CHAPTER I

INTRODUCTION

ABOUT THE PROBLEM

Heavily doped semiconductors are semiconductors that are doped with a large amount of impurities. These materials play important roles in both industries and education. In industries, heavily doped semiconductors are used in many devices such as tunnel diodes, lasers and thermoelectric devices. In physics circumstance, both theorists and experimentalists are challenged to describe and characterize their behaviours. Moreover, the theory of heavily doped semiconductors and disordered systems are good partners that contribute and interfere each other in developing their theories.

From elementary solid state physics, we know that solids can be described on energy-band schemes and the density of states, which gives a number of states that are able to occupy at each energy level, is the most important function to give the description of a band structure. Unlike the ordinary crystals, the density of states for heavily doped semiconductors has a strange behaviour in its band edges. This unusual characteristic is derived from the tunnelling, absorption and luminescence data. These data tell us that there are energy states in the forbidden gaps or a band-gap narrowing. Why heavily doped semiconductors have these special characters becomes an

interesting problem, which is our interest as well. The band-gap narrowing consists of both an energy-band shift and a band deformation or band tailing. The main contributions giving to such a phenomenon are the electron-impurity and electron-electron interactions. The former can be regarded as the randomness contribution, and the latter is the many-body effect. Even though the theory has been developed so much, there are still many physicists giving an attention to improve it. This is because only the one-dimensional Gaussian-white-noise case can be performed exactly. Recently, Sa-yakanit and Haβ (to be published) succeeded to interpolate the density of states between the high and low energy parts.

Before going on to the next section, to make understanding, we shall briefly elaborate about heavily doped semiconductors. When we dope an impurity into a semiconductor, the impurity level occurs in the forbidden gap between the conduction and valence bands. If this level appears near the conduction band, it is named a donor level. Conversely, an acceptor level means the level appearing near the valence band. As increase a number of doping impurities, the level becomes a degenerate level and ultimately, more doping concentration, the impurity band forms around the original level. This formation is similar to the ordinary bands in the sense of resulting from the overlapping of wave functions, but different in the kind of states. The states of an impurity band are localized states while the ordinary ones are extended or delocalized states. The impurity band still continues expanding, if the doping concentration increases, until it merges with the corresponding band. At this or more concentration limit, we shall call it a very highly or heavily doped semiconductor which has a

distinctive character that the impurity and its corresponding bands can not be divided obviously.

DEVELOPMENT OF THE THEORY

Around the mid of 1950s, the perturbation method so-called "virtual crystal approximation" was used to solve the band-tail problem by Parmenter (1955, 1956). He obtained the density of states without tails. Later, Wolff (1962) showed that the perturbation method is not sufficient for treating this problem and also suggested that the modified green's function technique is required inevitably. In addition, from the "first principle", the effect of electron-electron interactions is to screen a Coulomb potential and to shift the conduction band downward rigidly.

Since the problem seems not easily, indeed very complicated, in three dimensions, an one-dimensional chain of atoms then becomes an interesting problem, which one expects to understand and generalize it into the "real problem". Lax and Phillips (1958) has calculated on the IBM 650 computer and compared with local density and Schmidt's models. Analytically, Schmidt (1957), Frish and Lloyd (1960), Borland (1961), and Halperin (1965) are concerned with a special case called a Gaussian-white-noise case where the potentials at two points are uncorrelated. The exact asymptotic form of the density of states was obtained by Halperin (1965).

Kane (1963), using a semiclassical or Thomas-Fermi method in three dimensions, has obtained the density of states valid for all energy ranges. The important assumption used was the concept of the local density of states, which reduces the problem to finding the distribution of potentials. Due to neglecting the

quantum effect, the result should be overestimated in the tail region of the density of states. However, the advantage of such method has been found for its simplicity and convenience, leading to the generalization of a semi-classical method presented by Van Miegham, Borghs, and Mertens (1991).

In 1966, Halperin and Lax (1966, 1967) has resolved this problem by using a quantum mechanical approach called the minimum counting method. They focused their attention on the deep tail only. The wave functions in very low-lying states have a unique form for each energy and the Gaussian statistics are adequate for describing the potential fluctuations. These assumptions were supposed and a variational principle was also applied. The expression for the density of states is in a closed form with one constraint equation imposed on. Zittartz and Langer (1966) claimed that a mathematical treatment used by Halperin and Lax is not rigorous, which caused they recalculated it systematically based on a function-space formulation.

In the meantime, path integrals has been applied intensively to the theory of disordered systems and this problem. Edwards and Gulyaev (1964; see also Jones and Lukes, 1969; and Bezak, 1970) has derived the exact path integral for the density of states. Nevertheless, in order to calculate this path integral, the approximate method is needed. By using the method similar to the polaron theory of Feynman (1955), Samathiyakanit (1974) was first successful for approximating the path integral so that the Halperin and Lax' result was obtained. The series of works on this method (Sa-yakanit, 1979; Sa-yakanit and Glyde, 1980; and Sa-yakanit, Sritakool and Glyde, 1982) were confined within an one-parameter variational approach and used both the

Lloyd and Best' and Halperin and Lax' variational principles (Halperin and Lax, 1966; Lloyd and Best, 1975).

Relying on the Ginzburg-Landau field theory, Cardy (1978) and Brezin and Parisi (1978, 1980) have obtained the exponential tail of the density of states as well but different from that of Halperin and Lax. However, Van Miegham (1992) argued that this method was more general and powerful than the path integrals. In addition, there are some unsuccessful attempts (Thouless, 1976; Edwards, Greens and Srinivasan, 1977; Sa-yakanit, 1978) which tried to deduce the problem in four into three dimensions based on the analogy of the polymer problem and the electrons in four dimensions. For more details, the review on this theory has been given by Van Miegham (1992).

OUR PURPOSES AND METHODS

In this work, the main aim is to study the density of states for heavily doped semiconductors, especially in the tail region. The path-integral method was used to solve this problem variationally as Sa-yakanit (1979) but the two-parameter trial action is used instead of the one-parameter (Samathiyakanit, 1974). We expect that the improvement of the density of states should be obtained.

At outset, we shall confine ourselves within the one-electron theory and the effective mass approximation. Moreover, only one kind of impurities is doped into the semiconductor. The heavily doped semiconductor can then be modelled as a system of an electron moving in weak and dense scatterers or in a Gaussian random potential. Two types of the potential, Gaussian and screened Coulomb potentials, will be

considered. In path-integral representation, the exact density of states is obtained (Edwards and Gulyaev, 1964), but it cannot be solved explicitly.

As suggested by Samathiyakanit (1974), using a modelled system for a two-parameter trial action, the complicated average propagator is derived within the first cumulant expansion. In a low-lying energy limit, the variational density of states is performed through some certain assumptions, which is called the "full-ground-state" approximation. Using Halperin and Lax' approach (1966), or the so-called "deep-tail" approximation, the density of states like that of them is obtained. Lastly, in order to find the value of parameters, we have applied two variational principles. In the last chapter, the numerical results with comparison to the one-parameter theory and some conclusions are presented.