CHAPTER V

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THE VARIATIONAL PRINCIPLE

As pointed out by Halperin and Lax[24] one can reach the low - energy tail in two different but equivalent ways, i.e., by letting $E \longrightarrow -\infty$ or by keeping E constant and reducing the magnitude of the potential fluctuations and letting $\xi \longrightarrow 0$

Since $\rho(E)$ has the form $A(E)\exp(-\frac{B(E)}{2\xi})$ containing the limit $\xi \longrightarrow 0$, we can maximize $\rho(E)$ by minimizing function $-B(E)/2\xi$. This condition is correct in the limit where the eigenfunctions are localized and trapped in local potential fluctuations without overlapping spatially . Typical value of ξ are 0.5, 5 etc. As shown in Fig 3.1 , the unphysical region occurs in the region where the curve bends down.

Sayakanit[31] has used Halperin and Lax's limit to maximized $\rho(E)$ by minimizing the exponential term $\exp(-\frac{B(E,z)}{2\xi})$ To determine the best choice of z. He obtained the same results as Halperin and Lax's. He also pointed out that Halperin and Lax's limit is not based on the variational principle. He suggested that Lloyd and Best variational principle[34] could be used in this connection.

In this chapter we determine the variational parameter z based on the Lloyd and Best variational principle and study the asymptotic solution of z , $n(\nu)$, $b(\nu)$, $a(\nu)$ and $T(\nu)$.

5.1 The Exact Variational Principle.[27,33,34]

In quantum mechanics, if we need to determine the ground state energy of the system which has the Hamiltonian H, we can assume the trial wave function $\psi(r,\lambda)$ where λ is a parameter. We obtain the ground state energy.

$$E_1 = \int \psi^* H \psi \, d\tau \qquad 5.1.1$$

The above expression may be expressed in term of the variational principle, i.e.,

$$E_o < E_1 \qquad 5.1.2$$

where E_o is the true ground state energy of the system.

In a many fermion system, we can determine the ground state energy E_o in term of the density of states,

$$E_o = \int^{\mu} E \, \rho(E) \, dE \qquad 5.1.3$$

where the density of states $\rho(E)$ (from definition) can be written as

$$\rho(E) = \frac{1}{\Omega} \sum_{\alpha} \delta(E - E_{(\alpha)}) \qquad 5.1.4$$

and μ in this case is the Fermi energy

If we assume the trial wave function $\psi_\alpha(r,z)$ as the single particle states, similarly as (5.1.4), we obtain

$$\rho(E, z) = \frac{1}{\Omega} \sum_\alpha \delta(E - \langle\alpha| H |\alpha\rangle) \qquad 5.1.5$$

To obtain the true density of states we have to choose the most appropriate value of z For obtaining the best choice of z , Lloyd and Best suggested that one should maximize the pressure P(E). The non - interacting many fermion equation can be written in the form

$$P(\mu) = \frac{1}{\beta} \int_{-\infty}^{+\infty} \rho(E)\, dE \ln(1 + \exp(-\beta(E - \mu))) \qquad 5.1.6$$

Differentiating (5.1.6) with respect to μ under condition of T(temperature) and Ω (volume) being constant , we obtain

$$\left.\frac{\partial P(\mu)}{\partial \mu}\right|_{T,\Omega} = \frac{1}{\beta} \int_{-\infty}^{\infty} \rho(E)\, dE \, \frac{\beta . e^{-\beta(E-\mu)}}{1 + e^{-\beta(E-\mu)}}$$

$$= \int_{-\infty}^{\infty} \frac{\rho(E)\, dE}{1 + e^{-\beta(\mu - E)}}$$

When $\beta \rightarrow \infty$ (T = 0) , We have

$$\left.\frac{\partial P}{\partial \mu}\right|_{T,\Omega} = \int_{-\infty}^{\mu} \rho(E)\,dE = N(\mu) \qquad 5.1.7$$

where $N(\mu)$ is the number of particles .

We can write $P(\mu)$ as

$$P(\mu) = \int_{-\infty}^{\mu} dE \int_{-\infty}^{\mu} \rho(E)\,dE \qquad 5.1.8$$

We notice that (5.1.4) define $\rho(E)$ in the form of delta function,

$$\rho(E) = \sum_{E'} \delta(E - E') \qquad 5.1.9$$

The above equation can be rewritten in terms of Heaviside step function as

$$\rho(E) = \sum_{E'} \left\{ \frac{d\Theta(E-E')}{d(E-E')} \right\} \qquad 5.1.10$$

where $\Theta(X)$ is Heaviside step function defined for $X < 0$, $\Theta(X) = 0$ and in the domain $X > 0$, $\Theta(X) = 1$.

On integrating the above eauation,

We have

$$\int_{-\infty}^{E} \rho(E)\,dE = \int_{-\infty}^{E} \sum_{E'} \left\{ \frac{d\Theta(E-E')}{d(E-E')} \right\}$$

$$= \frac{1}{\Omega} \sum_{E'} \theta(E - E') \qquad 5.1.11$$

We repeat the above procedure and obtain

$$\int_{-\infty}^{E} dE' \int_{-\infty}^{E} \rho(E'')dE'' = \frac{1}{} \sum_{E'} (E-E')\, \theta(E - E') \qquad 5.1.12$$

It is convenient to study the function $X\theta(X)$ which has the property that the first and second derivatives are greater than zero. The function therefore belongs to a class of convex function. According to the convexity theorem which states that if f(X) is a convex function then

$$< f(X) > \geqslant f(<X>) \qquad 5.1.14$$

From (5.1.14) we have the approximate value of $\rho(E, z)$, and we can write,

$$P(E, z) = \int_{-\infty}^{E} dE' \int_{-\infty}^{E'} dE'' \rho(E'', z)$$

$$= \int_{-\infty}^{E} dE' \int_{-\infty}^{E'} dE'' \frac{1}{\Omega} \sum_{\alpha} \delta(E'' - <\alpha|H|\alpha>)$$

5.1.15

By using the above theorem we get

$$P\ (E) \geqslant \max_{\lambda} \int_{-\infty}^{E} dE' \int_{-\infty}^{E'} dE''\ \rho(E'', z)$$

To simplify the above expression we integrate by part and obtain

$$P(E,\ z) = E' \int_{-\infty}^{E'} dE''\ \rho(E'',\ z) \Big|_{-\infty}^{E} - \int_{-\infty}^{E} E'\ \rho\ (E',z)dE'$$

Since the first term of right hand side can be evaluated by using the fact that dummy variable can be changed, we have

$$P(E,\ z) = \int_{-\infty}^{E} (E - E'),\ \rho(E',\ z)dE'$$

To proceed further, we change the variable E to the dimensionless energy $\nu = \frac{E-E_o}{E_Q}$, and we have

$$P(\nu,\ z) = -E_Q^2 \int_{\nu}^{\infty} (\nu - \nu')\ ,\rho\ (\nu',\ z)d\nu' \qquad 5.1.14$$

The best value of Z can be obtained by solving the equation

$$\frac{dP(\nu,z)}{dz} = 0 \qquad 5.1.15$$

So differentiating (5.1.14) , we obtain

$$\frac{dP(\nu, z)}{dz} = -E_Q^2 \int_{\nu}^{\infty} (\nu - \nu'), \frac{d\rho(\nu', z)}{dz} d\nu' \qquad 5.1.16$$

Next we consider $\frac{d\rho}{dz}(\nu, z)$, it is convenient to determine

$\frac{d\ln}{dz} \rho(\nu, z)$ by using (4.5.6) for $\rho(\nu, z)$,

$$\frac{d}{dz} \ln \rho(\nu, z) = \frac{d}{dz} \ln a(\nu, z) - \frac{1}{2\xi} \frac{db}{dz}(\nu, z) \qquad 5.1.17$$

Considering the first term on the right hand side of (5.1.17), we have

$$\frac{d}{dz} \ln a(\nu, z) = \frac{d}{dz}\left(\frac{3}{2} \ln \left(\frac{3}{2} z^{-2} + \nu\right) - 6 \ln z - \frac{z^2}{2} - 2 \ln D_{-3}(z)\right)$$

$$5.1.18$$

To evaluate (5.1.18) we use the recursion formula for the parabolic cylinder function

$$\frac{dD_p(z)}{dz} = \frac{-1z}{2} D_p(z) + pD_{p-1}(z) \qquad 5.1.19$$

Carrying out the differentiation and using (5.1.19), we can write (5.1.18) as

$$\frac{d}{dz} \ln a(\nu, z) = 6\left(\frac{D_{-4}(z)}{D_{-3}(z)} - \frac{3 z^{-3}}{4(\frac{3}{2} z^{-2} + \nu)} - \frac{1}{z}\right) \qquad 5.1.20$$

Next we consider the second term on the right hand side of (5.1.17). We can differentiate ln b(ν,z) to get

$$\frac{d}{dz}\ln b(\nu, z) = \frac{1}{b(\nu, z)} \frac{db}{dz}(\nu, z) =$$

$$= \frac{d}{dz}\left(2\ln\left(\frac{3}{2} z^{-2} + \quad\right) - \frac{z^2}{4} - \ln D_{-3}(z)\right) \qquad 5.1.21$$

Carrying out the differentiation and using the recursion formula (5.1.19), we can write the above equation as

$$\frac{db}{dz}(\nu, z) = 3b(\nu, z)\left(\frac{D_{-4}(z)}{D_{-3}(z)} - \frac{2z^{-3}}{\frac{3}{2}z^{-2} + \nu}\right) \qquad 5.1.22$$

On substituting (5.1.20) and (5.1.21) in (5.1.17), we obtain

$$\frac{d}{dz}\ln \rho(\nu, z) = 3\left(\frac{2D_{-4}(z)}{D_{-3}(z)} - \frac{3 z^{-3}}{2(3/_2 z^{-2} + \nu)} - \frac{2}{z}\right)$$

$$- \frac{b(\nu, z)}{2\xi}\left(\frac{D_{-4}(z)}{D_{-3}(z)} - \frac{2z^{-3}}{(\frac{3}{2}z^{-2} + \nu)}\right)$$

Since $\frac{d}{dz}\ln \rho(\nu, z) = \frac{1}{\rho(\nu, z)} \frac{d\rho}{dz}(\nu, z)$ We can write the above equation as

$$\frac{d\rho}{dz}(\nu,z) = 3\,\rho(\nu,z)\left[\left\{\frac{2D_{-4}(z)}{D_{-3}(z)} - \frac{3z^{-3}}{2(3/_2 z^{-2}+\nu)} - \frac{2}{z}\right\}\right.$$

$$\left. - \frac{b(\nu,z)}{2\xi}\left\{\frac{D_{-4}(z)}{D_{-3}(z)} - \frac{2z^{-3}}{(\frac{3}{2}z^{-2}+\nu)}\right\}\right] \qquad 5.1.23$$

Putting (5.1.23) in (5.1.16), we obtain

$$\frac{dP(\nu,z)}{dz} = E_Q^2\int_\nu^\infty d\nu'(\nu-\nu')a(\nu',z)e^{-b(\nu',z)/2\xi}$$

$$\left[\frac{2D_{-4}(z)}{D_{-3}(z)} - \frac{3z^{-3}}{2(\frac{3}{2}z^{-2}+\nu)} - \frac{2}{z} - \frac{b(\nu,z)}{2\xi}\left\{\frac{D_{-4}(Z)}{D_{-3}(Z)} - \frac{2z^{-3}}{(\frac{3}{2}z^{-2}+\nu)}\right\}\right] \qquad 5.1.24$$

Setting (5.1.24) equal to zero, we obtain the variational equation for z

$$\int_\nu^\infty d\nu'(\nu-\nu')a(\nu',z)e^{-b(\nu',z)/2\xi}$$

$$X\left[\frac{2D_{-4}(z)}{D_{-3}(z)} - \frac{1}{z}\left(\frac{T}{T+\nu}+2\right) - \frac{b(\nu',z)}{2\xi}\left\{\frac{D_{-4}(z)}{D_{-3}(z)} - \frac{2z^{-3}}{(T+\nu')}\right\}\right] = 0$$

where $T = \frac{3}{2}z^{-2}$. 5.1.25

For comparison we study the further two cases :

Maximizing $\rho(\nu,z)$: case II

This case corresponds to maximizing $\rho(\nu,z)$. As before it is more convenient to maximize $\ln \rho_1(\nu,z)$. Thus we set (5.1.23) equal to zero and obtain

$$\frac{2D_{-4}(z)}{D_{-3}(z)} - \frac{1}{Z}\left(\frac{T}{T+\nu} + 2\right) - \frac{b(\nu,z)}{2\xi}\left[\frac{D_{-4}(z)}{D_{-3}(z)} - \frac{2z^{-3}}{(T+\nu)}\right] = 0$$

5.1.26

Here we neglected the constant factor which plays no role upon differentiation

Minimizing $b(\nu,z)$: case III

The variational equation is obtained by minimizing $b(\nu,z)$. Thus we set (5.1.22) equal to zero and obtain

$$\frac{D_{-4}(z)}{D_{-3}(z)} - \frac{2z^{-3}}{(T+\nu)} = 0 \qquad 5.1.27$$

It is interesting to note that if we neglected the first square bracket term of (5.1.26) which correspond to setting $\frac{\delta a(\nu,z)}{dz} = 0$ we then obtain (5.1.27). The expression plus one of the three equation (5.1.25), (5.1.26) or (5.1.27) completly determines the density of states in the band tail region

By using the variational (5.1.27), Sayakanit showed in his works that this approach correspond to the Halperin and Lax's results.

5.2 Asymptotic Solutions[31]

Following the same consideration as in Sayakanit's work, we consider two limiting values of ν, i.e., for $\nu >> 1$ and $\nu << 1$.

Case III (minimizing the exponent)

a $\nu >> 1$

This limit corresponds to the weak screening ($Q \rightarrow 0$) or $z \longrightarrow 0$ (since $z = \frac{\sqrt{2E_Q}}{\sqrt{E_\omega}}$). We let $z \longrightarrow 0$ and use the asymptotic properties of the parabolic cylinder function

$$D_p(z) = \frac{\sqrt{\pi} \quad 2^{P/2}}{\Gamma(\frac{1}{2} - {P/2})} \qquad 5.2.1$$

Eq. (5.2.7) becomes

$$\frac{1}{2}\sqrt{\frac{1}{2}\pi} = \frac{1}{6} z^3(\frac{3}{2}z^{-2} + \nu)$$

where $D_{-3}(z) \sim \frac{1}{2}\sqrt{\frac{1}{2}\pi}$ and $D_{-4}(z) \sim \frac{1}{3}$

Rewriting the above equation, we obtain

$$z^3\nu + \frac{3}{2}z - 3\sqrt{\frac{\pi}{2}} = 0 \qquad 5.2.2$$

If $z^2\nu << 1$ the first term of (5.2.2) can be neglected and we obtain the solution $z = 2\sqrt{\frac{\pi}{2}}$. However this solution is not an acceptable solution because it is in contradicts with our assumption that $z \to 0$. Thus the acceptable solution must come form $z^2\nu >> 1$. Indeed we obtain

$$z = (3\sqrt{\tfrac{\pi}{2}})^{\frac{1}{3}} \; \nu^{-\frac{1}{3}} \qquad 5.2.3$$

Physically the condition $z^2\nu >> 1$ implies the ratio of kinetic energy of localization $T = \frac{3}{2} z^{-2}$ is much less than ν .

thus
$$a(\nu,z) = \frac{(\frac{3}{2} + z^2\nu)^{\frac{3}{2}}}{8\pi\sqrt{2}\, z^9 \exp(z^2/2)(D_{-3}(z))^2} \qquad 5.2.4$$

and
$$b(\nu,z) = \frac{\sqrt{\pi}\;(\frac{3}{2} + z^2\nu)^2}{2\sqrt{2}\, z^4 \exp(z^2/4) D_{-3}(z)} \qquad 5.2.5$$

We can calulate the above limiting values by substituting (5.2.3) in (5.2.4), (5.2.5) and use the asymptotic properties of parabolic cylinder function (5.2.1). We get

$$a(\nu,z) = \frac{(\frac{3}{2}z^{-2} + \nu)^{\frac{3}{2}} e^{-\frac{1}{2}z^2}}{8\pi\sqrt{2}\;(\frac{9}{2}\pi)\,\nu^{-2}\,\frac{1}{8}\pi}$$

Rewriting the above expression by using $z^2\nu >> 1$, we obtain

$$a(\nu,z) \simeq \frac{2}{9\pi^3}\,\nu^{7/2} \qquad 5.2.6$$

Similarly the limiting value of $b(\nu,z)$ becomes

$$b(\nu,z) \sim \frac{\sqrt{\pi}}{2\sqrt{2}} \left(\frac{3}{2} + z^2\nu\right)^2 \cdot \frac{1}{z^4} \quad 2\sqrt{\frac{2}{\pi}} = \left(\frac{3}{2}z^{-2} + \nu\right)^2$$

$$\sim \nu^2 \qquad 5.2.7$$

We can consider the limiting value of the logarithmic derivative of the exponent $b(\nu,z)$, i.e.,

$$n(\nu) = \frac{d \ln b(\nu,z)}{d \ln \nu}$$

$$= \frac{\nu}{b(\nu,z)} \frac{db}{d\nu}(\nu,z) \qquad 5.2.8$$

To obtain $n(\nu)$ we differentiate (5.2.5) and substitute into (5.2.8). We have

$$n(\nu) = \frac{2\sqrt{2}}{\sqrt{\pi}} \cdot \frac{\nu \cdot \exp\left({}^1/_4 z^2\right) D_{-3}(z)}{\left(\frac{3}{2}z^{-2} + \nu\right)^2} \cdot \frac{2\sqrt{\pi}\left(\frac{3}{2}z^{-2} + \nu\right)}{2\sqrt{2}\ \exp(z^2/4)\, D_{-3}(z)}$$

$$= \frac{2\nu}{\left(\frac{3}{2}z^{-2} + \nu\right)} \qquad 5.2.9$$

We can obtain the limiting value of $n(\nu)$ by substituting the limiting value z into (5.2.9)

$$n(\nu) \simeq \frac{2\nu}{\nu} = 2 \qquad 5.2.10$$

The other quantity of interest is the kinetic energy of localization $T = \frac{3}{2}z^{-2}$ which can be obtained by using the limiting value of z (5.2.3), i.e.,

$$\frac{T}{\nu} \simeq \frac{3}{2Z^2\nu} = \frac{3}{2(3\sqrt{\frac{1}{2}}\,\pi)^{\frac{1}{3}}}\frac{\nu^{-1/3}}{\nu} \simeq 0 \qquad 5.2.11$$

b. $\nu << 1$

This condition corresponds to the strong screening case where we can obtain the limit by letting $z \rightarrow 0$ and using the asymptotic properties of the parabolic cylinder function

$$D_P(z) = \begin{cases} e^{-z^2/4}\, z^P & z >> 1 \\ -\frac{\sqrt{2\pi}}{\Gamma(-P)}\, e^{z^2/4}\, z^{P-1}\, e^{P\pi i} & z << 1 \end{cases} \qquad 5.2.12$$

As in (a) the asymptotic solution of z can be obtained by substituting the asymptotic values of the parabolic cylinder function (5.2.12) where $\underset{z>>1}{D_{-3}(z)} \simeq \frac{e^{-z^2/4}}{z^3}$ and $\underset{z>>1}{D_{-4}(z)} \simeq \frac{e^{-z^2/4}}{z^4}$ in (5.1.27) . Hence we obtain

$$z \simeq \sqrt{\frac{1}{2\nu}} \qquad 5.2.13$$

The limiting values of $a(\nu,z)$, $b(\nu,z)$, $n(\nu)$ and $T(\nu)$ can be obtained by using (5.2.12) and (5.2.13). We have

$$a(\nu,z) \simeq \frac{1}{\sqrt{2}\,\pi}\,\nu^{3/2} \qquad 5.2.14$$

$$b(\nu,z) \simeq (2\nu)^{1/2}\frac{2\sqrt{\pi}}{2\sqrt{2}}\left(\frac{3}{2}+\frac{\nu}{2\nu}\right)^2$$

$$\simeq 2\sqrt{\pi}\,\nu^{1/2} \qquad 5.2.15$$

The kinetic energy of localization

$$\frac{T}{\nu} \simeq \frac{3}{2}\cdot\frac{2\nu}{\nu} = 3 \qquad 5.2.16$$

and

$$n(\nu) \simeq \frac{2\nu}{(3\nu+\nu)} = \frac{1}{2} \qquad 5.2.17$$

For comparison, it is interesting to note that the asymptotic behavior obtained by the path integral method and the method of Halperin and Lax give the identical limiting values for $n(\nu)$ and $\frac{T(\nu)}{\nu}$ but slightly different values for $a(\nu)$ and $b(\nu)$

case II (maximizing $\rho(\nu,z)$)

a. $\nu \gg 1$

We begin to study (5.1.26) that is

$$\left[-\frac{2D_{-4}(z)}{D_{-3}(z)} - \frac{1}{\varepsilon}\left(\frac{T}{T+\nu} + 2\right)\right] - \frac{b(\nu,z)}{2\xi}\left[\frac{D_{-4}(z)}{D_{-3}(z)} - \frac{2z^{-3}}{(T+\nu)}\right] = 0 \qquad 5.2.18$$

Following the same procedure as in case IIIa, we let $z \longrightarrow 0$ then the above equation becomes

$$\left[-\frac{4}{3}\sqrt{\frac{2}{\pi}} - \frac{3}{2}\frac{1}{z^3\nu} - \frac{2}{z}\right] - \frac{\nu^2}{2\xi}\cdot\left[\frac{2}{3}\sqrt{\frac{2}{\pi}} - \frac{2}{z^3\nu}\right] = 0 \qquad 5.2.19$$

where we have used the asymptotic properties of parabolic cylinder function (5.2.1) and the asymptotic property of $b(\nu,z)$(5.2.7) ,i.e, $b(\nu,z) \simeq \nu^2$ for $z \rightarrow 0$. Now if $z^2\nu \ll 1$, the second term in both brackets are dominating . In this situation , we find no solution. For $z^2\nu \gg 1$ the third term in the first bracket dominates and by inspection shows that there exists solutions. Since we know that the first bracket is generally smaller than the second bracket, then the first order approximation by iteration technique we can substitute z in the first bracket. Using z obtain in (5.2.3), we have

$$-\frac{2\nu^{1/3}}{(3\sqrt{\frac{\pi}{2}})^{1/3}} - \frac{1}{3}\frac{\nu^2}{\xi_1}\sqrt{\frac{2}{\pi}} + \frac{\nu^2}{\xi}\cdot\frac{1}{z^3\nu} = 0$$

Rearranging the above expression we get the solution

$$z \simeq \left(3\sqrt{\frac{\pi}{2}}\right)^{\frac{1}{3}} \nu^{\frac{1}{3}} \left[1 + \frac{2\,\xi}{\nu^{5/3}} \left(3\sqrt{\frac{\pi}{2}}\right)^{\frac{2}{3}}\right]^{-\frac{1}{3}} \qquad 5.2.20$$

We can see that for $\xi \longrightarrow 0$, $\nu >> 1$ (5.2.20) the second term in the bracket is much less then 1, then reduces to (5.2.3). Therefore the limiting values of $a(\nu)$, $b(\nu)$, $n(\nu)$ and $\frac{T(\nu)}{\nu}$ must be equivalent to case III(a).

b. $\nu << 1$

As before we let $z \longrightarrow \infty$ and use asymptotic properties of the parabolic cylinder function (5.2.12). We obtain

$$b(\nu,z) \simeq \frac{\sqrt{\pi}}{2\sqrt{2}} \left(\frac{3}{2} + z^2\nu\right)^2 \cdot \frac{1}{z} \qquad 5.2.21$$

On substituting (5.2.21) in (5.2.18) we have

$$\left[\frac{-4}{z} - \frac{3}{2z} \cdot \frac{1}{\left(\frac{3}{2} + z^2\nu\right)}\right] - \frac{1}{2\xi} \cdot \sqrt{\frac{\pi}{2}} \cdot \frac{1}{2}\left(\frac{3}{2} + z^2\nu\right)^2$$

$$\cdot \frac{1}{z} \cdot \left[\frac{1}{z} - \frac{2}{z\left(\frac{3}{2} + z^2\nu\right)}\right] = 0 \qquad 5.2.22$$

If $z^2\nu >> 1$, the second term in the first square bracket and the second square bracket approach zero. Thus the above equation becomes

$$\frac{-4}{z} - \frac{1}{2\xi}\, \frac{1}{2}\sqrt{\frac{\pi}{2}}\, \frac{z^4\nu^2}{z} \left(\frac{1}{z}\right) = 0 \qquad 5.2.23$$

Eq. (5.2.23) can be solved by using De moivre's theorem and we obtain three distinguish solutions of z , i.e.,

$$z_1 = \xi^{\frac{1}{3}} \nu^{-2/3} \quad (16\sqrt{\tfrac{2}{\pi}})^{\frac{1}{3}} (\tfrac{1}{2} + \tfrac{i\sqrt{3}}{2}) ,$$

$$z_2 = \xi^{\frac{1}{3}} \nu^{-2/3} \quad (16\sqrt{\tfrac{2}{\pi}})^{1/3} (-\tfrac{1}{2} + i\sqrt{\tfrac{3}{2}})$$

and $z_3 = -\xi^{\frac{1}{3}} \nu^{-2/3} \cdot (16\sqrt{\frac{2}{\pi}})^{1/3}$. One can see that these solutions cannot be considered as acceptable solutions because their values are complex. Thus the asymptotic solution of ξ can be obtained by taking the limit $\nu << 1$ in(5.2.18). In this case we obtain trancendental equation

$$-\frac{2D_{-4}(z)}{D_{-3}(z)} - \frac{3}{Z} - \frac{1}{2\xi}\frac{9}{16}\sqrt{\frac{\pi}{2}}\frac{e^{-z^2/4}}{z^4} \cdot \frac{1}{D_{-3}(Z)} \left\{ \frac{D_{-4}(z)}{D_{-3}(z)} - \frac{4}{3z} \right\} = 0 \tag{5.2.24}$$

It is clear from this equation that z is independent of ν but depend on . It is interesting to confirm this result from the numerical calculation.

case I (Maximizing $P(\nu,z)$)

a. $\nu >> 1$

We now consider (5.1.25), i.e.,

$$\int_{\nu}^{\infty} d\nu' \, (\nu-\nu') a(\nu',z) e^{-b(\nu',z)/2\xi} \cdot \left[\frac{-2D_{-4}(z)}{D_{-3}(z)} - \frac{1}{z} \cdot \left[\frac{\frac{3}{2}z^{-2}}{\frac{3}{2}z^{-2} + \nu'} + 2 \right] \right.$$

$$\left. - \frac{b(\nu',z)}{2\xi} \left[\frac{D_{-4}(z)}{D_{-3}(z)} - \frac{2z^{-3}}{3/_2 z^{-2} + \nu'} \right] \right] = 0 \qquad (5.2.25)$$

$$\text{where} \quad a(\nu,z) = (\tfrac{3}{2}z^{-2} + \nu)^{3/2} \Big/ \; 8\pi\sqrt{2}\, z^{6} \exp(z^{2}/_{2}) D^{2}_{-3}(z)$$

$$(5.2.26)$$

As in case II (a) we study the limit where $z \to 0$.

Using the asymptotic limit of parabolic cylinder function ,i.e., $D_{-3}(z) \sim \frac{1}{2} \cdot \sqrt{\frac{1}{2}\pi}$, $D_{-4}(z) \sim \frac{1}{3}$ then we obtain $b(\nu) \sim \nu^{2}$. Now we consider terms in first square bracket, by using the condition $z^{2}\nu >> 1$ and asymtotic limit of parabolic cylinder, function.This term becomes $-\frac{4}{3} \cdot \sqrt{\frac{2}{\pi}} - \frac{3}{2z^{3}\nu}$. The second square bracket can also be considered as above. This term becomes $\nu'^{2} \cdot \left[\frac{2}{3}\sqrt{\frac{2}{\pi}} - \frac{2}{z^{3}\nu} \right]$

Next, the limit of $a(\nu',z)$ can be written as $\dfrac{\nu'^{3/2}}{\sqrt{2}\,\pi^{2} z^{6}}$ where we use the condition $z^{2}\nu >> 1$ and the asymptotic behavior of parabolic cylinder function.

From the above consideration, these asymptotic quantities can be substituted in (5.2.26) and we obtain

$$\int_{\nu}^{\infty} d\nu' (\nu-\nu') \, \nu'^{3/2} \, e^{-\nu'^{2}/2\xi} \left[-\frac{4}{3} \sqrt{\frac{2}{\pi}} - \frac{3}{2z^{3}\nu'} \; \nu'^{2} \cdot \left(\frac{2}{3}\sqrt{\frac{2}{\pi}} - \frac{2}{z^{3}\nu'} \right) \right] = 0$$

For the case $\nu \gg 1$, ν' in the first bracket can be dropped out. Thus we can write the above equation as

$$\int_{\nu}^{\infty} d\nu' (\nu - \nu')\, \nu'^{7/2}\, e^{-\nu'^2/2\xi} \cdot \left(\frac{2}{\xi} \sqrt{\frac{2}{\pi}} - \frac{2}{z^3 \nu'} \right) = 0$$

We now change the variable $\frac{\nu'^2}{2\xi} = x$, or $d\nu' = \frac{\xi}{\nu'} \cdot dx$.

Then the above equation becomes

$$\xi \int_{\frac{\nu^2}{2\xi}}^{\infty} dx e^{-x} \left(2\xi x \right)^{5/4} \cdot \left[\left(\frac{2}{3} \sqrt{\frac{2}{\pi}} + \frac{2}{z^3} \right) - \frac{2}{z^3} (2\xi x)^{3/4} - \frac{2}{3} \sqrt{\frac{2}{\pi}} (2\xi x)^{7/4} \right]$$

$$= 0 \qquad (5.2.27)$$

Eq. (5.2.27) can be integrated by using the formula[22]

$$\int_{u}^{\infty} x^{\alpha - 1} e^{-\mu x} dx = \mu^{-\alpha} \Gamma(\alpha, \frac{u}{\mu}) \quad \text{for } u > 0 \text{ , Re } \mu > 0$$

We then obtain

$$\left(\frac{2}{3} \sqrt{\frac{2}{\pi}} + \frac{2}{z^3} \right) \Gamma\left(\frac{9}{4}, \frac{\nu^2}{2\xi}\right)(2\xi)^{5/4} - \frac{2}{z^3}(2\xi)^{3/4} \Gamma\left(\frac{7}{4}, \frac{\nu^2}{2\xi}\right) - \frac{2}{3} \sqrt{\frac{2}{\pi}} (2\xi)^{7/4} \Gamma\left(\frac{11}{4}, \frac{\nu^2}{2\xi}\right)$$

$$= 0 \qquad (5.2.28)$$

where $\Gamma(\alpha, \frac{u}{\mu})$ denotes the incomplete Gamma function. To obtain the solution we use the asymptotic formula for the incomplete gamma function,[22]

$$\Gamma(\alpha, \frac{u}{\mu}) = (\frac{u}{\mu})^{\alpha-1} e^{-u/\mu} \left(\sum_{M=o}^{M-1} \frac{(-1)^m \Gamma(1-\alpha+m)}{(\frac{u}{\mu})^m \Gamma(1-\alpha)} + O(\left|\frac{u}{\mu}\right|^{-M}) \right)$$

$$\left|\frac{u}{\mu}\right| \longrightarrow \infty \quad , -\frac{3\pi}{2} < \arg x < \frac{3\pi}{2} \, , \; M = 1,2\ldots$$

Substituting the first term of the above series in (5.2.28), we have

$$(\frac{2}{3}\sqrt{\frac{2}{\pi}} + \frac{2}{z^3})(2\xi)^{5/4} (\frac{\nu^2}{2\xi})^{5/4} e^{-\nu^2/2\xi} - \frac{2}{z^3}(2\xi)^{3/4}(\frac{\nu^2}{2\xi})^{3/4} e^{-\nu^2/2\xi}$$

$$- \frac{2}{3}\sqrt{\frac{2}{\pi}} (2\xi)^{7/4} (\frac{\nu^2}{2\xi})^{7/4} e^{-\frac{\nu^2}{2\xi}} = 0$$

Rearranging the above expression, we obtain

$$(\frac{2}{3}\sqrt{\frac{2}{\pi}} + \frac{2}{z^3}) \nu^{5/2} - \frac{2}{z^3} \nu^{3/2} - \frac{2}{3}\sqrt{\frac{2}{\pi}} \nu^{7/2} = 0$$

The above equation has solution $z = (3\sqrt{\frac{\pi}{2}})^{1/3} \nu^{-1/3}$ which is the same as case II(a) and case III(a).

b. $\nu \ll 1$

In this case we can neglect ν compared to ν' and extend the integration from zero to infinity then (5.2.25) becomes

$$\int_0^\infty d\nu'\, \nu' a(\nu',z)\, e^{-b(\nu',z)/2\xi} \left[-\frac{2D_{-4}(z)}{D_{-3}(z)} - \frac{1}{z}\left(\frac{T}{T+\nu'} + 2\right) - \frac{b(\nu',z)}{2\xi} \right.$$

$$\left. X \left(\frac{D_{-4}(z)}{D_{-3}(z)} - \frac{2z^{-3}}{(T+\nu')} \right) \right] = 0 \qquad 5.2.29$$

Since $a(\nu,z) = (T+\nu)^{3/2} / 8\pi\sqrt{2}\, z^6 \exp(z^2/2)\, D^2_{-3}(z)$, the term $8\pi\sqrt{2}\, z^6 \exp(z^2/2)\, D^2_{-3}(z)$ can be neglected. We then have

$$\int_0^\infty d\nu\nu (T+\nu')^{3/2} e^{-b(\nu',z)/2\xi} \left[-\frac{2D_{-4}(z)}{D_{-3}(z)} - \frac{1}{z}\left(\frac{T}{T+\nu} + 2\right) - \frac{b(\nu',z)}{2\xi} \right.$$

$$\left. X \left(\frac{D_{-4}(z)}{D_{-3}(z)} - \frac{2z^{-3}}{(T+\nu')} \right) \right] = 0 \qquad 5.2.30$$

Proceeding further we write $\frac{b(\nu,z)}{2\xi} = (T+\nu)^2$ where

$$\alpha = \frac{\sqrt{\pi}}{2\xi} / 2\sqrt{2} \exp(z^{2/4})\, D_{-3}(z), \text{ and } \beta = \frac{D'_{-4}(z)}{D_{-3}(z)}, \qquad (5.2.30)$$

becomes $\int_0^\infty \nu' d\nu' (T+\nu')^{3/2} e^{-\alpha(T+\nu')^2}$

$$\cdot \left[-2\beta - \frac{1}{z}\frac{T}{T+\nu} - \frac{2}{z} - \alpha\beta(T+\nu')^2 + \frac{2\alpha}{z^3}(T+\nu') \right] = 0 \qquad 5.2.31$$

Rewriting the above expression, we have

$$-(2\beta + \frac{2}{z})\int_0^\infty d\,\nu' e^{-\alpha(T+\nu')^2}\,\nu'(T+\nu')^{3/2} - \frac{T}{z}\int_0^\infty d\,\nu' e^{-\alpha(T+\nu')^2}\,\nu(T+\nu')^{\frac{1}{2}}$$

$$-\alpha\beta\int d\,\nu' e^{-\alpha(T+\nu')^2}(T+\nu')^{7/2} + \frac{2\alpha}{z^3}\int_0 d\,\nu'\nu' e^{-\alpha(T+\nu')^2}(T+\nu')^{5/2} = 0$$

5.2.32

To simplify the above integrals, we let $\alpha(T+\nu) = x$, and then (5.2.32) becomes

$$0 = -(2\beta + \frac{2}{z})\int_{\alpha T^2}^\infty \frac{dx}{2(\alpha x)^{1/2}}\,((\frac{x}{\alpha})^{1/2} - T)(\frac{x}{\alpha})^{3/4}$$

$$-\frac{T}{z}\int_{\alpha T^2}^\infty \frac{dx}{2(\alpha x)^{1/2}}\,((\frac{x}{\alpha})^{1/2} - T)(\frac{x}{\alpha})^{1/4}$$

$$-\alpha\beta\int_{\alpha T^2}^\infty \frac{dx}{2(\alpha x)^{1/2}}\,((\frac{x}{\alpha})^{1/2} - T)(\frac{x}{\alpha})^{7/4} + \frac{2\alpha}{z^3}\int_{\alpha\Gamma^2}^\infty \frac{dx}{2(\alpha x)^{1/2}}((\frac{x}{\alpha})^{1/2} - T)(\frac{x}{\alpha})^{5/4}$$

5.2.33

The above integrals can be evaluated by using the formula

$$\Gamma(\alpha,x) = \int_x^\infty e^{-t}\,t^{\alpha-1}\,dt$$

to obtain

$$0 = -(2\beta + \frac{2}{z})\left(\frac{1}{2\alpha^{7/4}} \Gamma(\frac{7}{4}, \alpha T^2) - \frac{T}{2\alpha^{5/4}} \Gamma(\frac{5}{4}, \alpha T^2) \right)$$

$$- \frac{T}{z}\left(\frac{\Gamma(5/4, T^2)}{2\alpha^{5/4}} \quad \frac{T\,\Gamma(3/4, \alpha T^2)}{2\alpha^{3/4}} \right)$$

$$- \alpha\beta\left(-\frac{\Gamma(11/4, \alpha T^2)}{2\alpha^{11/4}} \quad \frac{T}{2\alpha^{9/4}} \Gamma(7/4, \alpha T^2) \right) + \frac{2\alpha}{z^3}\left(\frac{\Gamma(9/4, \alpha T^2)}{2\alpha^{9/4}} - \frac{T\,\Gamma(7/4, \alpha T^2)}{2\alpha^{7/4}} \right)$$

Rearranging the above expression we get

$$0 = \frac{1}{2\alpha^{7/4}} \Gamma(7/4, \alpha T^2)\left(-(2\beta + 2z) - \frac{2\alpha}{z^3} \right) + \frac{T}{2\alpha^{5/4}} \Gamma(5/4, \alpha T^2)\left(2\beta + \frac{1}{z} \right)$$

$$+ \frac{1}{2\alpha^{9/4}} \Gamma(9/4, \alpha T^2)\left(\alpha\beta + \frac{2\alpha}{z^3} \right) + \frac{T^2}{2z\alpha^{3/4}} \Gamma(3/4, \alpha T^2) - \frac{\alpha\beta}{2\alpha^{1/4}} \Gamma(11/4, \alpha T^2)$$

5.2.34

Next we use the relation $\Gamma(\alpha+1, x) = \alpha\Gamma(\alpha, x) + x^{\alpha} e^{-x}$,

(5.2.34) becomes

$$0 = \alpha^{1/2} \Gamma(\frac{5}{4}, \alpha T^2)\left(\frac{T}{2}(2\beta + \frac{1}{z}) + \frac{5}{4}(\beta + \frac{2}{z^3}) \right) + \frac{T^2 \alpha^{3/4}}{2z} \Gamma(\frac{3}{4}, \alpha T^2)$$

$$- \Gamma(\frac{7}{4}, \alpha T^2)\left(z + \frac{2}{z^3} + \frac{15}{4}\beta \right) + T^2 \alpha^{7/4} e^{-\alpha T^2}\left(\beta(1 - \frac{T}{2}) + \frac{2}{z^3} \right)$$

5.2.35

where α and β have defined. We can see from (5.2.35) that z is independent of ν but depends on ξ as in case II(b)

The value of z determined from the Lloyd and Best variational principle cannot be solved analytically. However we can see that in the limit of very deep tail condition, the three cases give the same asymptotic value of z. In conridering the limit ($\nu \ll 1$) , we can see that Halperin and Lax's limit gives the increasing value of z. But in case of maximization of pressure $P(\nu, z)$ and $\rho(\nu, z)$, the value of z becomes finite also depending on ξ .