2 (\tilde{x}_c^4 - 2\tilde{x}_c^2 + 3 - 4\tilde{x}_c^2) - (\langle K\rangle^c)^2$$

$$\left. + 2\langle K\rangle^c \zeta_c \sigma_x(c)(\tilde{x}_c^3 - \tilde{x}_c - 2\tilde{x}_c) \right]$$

$$= \frac{\rho_o^c(x)}{\sigma_o^2(c)} \left[((\langle K\rangle^c)^2 + \sigma_k^2(c))\, He_2(\tilde{x}_c) + \zeta_c^2 \sigma_k^2(c)\, He_4(\tilde{x}_c) \right.$$

$$\left. + 2\langle K\rangle^c \zeta_c \sigma_k(c)\, He_3(\tilde{x}_c) \right].$$

$$\therefore \left.\frac{\partial^2 F_\alpha(E)}{(\partial\alpha)^2}\right|_{\alpha=0} = \sum_c \int_{-\infty}^{E} \frac{dc}{D} \left.\frac{\partial^2 \rho_\alpha(x)}{(\partial\alpha)^2}\right|_{\alpha=0} dx$$

$$= \sum_c \int_{-\infty}^{E_c} \frac{dc}{D}\, \sigma_o(c) \left.\frac{\partial^2 \rho_\alpha^c(\tilde{x}_c)}{(\partial\alpha)^2}\right|_{\alpha=0} dx_c$$

$$= \sum_c \frac{\sigma_o(c)}{\sigma_o^2(c)} \frac{dc}{D} \int_{-\infty}^{E_c} \rho^c(\tilde{x}_c) \, [(\langle K\rangle^{c\,2} + \sigma_k^2(c)) \, He_2(\tilde{x}_c)$$

$$+ \tau_c^2 \, \sigma_k^2(c) \, He_4(\tilde{x}_c) + 2\langle K\rangle^c \, \tau_c \, \sigma_k(c) \, He_3(\tilde{x}_c)] \, d\tilde{x}_c$$

$$= - \sum_c \frac{d_c}{D} \frac{\rho_o^c(E_c)}{\sigma_o(c)} \Big\{ (\langle K\rangle^{c\,2} + \sigma_k^2(c)) \, He_1(E_c) + \tau_c^2 \, \sigma_k^2(c) \, He_3(E_c)$$

$$+ 2\langle K\rangle^c \tau_c \, \sigma_k(c) \, He_2(E_c) \Big\} .$$

Now $\displaystyle \frac{\partial F_\alpha(E)}{\partial \alpha} \Big|_{\alpha=0} = - \sum_c \frac{dc}{D} \rho_o^c(E_c) [\langle K\rangle^c + \tau_c \, \sigma_k(c) \, E_c]$

For evaluation of the second term in the expression for $S_2(E)$, we need

$$\frac{\partial}{\partial E} \frac{1}{\rho(E)} \left(\frac{\partial F_\alpha(E)}{\partial \alpha} \Big|_{\alpha=0} \right)^2$$

$$= \left(\frac{\partial F_\alpha(E)}{\partial \alpha} \Big|_{\alpha=0} \right)^2 \frac{\partial}{\partial E} \left(\frac{1}{\rho(E)} \right) + \frac{1}{\rho(E)} \, 2 \frac{\partial}{\partial \alpha} F_\alpha(E) \Big|_{\alpha=0}$$

$$+ \frac{\partial}{\partial E} \left(\frac{\partial}{\partial \alpha} F_\alpha(E) \Big|_{\alpha=0} \right)$$

Now $\displaystyle \frac{\partial}{\partial E} \left(\frac{1}{\rho(E)} \right) = \frac{-1}{(\rho(E))^2} \frac{\partial \rho(E)}{\partial E}$

$$= \frac{1}{(\rho(E))^2} \sum_c \frac{dc}{D} \frac{1}{\sqrt{2\pi}\sigma_o(c)} (-) \left(\frac{E - \epsilon_o(c)}{\sigma_o(c)} \right) \frac{\exp\left[-1/2 \left\{ \frac{E - \epsilon_o(c)}{\sigma_o(c)} \right\}^2 \right]}{\sigma_o(c)}$$

$$= \frac{1}{(\rho(x))^2} \sum_c \frac{dc}{D} \frac{\rho^c(E_c)}{\sigma_0(c)} E_c$$

$$\therefore \frac{\partial}{\partial E} \left(\frac{\partial F_\alpha(E)}{\partial \alpha} \Big|_{\alpha=0} \right) = \frac{\partial}{\partial E} \left\{ - \sum_c \frac{dc}{D} \rho^c(E_c) \left(\langle k \rangle^c + \zeta_c \sigma_k(c) E_c \right) \right\}$$

$$= \sum_c \left(\langle K \rangle^c + \zeta_c \sigma_k(c) E_c \right) \frac{x_c}{D} * \frac{\rho^c(E_c)(-E_c)}{\sigma_0(c)}$$

and $\frac{\partial}{\partial E} \left\{ \frac{1}{\rho(E)} \left(\frac{\partial F_\alpha(E)}{\partial \alpha} \Big|_{\alpha=0} \right)^2 \right\}$

$$= \frac{1}{(\rho(E))^2} \left[\sum_c \frac{dc}{D} \rho^c(E_c) \left(\langle K \rangle^c + \sigma_k(c) E_c \right) \right]^2 \sum_c \frac{dc}{D} \rho^c(E_c) \frac{E_c}{\sigma_0(c)}$$

$$+ \frac{2}{\rho(E)} \sum_c \frac{dc}{D} \rho^c(E_c) \left(\langle K \rangle^c + \zeta_c \sigma_k(c) E_c \right)$$

$$* \sum_c \frac{dc}{D} \frac{\rho^c(E_c)}{\sigma_0(c)} \left[E_c \langle K \rangle^c + \zeta_c \sigma_k(c) He_2(E_c) \right]$$

$$S_2(E) = \frac{1}{2\rho(E)} \left[\frac{\partial^2 F_\alpha(E)}{\partial \alpha^2} \Big|_{\alpha=0} - \frac{\partial}{\partial E} \left(\frac{1}{\rho(E)} \left(\frac{\partial F_\alpha(E)}{\partial \alpha} \Big|_{\alpha=0} \right)^2 \right) \right]$$

$$= \frac{1}{2\rho(E))^3} \left\{ \sum_c \frac{dc}{D} \rho_0^c(E) \left[\left(\langle K \rangle^c + \zeta_c \sigma_k(c) E_c \right] \right\}^2 \sum_c \frac{dc}{D} \frac{\rho^c(E_c) E_c}{\sigma_0(c)}$$

$$- \frac{1}{(\rho(E))^2} \cdot \sum_c \frac{dc}{D} \rho_0^c(E_c) \left(\langle K \rangle^c + \zeta_c \sigma_k(c) E_c \right)$$

$$* \sum_c \frac{dc}{D} \frac{\rho_0^c(E_c)}{\sigma_0(c)} \left[E_c \langle K \rangle^c + \zeta_c \sigma_k(c) He_2(E_c) \right]$$

$$\frac{-1}{2\rho(E)} \sum_c \frac{dc}{D} \frac{\rho_0^c(E_c)}{\sigma_0(c)} \left\{ \left((\langle K \rangle^c)^2 + \sigma_K^2(c) \right) He_1(E_c) + \zeta_c^2 \sigma_K^2(c) He_3(E_c) \right.$$
$$\left. + 2 \langle K \rangle^c \zeta_c \sigma_K(c) He_2(E_c) \right\}$$