CHAPTER VI

DISCUSSIONS AND CONCLUSIONS

We shall begin with the summary of the main results obtained in this work. Discussion and comparison will then be considered intensively. Finally, the extension to the excited-state contribution will be given without a detailed calculation.

The approximate density of states of the heavily doped semiconductor is calculated by using the two-parameter variational method via path integrals. The expressions for the density of states are given in the closed forms for both the full-ground-state and deep-tail approximations. Their corresponding variational equations are derived, relying on two well-known variational principles. Lastly, the two-parameter and one-parameter theories are performed numerically. The calculated density of states are shown in Tables 1-8.

According to previous chapter, there are three categories of constraints for evaluating the density of states :

1) Lloyd and Best' variational principle or maximizing the pressure,

2) strong Halperin and Lax' variational ansatz or maximizing the density of states,

3) weak Halperin and Lax' variational ansatz or maximizing exponent.

For the third case, it is found that one of two variational equations will impose on the two parameters to have the same value. Since the full-ground-state and deep-tail

approximations give no different variational equations, it may then be concluded that all the density of states obtained by maximizing the exponent are not dependent on the number of parameters and the approximation method used. That is, the two-parameter theory does not improve anything from the one-parameter theory in this case.

To verify this theory, the simple but active method we shall use first is to reduce the results from two-parameter to one-parameter forms and compare it with the results of one-parameter theory, which should be equal. This can be done by letting $\gamma^2 \to 0$ or equivalently setting $x = x'$ in the Gaussian case (or $z = z'$ in the screened Coulomb case). For the density of states, the similarity between both theories are obviously seen while the derivation of one variational equation from the coupled variational equations requires the help of (5.3). This suggests us to set both parameters equal and combine both variational equations together. This leads to the variational equation like that of the one-parameter theory.

Graphically, the two-parameter and one-parameter density of states, by maximizing the exponent and the density of states in both approximations, are shown below (Figures 6.1 and 6.2). There are also Kane's and free-particle density of states given in these pictures. Note that we have plotted the density of states in units of
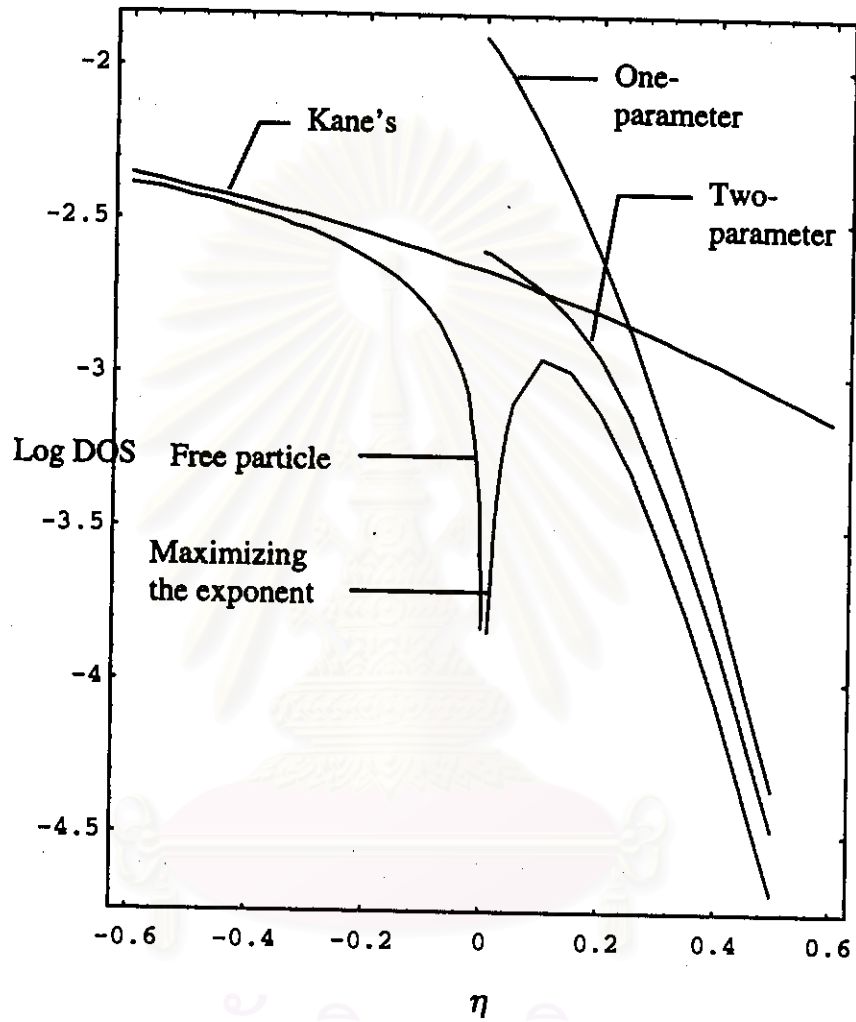
$$\frac{Q^3}{E_Q \xi_Q'^2} \cdot$$

Figure 6.1 The logarithm of the density of states (Log DOS) versus η when ξ'_Q =0.5. The *one-parameter* and *two-parameter* are in the full-ground-state approximation.
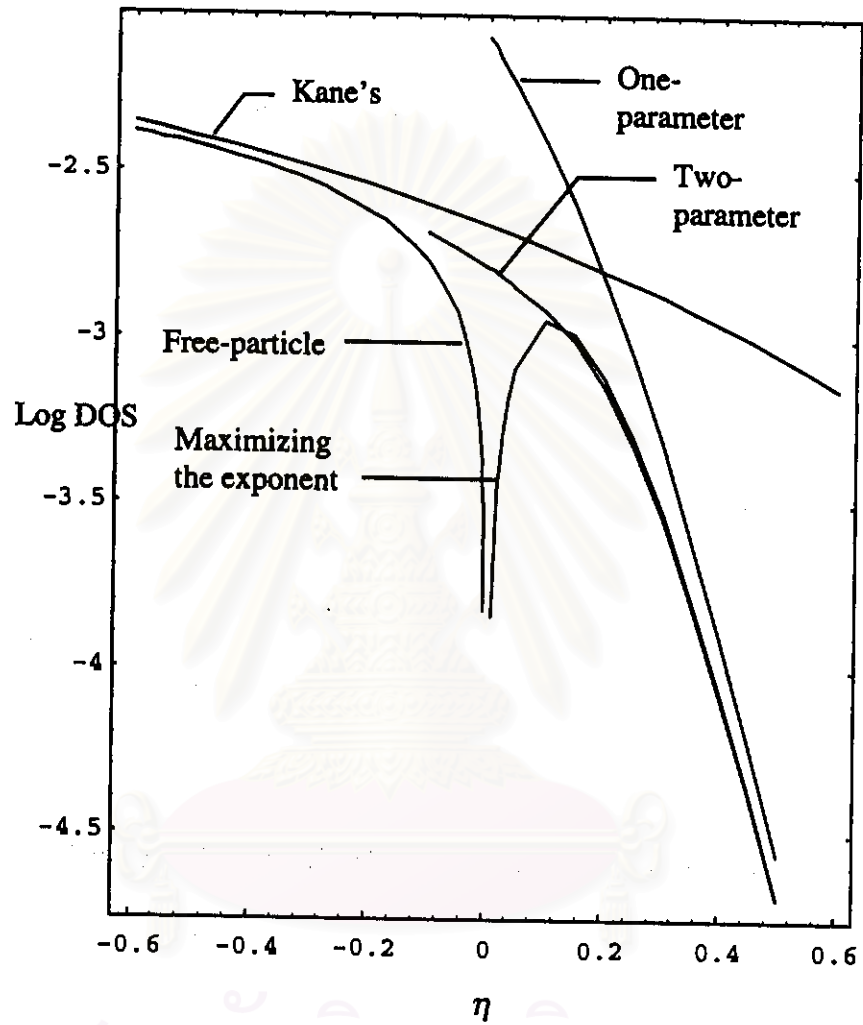
Figure 6.2 The logarithm of the density of states (Log DOS) versus η when $\xi'_Q = 0.5$.

The *one-parameter* and *two-parameter* are in the deep-tail approximation.

The expression for Kane's density of states (Kane, 1963; Sa-yakanit and Glyde, 1980), which is obtained by using the Thomas-Fermi or semiclassical method, can be written as

$$\rho(\eta) = \frac{Q^3}{E_Q \xi_Q'^2} \times \frac{\xi_Q'^{\frac{1}{4}}}{8\sqrt{2}\pi^2} \exp\left[-\frac{\eta}{4\xi_Q'}\right] D_{-\frac{1}{2}}\left(\frac{\eta}{\sqrt{\xi_Q'}}\right). \tag{6.1}$$

It has been shown that the validity range of this covers all energy range but overestimated in the tail region. For the free-particle one, the density of states is given by (Sa-yakanit and Glyde, 1980)

$$\rho(\eta) = \frac{Q^3}{E_Q \xi_Q'^2} \times \frac{\xi_Q'^2}{4\pi^2} \sqrt{|\eta|} \ H(-\eta). \tag{6.2}$$

Look at Figures 6.1 and 6.2, one point which tells us the validity of the two-parameter theory is its alignment, due to the suggestion of Sa-yakanit (1979) that a good tail should be smaller than that of Kane. This consideration implies that the part of the graph above the cross with Kane's is not correct at all. The raising of the curve as the energy increases (η decreases) is also the property which should be obtained by a good method. Next, it is found that the density of states for the two-parameter theory in both cases are smaller than those of the one-parameter theory, especially in the tail region. These shifts show their improvement over the other.

Moreover, the interpolation of these band tails with the density of states obtained by Kane (1963) is of interest. But no such consideration is given here, we shall refer to the work of Sa-yakanit and Haβ (to be published) for completion.

Briefly, in that work, they tried to interpolate the one-parameter density of states by maximizing the density of states with that of Kane, which is valid for the high energy range. In this aspect, we expect that the two-parameter density of states may join with Kane's more smoothly than the one-parameter one.

It is possible to extend our method by considering also the excited-state contribution. Such a contribution can be obtained by expanding (4.36)-(4.39) up to the second order. That is, all these equations will be replaced by

$$\frac{\sin\frac{1}{2}v\,x\sin\frac{1}{2}v(t-x)}{\sin\frac{1}{2}v\,t} \cong \frac{1}{2i}\left(1+\exp[-iv t]-\exp[-iv x]-\exp[-iv(t-x)]\right), \quad (6.3)$$

$$\sin\frac{1}{2}\omega t \cong \frac{1}{2}v\gamma\,t -\frac{1}{8}\frac{v^3\gamma^3\,t^3}{3!}, \qquad (6.4)$$

$$\left(\sin\frac{1}{2}v\,t\right)^{-3} \cong -8i\exp\left[-i\frac{3}{2}v\,t\right]\left(1+3\exp[-iv t]\right), \qquad (6.5)$$

$$\frac{1}{2}v\,t\cot\frac{1}{2}v\,t-1 \cong \frac{i}{2}v\,t\left(1+2\exp[-iv t]\right). \qquad (6.6)$$

This extension is not easily to solve analytically to be in the closed form. But if we focus only on the main term, say (6.5), the "new" density of states can be written in terms of the old one as, for the screened Coulomb case,

$$\rho_s' = \rho_s +3\rho_s\exp\left[\frac{q'^2-q^2}{8\beta^2}\right]D_{\frac{1}{2}}\left(\frac{q'}{\sqrt{2}\beta}\right)\Big/D_{\frac{1}{2}}\left(\frac{q}{\sqrt{2}\beta}\right), \qquad (6.7)$$

where

$$q' = \frac{E_Q}{\hbar}\left(4z^{-2} - \frac{3}{2}z^{-4}z'^2 + \eta\right),$$ (6.8)

$$q = \frac{E_Q}{\hbar}\left(3z^{-2} - \frac{3}{2}z^{-4}z'^2 + \eta\right),$$ (6.9)

and $$\beta^2 = \frac{\sqrt{2}}{\sqrt{\pi}\hbar^2}\xi_Q' \exp\left[\frac{z'^2}{4}\right]D_{-3}(z').$$ (6.10)

However, the variational equations are very complicated, the numerical calculation are not given.

From all above discussions, we may conclude that the two-parameter theory we have presented has improvements and advantages over previous results.