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ELECTRON DENSITY OF STATES IN DISORDERED SYSTEMS

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Summary

This paper gives a review of the theory of noninteracting electrons in the disordered environment arising from either disordered positions of the ions in the solid or from impurities substituted at random through out the solid. The discussion is focussed on the density of states available to electrons in disordered systems. The specific example considered is the heavily doped semiconductors. A detailed discussion is given concerning with the methods used to find the density of states both in the main part of the band and in the tail part of the band. Special emphasis is paid to the method introduced by one of us (V.S). An interpolation scheme is proposed whtch combines the high and low energies to obtain the density of staies at all energies.

Introduction

In this review we study electrons in a disordered solid. A heavily doped semiconductor is a specific example[1]. The electrons are the particles of interest and the disordered environment is due to either disordered positions of the ions in the solid or to impurities substituted at random throughout the solid. Such a system is called a "disordered system"[2]. There are many other examples of disordered systems, such as phonons, magnons or polarons in a disordered array of ions or impurities[3]. Electrons in disordered systems is a wide field and a subject of intense activity at present. Of particular interest is the conditions under which the electrons are "localized" and non-conducting or are "delocalized" and can contribute to electrical conductivity[4-15]. Here we focus on the density of states available to electrons in disordered systems[9,14]. The density of states is needed to determine almost all properties of the electrons[1]. To begin we consider electrons in an ordered solid.

The Ordered Solid

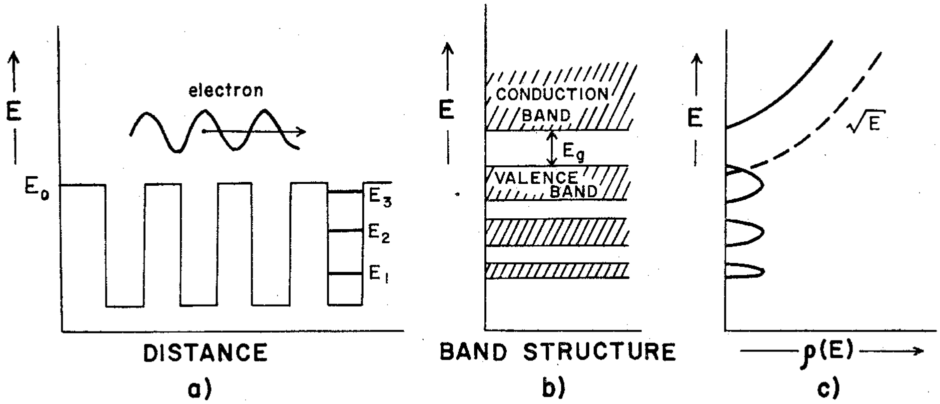
In an ordered solid the identical ions form an ordered array with no impurities. The electrons see a potential due to each ion. Since the ions are ordered, the potential in the solid is an ordered, regular, repeating potential. If we model the potential due to each ion by a square well, then the electron in the solid sees a regular, ordered array of square wells. A one-demensional example of this model is depicted in Fig. 1a.

If the electron saw only one ion (i.e. the electron was in one square well) it would have bound states for $E < E_0$ and travelling wave states for $E > E_0$. In Fig. 1a we have depicted the possible bound state energies (suppose for argument there are only three bound states) by E_1, E_2 and E_3. When the electron is in an array of these square wells, the electron states spread out into bands of states[16,17] as depicted in Fig. 1b. When we "add" the electrons to the solid, the electrons fill up the lowest energy bands first. The highest energy band that is completely filled is called the "valence" band. Electrons in completely filled bands cannot contribute to conductivity and therefore are of little interest and we can ignore them for the remainder of the discussion.

The unfilled or partly filled band is called the conduction band. In this band the electrons can readily change momentum states in an applied electric field and contribute to a net flow of electrons (electrical conductivity) in a crystal. An insulator is a solid in which the valence band is full, the conduction band is empty and the energy gap E_g between them is too large to excite electrons across E_g. A metal is a solid in which the conduction band has many electrons in it, but the band is not completely filled.

In a semiconductor there are only a few electrons in the conduction band or a few unfilled states (holes) in the valence band which makes only limited conduction possible. In this last case the size of E_g is most important. If we added to the semiconductor impurities which attract the electrons (attractive impurities) the attracted electrons have states which lie below the conduction band in the energy gap. If we add many impurities these "impurity states" themselves form a band and effectively lower the edge of the conduction band. This substantially increases the conductivity. The density of electron states in these impurity bands determines the conductivity of the semiconductor.

To get an idea of the density of states in the conduction band, suppose the electrons are "classical" in the sense that they cannot have energy $E < E_0$ and for $E > E_0$ they are "free electrons". From Schrödinger's quantum mechanics the energy



Fig, 1. Potential and density of states in an ordered solid.

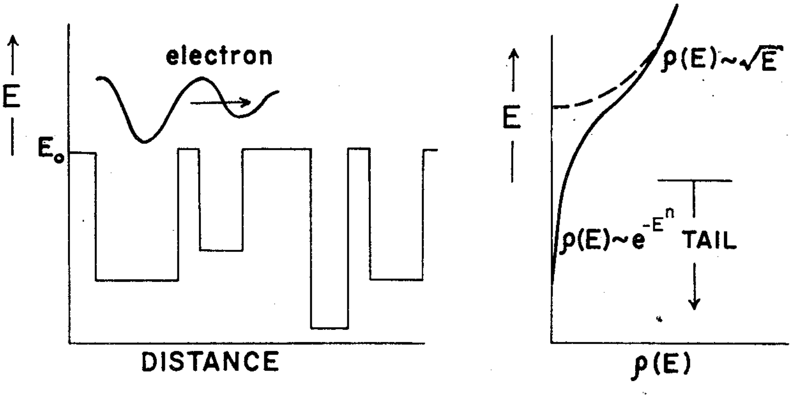


Fig. 2. Potential and density of states in a disordered solid.

of a free electron having wave vector k is $E_k = \hbar^2k^2/2m$ (measured from E_o). The number of states having energy up to E_k is found by summing over the possible k values (up to $k = (2mE_k/\hbar^2)^{\frac{1}{2}}$),

$$N(E_k) = \sum_{\vec{k}} 1 = \frac{\Omega}{(2\pi)^3} \int d\vec{k}$$

with one state per k' value. Here Ω denotes the volume of the system. Since $E_k \propto k^2$ the vector nature of $\vec{k}$ is not important and

$$\begin{aligned} N(E_k) &= \frac{\Omega}{(2\pi)^3} \int_0^k 4\pi k'^2 dk' = \frac{\Omega}{(2\pi)^3} \frac{4}{3} \pi k^3 \\ &= \frac{\Omega}{(2\pi)^3} \frac{4\pi}{3} \left(\frac{2m}{\hbar^2}\right)^{3/2} E_k^{3/2} \end{aligned}$$

The density of states per unit volume, $\rho(E)$, at energy E is defined as the number of states per energy interval dE,

$$\rho(E) = \frac{1}{\Omega} \frac{dN(E)}{dE} = \left(\frac{m^{3/2}}{\sqrt{2}\pi^2\hbar^3}\right)E^{\frac{1}{2}} \tag{1.1}$$

This density of states is shown as the dashed line in Fig. 1c and is the standard free electron density of states. In deriving it we took $E_o = 0$ so in fact $\rho(E) \propto (E - E_o)^{\frac{1}{2}}$. If we allowed two electrons per state, the density of states for both spins, we should multiply $\rho(E)$ by 2. The density of states in the real solid is shown schematically as solid lines in Fig. 1c.

The Disordered Solid

In this case the ions or added impurities form a disordered pattern throughout the solid. If the potential due to each ion or impurity is represented by a square well, then the potential seen by the electron is shown schematically in Fig. 2a. In regions of high impurity concentration the potential is deep. In regions of low concentration the potential is weak. Because of this random arrangement the electron states do not fall in well defined bands of energy. Particularly the "conduction" band has a long tail which reaches down into the energy gap toward the "valence band". Since conduction is dominated by the properties of the conduction band we are interested only in this energy region and can neglect the filled states at lower energy. The density of states in a disordered solid is shown schematically in Fig. 2b.

The electronic properties of a disordered solid depends largely on the "tail" in the density of states depicted in Fig. 2b. For this reason theories of disordered systems focussed on determining density of states in this tail. Kane[18] and others[12,19] used a semi-classical treatment of the electrons to show that in the tail $\rho(E) \propto e^{-E^2}$. To do this, Kane[18] assumed that $\rho(E) \propto (E - V)^{\frac{1}{2}}$ where V, the potential seen by the electron, fluctuates from point to point in the solid. This is valid only if V is slowly varying in the solid. Halperin and Lax[20] use the full quantum theory of

Schrödinger to determine $\rho(E)$. This, however, was numerically very complicated and both approaches are valid only at low E deep in the tail region of the impurity band. More recently, Sa-yakanit[21] proposed a new theory of $\rho(E)$ based on the Path Integral formulation of quantum mechanics developed in 1948 by Feynman[22]. Sa-yakanit obtained an expression for $\rho(E)$ valid at all energies E. Also the $\rho(E)$ reduced to a simple analytic expression in the tail region.

The path integral method has the advantage that the electron is treated much like a classical point particle rather than like a wave. This means many of the ideas suggested by Kane[18] can be employed. The important quantum nature of the electron is then included although the system is treated classically (for example using numbers rather than operators). The quantum nature is incorporated by summing over all possible "classical" paths of the electron.

To anticipate the results we consider first free electrons ($V = 0$) and find $\rho(E) \propto \sqrt{E}$ as expected. Kane's semi-classical theory is then developed which yields $\rho(E) \propto \exp(-E^2)$, valid in practice only for long range potentials. The quantum theory of Halperin and Lax, which uses the Schrödinger representation and yields $\rho(E) \propto \exp(-E^n)$ with $\frac{1}{2} < n < 2$, is then outlined. They obtained the explicit form

$$\rho(E) = a(E)\, e^{-b(E)}$$

where a(E) and b(E) must be calculated numerically. Finally the recent theory developed by Sa-yakanit using Feynman's path integral representation of quantum mechanics is discussed. In this case, the a(E) and b(E) are obtained analytically and $\rho(E)$ is evaluated explicitly for a number of cases.

Potential in a Disordered System

An electron in a disordered solid sees a potential $V(\vec{r})$ that varies unexpectedly from point to point in the solid. The V is not zero as in the free electron case, it is not periodic as in the ordered solid case. The $V(\vec{r})$ could be due to the N ions which make up an amorphous solid so that

$$V(\vec{r}) = \sum_{i=1}^{N} v(\vec{r} - \vec{R}_i), \tag{2.1}$$

where $v(\vec{r} - \vec{R}_i)$ is the potential at $\vec{r}$ due to ion at point $\vec{R}_i$. $V(\vec{r})$ in (2.1) could also be due to N impurity ions substituted at random in an otherwise periodic solid. The $V(\vec{r})$ is then a fluctuating potential superimposed on a periodic potential.

In the present model we ignore electron-electron interactions so that we may treat one single electron at one time in $V(\vec{r})$. (The electron-electron effects can be incorporated in an effective electron mass and in a shift in band energies in specific applications[23-25].) We also assume the $\vec{R}_i$ are randomly distributed throughout the solid. That is, the probability of observing impurity ion i in volume element $d\vec{R}$ is just $d\vec{R}/\Omega$, where Ω is the volume of the solid. This also ignores any possible correlation between the $\vec{R}_i$. Thus the model describes best impurities in a solid rather than amorphous solids. In amorphous solids there is always some correlation (short range) in the ionic positions (two ions cannot overlap). Even at high impurity concentration the impurities are widely separated so that two rarely are neighbours. In the case of impurities in an otherwise periodic solid, the electron states are band states (as discussed in ref. 1) perturbed by the impurities. We consider here only the electrons in the conduction band. We also assume that the band is parabolic ($E \propto k^2$) so that the electron can be treated as a free electron having an effective mass $E_k = (\frac{k^2\hbar^2}{2m^*})$, m* being larger or smaller than its real mass.

In summary the model is a single free electron moving in a random potential $V(\vec{r})$ due to N attractive impurity centres located at points $\vec{R}_i$ distributed at random throughout the solid.

The potential $V(\vec{r})$ in (2.1) will have deep wells where the impurity concentration is high. On the other hand V will be small (nearly zero) where the concentration is low. We can characterize V by its mean value V_o,

$$\begin{aligned} V_o \equiv \langle V(\vec{r})\rangle &= \int \frac{d\vec{R}_1}{\Omega} \cdots \frac{d\vec{R}_N}{\Omega} \sum_i v(\vec{r} - \vec{R}_i) \\ &= N \int \frac{dR}{\Omega} v(\vec{r} - \vec{R}) = n \int d\vec{R}\, v(\vec{r} - \vec{R}) \end{aligned} \tag{2.2}$$

(all impurities identical) and its mean square value ξ.

$$\xi = n \int d\vec{R}\, v^2(\vec{r} - \vec{R}). \tag{2.3}$$

Here n ($= N/\Omega$) is the impurity density.
The V_o and ξ set the mean and the magnitude of the fluctuation about the mean in the potential seen by the electron. We will also need the correlation of $V(\vec{r})$ at different points in the crystal which we denote by[20]

$$\begin{aligned} W(\vec{r} - \vec{r}') &\equiv \langle V(\vec{r})\, V(\vec{r}')\rangle - V_o^2 \\ &= n\int d\vec{R}\, v(\vec{r} - \vec{R})\, v(\vec{r}' - \vec{R}) \end{aligned} \tag{2.4}$$

Clearly from (2.3) and (2.4)

$$\xi = W(o) \tag{2.5}$$

so that ξ measures the magnitude of the correlations.

We also consider the high density limit. This means we have many impurities lying within the wave function of a single electron. The electron wave function can extend several hundred angstroms and high concentration begins in practice at $n \sim 10^{17}$ centres/cm^3. We also consider weakly attractive impurities (v small and negative) such that nv^2 = constant. In this case $nv^3 \ll nv^2$, for example.

A specific representation of the impurity potential we will consider is the screened Coulomb potential.

$$v(\vec{r} - \vec{R}) = - \frac{e^2}{\varepsilon|\vec{r} - \vec{R}|}\, e^{-Q|\vec{r} - \vec{R}|}, \tag{2.6}$$

where Q^{-1} is the screening length and ε the dielectric constant. In this case,

$$V_o = -n\frac{4\pi e^2}{\varepsilon Q^2}, \ \xi = n\frac{2\pi e^4}{\varepsilon^2 Q}, \tag{2.7}$$

and the correlation function is

$$W(\vec{r}-\vec{r}\,') = \xi\, e^{-Q|\vec{r}-\vec{r}\,'|}. \tag{2.8}$$

However for the moment we leave v arbitrary with V_o, ξ and $W(\vec{r}-\vec{r}\,')$ parametrizing its properties.

Free Electron Theory

In this case $V = 0$ and the electron wave functions are plane waves $\psi_{\vec{k}} = \Omega^{-\frac{1}{2}} e^{i\vec{k}.\vec{r}}$ corresponding to momentnm $\hbar\vec{k}$ and energy $E_k = \hbar^2k^2/2m^*$. The density of states per unit volume at energy E is defined as

$$\rho(E) = \frac{1}{\Omega}\sum_{\vec{k}} \delta(E - E_k) \tag{3.1}$$

where the sum is over the free electron energies E_k. Taking Ω large we may convert the sum over $\vec{k}$ to an integral

$$\sum_{\vec{k}} \rightarrow \frac{\Omega}{(2\pi)^3}\int d^3k$$

and

$$\begin{aligned}\rho(E) &= \frac{1}{(2\pi)^3}\int_0^\infty 4\pi k^2 dk\ \delta(E - E_k)\\ &= \frac{1}{(2\pi)^2}\left(\frac{2m^*}{\hbar}\right)^{3/2}\int_0^\infty dE_k\ E_k^{\frac{1}{2}}\ \delta(E - E_k)\end{aligned} \tag{3.2}$$

To use the properties of the delta function

$$\int_{-\infty}^{\infty} dx\ f(x)\ \delta(x - a) = f(a)$$

we introduce the Heaviside step function

$$H(E) = \begin{cases} 1 & E \geq 0 \\ 0 & E < 0 \end{cases} \tag{3.3}$$

so that

$$\rho(E) = \left(\frac{m^{*3/2}}{\sqrt{2}\pi^2\hbar^3}\right)\int_{-\infty}^{\infty} dE_k\ E_k^{\frac{1}{2}}\ H(E_k)\ \delta(E-E_k)$$

and

$$\rho(E) = f\ E^{\frac{1}{2}}\, H(E) \tag{3.4}$$

where

$$f \equiv \left(\frac{m^{*3/2}}{\sqrt{2}\pi^2\hbar^3}\right) \tag{3.5}$$

Hence $\rho(E) \propto E^{\frac{1}{2}}$ measured away from a potential $V = 0$.

The Kane Theory

Kane's theory[18] is a semiclassical treatment of an electron in a disordered solid. This means we ignore the zero point energy of the electron (a quantum effect). As noted above, the potential $V(\vec{r})$ varies from point to point in the solid. In regions where $V(\vec{r})$ is deep, we expect the electron wave function to be narrow (a highly localized electron). Since the kinetic energy is proportional to the curvature of the electron wave function the kinetic energy will be large in these regions. Conversely when $V(\vec{r})$ is nearly zero and flat, the kinetic energy is small (and slowly varying with $\vec{r}$).

The central assumption of Kane's theory is to ignore the variation of kinetic energy with $V(\vec{r})$ and assume the electrons can be treated as "free electrons" having the same kinetic energy everywhere in the solid for all $V(\vec{r})$. The $V(\vec{r})$ then simply sets the potential level from which we measure the energy of these "free electrons". The density of states at point $\vec{r}$ is then proportional to $\sqrt{E - V(\vec{r})}$. Explicity, using the free electron result,

$$\rho(E - V) = f\sqrt{E - V}\; H(E - V) \tag{4.1}$$

This $\rho(E - V)$ can be regarded as a function of V or $\vec{r}$ (through $V(\vec{r})$). The density of states for the solid is then (4.1) averaged over all points in the crystal (or equivalently all potential energy values V). That is,

$$\rho(E) = \langle\rho(E - V)\rangle_V \tag{4.2}$$

where

$$\langle\;\rangle_V = \int dV\; P(V) \tag{4.3}$$

and P(V) is the probability distribution of V, giving the probability of observing V in the range of V to V + dV. With this central assumption it remains only to determine P(V) to complete the calculation of $\rho(E)$. Ignoring the variation of the kinetic energy with $V(\vec{r})$ will be valid in practice when V is long range and slowly varying in space.

To calculate P(V) we use the assumption that the impurities are randomly distributed throughout the volume Ω of the solid. For a random distribution

$$P(V) = \int\cdots\cdots\int \frac{d\vec{R}_1}{\Omega}\;\cdots\cdots\;\frac{d\vec{R}_N}{\Omega}\;\delta\left(V - \sum_{i=1}^{N} v(\vec{r} - \vec{R}_i)\right) \tag{4.4}$$

when the delta function selects out those configurations which lead to a potential V. Using the integral representation of the delta function

$$\delta(V - \sum_{i=1}^{N} v(\vec{r} - \vec{R}_i)) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, e^{it(V - \sum_{i=1}^{N} v(\vec{r} - \vec{R}_i))}$$

we have

$$P(V) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, e^{it\,V}\left[\int \frac{d\vec{R}}{\Omega}\, e^{-it\,v(\vec{r} - \vec{R})}\right]^N$$

Employing,

$$[x]^N = [1 + (x - 1)]^N = e^{N(x - 1)},$$

where the last equality holds in the limit N → ∞,

$$\left[\int \frac{dR}{\Omega}\, e^{-it\,v(\vec{r} - \vec{R})}\right]^N = \exp\left\{N\int \frac{d\vec{R}}{\Omega}\,(e^{-it\,v(\vec{r} - \vec{R})} - 1)\right\}$$

and

$$P(V) = \frac{1}{2\pi}\int dt\, \exp\left\{(itV + n\int d\vec{R}\,(e^{-it\,v(\vec{r} - \vec{R})} - 1)\right\}.$$

We now use the fact that v is small to expand e^{-itv} in a power series in v. Since $nv^3 \ll nv^2$ we truncate the expansion after the term quadratic in v. It is here that we use the assumption of weak, dense scatterers. Then

$$\begin{aligned} P(V) &= \frac{1}{2\pi}\int dt\, \exp\left\{itV - itn\int d\vec{R}\, v(\vec{r} - \vec{R}) - \frac{t^2}{2}\, n\int d\vec{R}\, v^2(\vec{r} - \vec{R})\right\} \\ &= \frac{1}{2\pi}\int dt\, \exp\left\{it(V - V_o) - \frac{t^2\xi}{2}\right\}. \end{aligned} \tag{4.5}$$

In the last equality we have used the definitions of the average V_o, and variance, ξ, of the potential given in (2.2) and (2.3). Using

$$\int_{-\infty}^{\infty} dx\, e^{-ax^2 + bx} = \left(\frac{\pi}{a}\right)^{\frac{1}{2}} e^{b^2/4a}$$

we have

$$P(V) = (2\pi\xi)^{-\frac{1}{2}}\, e^{-\frac{1}{2}(V - V_o)^2/\xi}. \tag{4.6}$$

Finally to display the meaning of P(V) more clearly we use

$$(2\pi\xi)^{-\frac{1}{2}} = \int_{-\infty}^{\infty} dV\, e^{-\frac{1}{2}(V - V_o)^2/\xi}. \tag{4.7}$$

to write

$$P(V) = \frac{e^{-\frac{1}{2}(V - V_o)^2/\xi}}{\int_{-\infty}^{\infty} dV\, e^{-\frac{1}{2}(V - V_o)^2/\xi}} \tag{4.8}$$

The expressions (4.6) and (4.8) show that P(V) is a Gaussian distribution about the mean V_o. A potential having this distribution is called a "Gaussian Random Potential". This distribution follows (1) from assuming the impurities are equally likely to be in any volume element in the solid and (2) from retaining quadratic terms in V only. With these assumptions a Gaussian distribution is expected. For example, in equilibrium statistical mechanics we use the "equal a priori probability of phase space" assumption. This tells us that the variables $\vec{r}$ and $\vec{p}$ are equally likely to be found anywhere in phase space. This assumption leads to the Boltzmann disbribution, $e^{-\beta E}$ ($\beta = 1/k_BT$). If E is quadratic in the variables (e.g. $E = \frac{1}{2}mv^2$ for free particles, $E = \frac{1}{2}kr^2$ for a harmonic oscillator) then we obtain a Gaussian distribution as in (4.6) for the variables.

Using (4.6) for P(V) in (4.3) (and using the Heaviside function to reduce the integration up to E) we have

$$\begin{aligned}\rho(E) &= \int_{-\infty}^{\infty} dV\ P(V)\ f\ \sqrt{E-V}\ H(E-V) \\ &= (2\pi\xi)^{-\frac{1}{2}} = \int_{-\infty}^{E} dV\ (E-V)^{\frac{1}{2}}\ e^{-\frac{1}{2}\,(V-V_o)^2/\xi}. \end{aligned} \tag{4.9}$$

This is Kane's result for the density of states.

We consider two limits of (4.9). For high energy E>>V we can ignore V (i.e. set V = 0) and take $E \rightarrow \infty$. Then

$$\begin{aligned}\rho(E) &= f\ (2\pi\xi)^{-\frac{1}{2}}\ E^{\frac{1}{2}} \int_{-\infty}^{\infty} dV\ e^{-\frac{1}{2}\,(V-V_o)^2/\xi} \\ &= f\ E^{\frac{1}{2}} \end{aligned} \tag{4.10}$$

Thus Kane's result for high electron energies, where V is negligible goes over to the free electron value—as expected. For E<<V, that is electron energies deep in the potential region, we substitute z = E – V in (4.9) so that

$$\begin{aligned}\rho(E) &= f\ (2\pi\xi)^{-\frac{1}{2}} \int_{0}^{\infty} dz\ z^{\frac{1}{2}}\ e^{-\frac{1}{2}\,(E-z-V_o)^2/\xi} \\ &= f\ (2\pi\xi)^{-\frac{1}{2}}\ e^{-\frac{1}{2}\,(E-V_o)^2/\xi} \int_{0}^{\infty} dz\ z^{\frac{1}{2}}\ e^{-1/2\,(z^2-2z(E-V_o))/\xi} \end{aligned}$$

Then using the integral representation of the parabolic cylinder function D_{-p},

$$\int_{0}^{\infty} dz\ z^{p-1}\ e^{-\alpha z^2-\beta z} = (2\alpha)^{-p/2}\ \Gamma(p)\ e^{\beta^2/8\alpha}\ D_{-p}\left(\frac{\beta}{\sqrt{2\alpha}}\right), \tag{4.11}$$

where $\Gamma(p)$ is the Gamma function, we have

$$\rho(E) = f\ (2\pi\xi)^{-\frac{1}{2}}\ \xi^{3/4}\ \Gamma\left(\frac{3}{2}\right)\ e^{-\frac{1}{4}(E-V_o)^2/\xi}\ D_{-3/2}\left(-\frac{(E-V_o)}{\sqrt{\xi}}\right).$$

With $\Gamma(3/2) = \frac{1}{2}\ \Gamma(\frac{1}{2}) = \sqrt{\pi}/2$,

$$\rho(E) = \frac{f}{2\sqrt{2}}\,\xi^{\frac{1}{4}}\ e^{-\frac{1}{4}\,(E-V_o)^2/\xi}\ D_{-3/2}\left(-\frac{(E-V_o)}{\sqrt{\xi}}\right). \tag{4.12}$$

Finally, since $E - V_o$ is large and negative, we use the asymptotic expression for $D_{-3/2}$ valid at large argument,

$$D_p(x) \approx e^{-x^2/4}\ x^p,$$

so that

$$\rho(E) = \frac{f}{2\sqrt{2}}\, \xi\, (V_o - E)^{-3/2}\, e^{-\frac{1}{2}(E - V_o)^2/\xi}. \tag{4.13}$$

This is Kane's central result for the density of states at low energy in the "deep tail region". We see that $\rho(E) \propto e^{-E^2}$ has an exponential tail at low energies. This tail falls off as E^2 which we shall see is valid in practice for long range potentails v only. The existence of the tail in $\rho(E)$ is the new feature characterstic of a disordered system.

Finally, to make contact with Kane's original expressions we introduce the dimensionless energy and density of states variables used by him,

$$x \equiv \frac{(E - V_o)}{\sqrt{2\xi}} \qquad y \equiv \rho(E)\,/\,[2f(2\xi)^{\frac{1}{4}}] \tag{4.14}$$

The $\rho(E)$ in (4.12) is then

$$y = \frac{1}{2^{11/4}}\, e^{-x^2/2}\, D_{-3/2}\,(-\sqrt{2}x) \tag{4.15}$$

which is known as "Kane's function". The $D_{-3/2}$ can be obtained from standard tables[26] and the asymptotic values

$$D_{-3/2}\,(-\sqrt{2}x) \sim \begin{cases} e^{x^2/2} & x^{\frac{1}{2}} \qquad x >> 1 \\ e^{-x^2/2} & x^{-3/2} \qquad x << -1 \end{cases} \tag{4.16}$$

lead to the asymptotic forms

$$y \sim \begin{cases} \sqrt{x} & x >> 1 \\ x^{-3/2}\; e^{-x^2} & x << -1 \end{cases} \tag{4.17}$$

The dimensionless density of states y is sketched in Fig. 3.

The Halperin and Lax Theory

In Kane's semiclassical theory the kinetic energy of the electrons is assumed independent of the potential $V(\vec{r})$, In fact, in the regions of deep narrow potential wells the electrons will be highly localized and the kinetic energy of localization will be large. In regions of shallow or wide potentials the electron kinetic energy will be small. Hence the complete electron energy states, kinetic plus potential, will in general be higher than with the kinetic energy ignored, particularly in regions of deep wells. This is depicted schematically in Fig. 4.

Halperin and Lax[20] set out to include the kinetic energy in a full quantum mechanical calculation of the density of states. In this case the expression (4.1) used by Kane must be abandoned and replaced by

$$\rho(E) = \frac{1}{\Omega} \sum_i < \delta[E - E_i\,(V)] >_V \tag{5.1}$$

where $E_i(V)$ are the "exact" energy states of the electron in a potential V, including the kinetic energy. The average is again given by (4.3) and (4.6). In this case we

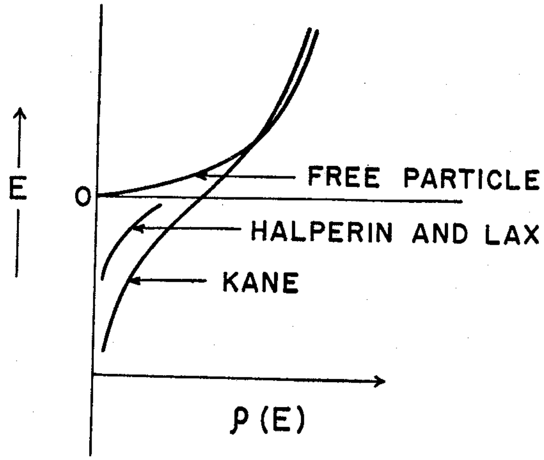


Fig. 3. The dimensionless density of states obtained by Kane.

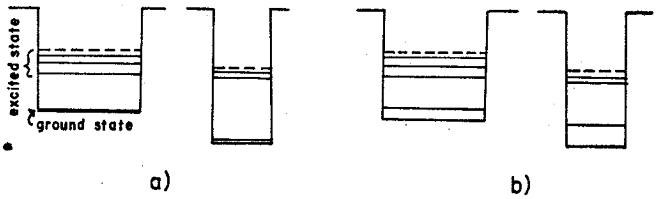


Fig. 4. a) Semiclassical energy levels,
b) Energy levels obtained using quantum theory including the zero point energy.

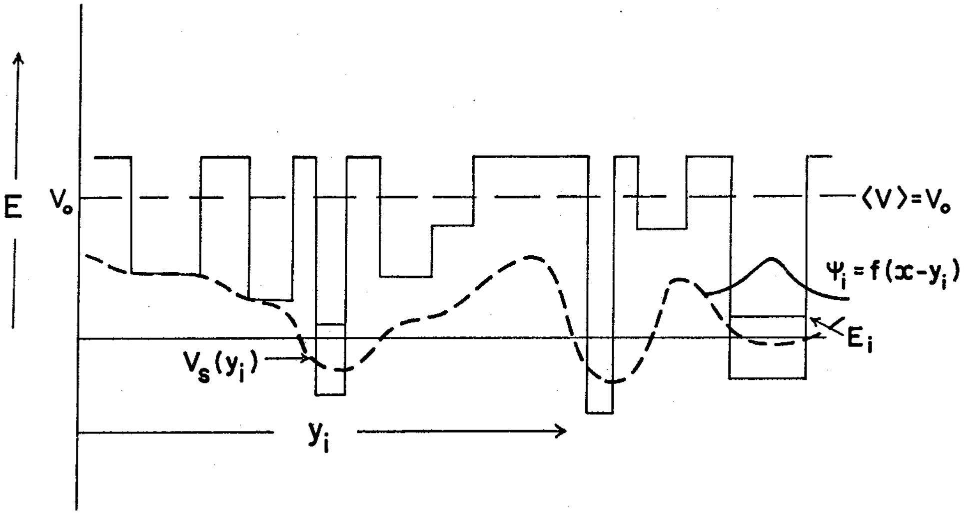


Fig. 5. Potential wells in a disordered solid.

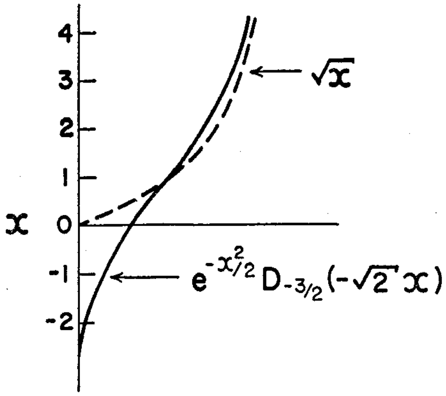


Fig. 6. The Halperin and Lax, Kane and free particle density of states.

use the central limit theorem to justify using the Gaussian potential distribution function P(V).

To evaluate (5.1) Halperin and Lax first emphasize that they are interested in $\rho(E)$ for low E in the band tail region. In this case only the lowest possible energy states found in regions of deep wells in $V(\vec{r})$ need be included in (5.1). Also they include only the ground states of the electrons in these deep wells. Secondly, at low E only a few states E_i will be low enough to satisfy the delta function in (5.1). As noted these will occur in regions of the crystal where the potential $V(\vec{r})$ has a deep well. However, if $V(\vec{r})$ is very deep it will also be narrow so that the kinetic energy will be large. Thus Halperin and Lax assume that for a given E there is an optimum well depth to get the most values of low E_i. They denote the wave function $\psi_i(\vec{r})$ for this optimum well by

$$\psi_i(\vec{r}) = f(\vec{r} - \vec{y}_i)$$

where $\vec{y}_i$ is the centre of $f(\vec{r} - \vec{y}_i)$. A one to one correspondence between the E_i and $\psi_i(\vec{r})$ is assumed and all other well shapes and $\psi_i(\vec{r})$ are ignored (assumed to occur much less often). The $f(\vec{r} - \vec{y}_i)$ is assumed real and normalized. Since the Hamiltonian of the disordered solid is given by

$$H = T + V(\vec{r}),$$

where

$$T = -\frac{\hbar^2}{2m^*}\nabla^2 + V_o$$

includes the mean value V_o of the random potential characterized by (2.1), (2.2) and (2.3), the energy corresponding to $f(\vec{r} - \vec{y}_i)$ is

$$\begin{aligned} E(\vec{y}_i) &= \int f(\vec{r} - \vec{y}_i)\left[-\frac{\hbar^2}{2m^*}\nabla^2 f(\vec{r} - \vec{y}_i)\right]d\vec{r} + V_o \\ &\quad + \int f^2(\vec{r} - \vec{y}_i)\, V(\vec{r})\, d\vec{r} \\ &= T_s + V_o + V_s(\vec{y}_i) \equiv \theta + V_s(\vec{y}_i). \end{aligned} \tag{5.2}$$

Here only the averaged potential $V_s(\vec{y}_i)$ depends on $\vec{y}_i$.

With the assumption that all E_i are given by the optimum $E(\vec{y}_i)$ we have

$$E_i \simeq E(\vec{y}_i) = \theta + V_s(\vec{y}_i) \tag{5.3}$$

and

$$\rho(E) = \frac{1}{\Omega}\sum_i <\delta[E - (\theta + V_s(\vec{y}_i))]> \tag{5.4}$$

Note that this density of states is effectively the same as used by Kane except that the kinetic energy θ corresponding to the smoothed $V_s(\vec{y}_i)$ is included and must be calculated for each $V_s(\vec{y}_i)$. The form of the smoothed potential is shown schematically in Fig. 5.

At this point we do not know the functions $f(\vec{y}_i)$. However since the $E(\vec{y}_i)$ are intended to represent ground states E_i we can use a variational principle to find

$f(\vec{y}_i)$. That is $E(\vec{y}_i)$ will always lie above E_i, and the best fit $f(\vec{y}_i)$ will make $E(\vec{y}_i)$ closest to E_i. (Also since the $E(\vec{y}_i)$ always lie above the true E_i the $\rho(E)$ calculated using the $E(\vec{y}_i)$ will always be too small at low E. Hence we could maximize $\rho(E)$ to find $f(\vec{y}_i)$.) In this variation $\vec{y}_i$ is treated as a variational parameter. Hence the optimum values of $\vec{y}_i$ occur when $\nabla E(\vec{y}_i) = 0$ or, since only $V_s(\vec{y}_i) >$ in (5.2) depends on $\vec{y}_i$, then

$$\nabla V_s(\vec{y}_i) = 0.$$

There are many $\vec{y}_i$ which satisfy this condition and to deal with this we insert a Dirac delta function in (5.4) so that

$$\rho(E) = \int \frac{d\vec{y}}{\Omega} < \sum_i \delta(\vec{y} - \vec{y}_i)\, \delta\,[E - (\theta + V_s(\vec{y})]>_V \tag{5.5}$$

After averaging, $\rho(E)$ is not a function of $\vec{y}$, or

$$\rho(E) = <\delta(\vec{y} - \vec{y}_i)\ \delta\ [E - (\theta + V_s(\vec{y}))]>_V \tag{5.6}$$

If we transform from the variable $\vec{y}$ to $\nabla V_s(\vec{y})$ by writing

$$\sum_i \delta(\vec{y} - \vec{y}_i) = \delta(\nabla V_s(\vec{y}))\,|\det\ \nabla\nabla V_s(\vec{y})|$$

we have

$$\rho(E) = <\delta[E - (\theta + V_s(\vec{y}))]\ \delta[\nabla V_s(\vec{y})]\,|\det \nabla\nabla\ V_s(\vec{y})|>_V \tag{5.7}$$

This expression for $\rho(E)$ is expressed entirely in terms of $V_s(\vec{y})$. Halperin and Lax then replace V by $V_s(\vec{y})$ in the averging and by a sophisicated analysis of Gaussian averaging obtain

$$\rho(E) = \frac{\sigma_1\sigma_2\sigma_3\ (\theta - E)^3}{(2\pi)^2\ \xi^2\ \sigma_o^7}\ \exp\left[-\frac{(\theta - E)^2}{2\xi\sigma_o^2}\right] \tag{5.8}$$

Here

$$\sigma_o^2 = \int f^2(\vec{r})\ \ f^2(\vec{r})\ \ W(\vec{r} - \vec{r}')\ d\vec{r}\ d\vec{r}'$$

where $W(\vec{r} - \vec{r}')$ is the correlation function of the potential given by (2.4). Note that from (2.5) $nW(o) = \xi$. The σ_1, σ_2 and σ_3 are the diagonal elements of $\nabla\nabla V_s(\vec{y})$.

To find the optimum wave function f, Halperin and Lax maximize $\rho(E)$. Since $\rho(E)$ is dominated by the exponent they approximate this by minimizing the exponent,

$$\frac{\partial}{\partial f}\left[\frac{\theta - E}{\sigma_o}\right]^2 = 0 \tag{5.9}$$

This leads to a Hartree-Fock like equation for f

$$Tf(\vec{r}) - \mu f(\vec{r}) \int f^2(\vec{r}')\ W(\vec{r} - \vec{r}')\ d\vec{r}' = E\, f(\vec{r}) \tag{5.10}$$

which must be solved numerically. Since E is given, the parameter μ corresponds to the eigenvalue in (5.10) and must be determined in the solution of (5.10). Once f is obtained the σ_o, its derivatives σ_1, σ_2, σ_3 and the mean kinetic energy θ can be calculated numerically for substitution in (5.8).

Halperin and Lax used the screened Coulomb potential (2.6) in the explicit calculation of $\rho(E)$. The result, expressed in terms of the dimensionless energy $\nu = -(E - V_o)/E_Q$ where $E_Q = \hbar^2 k^2/2m^*$ is the energy associated with the screened Coulomb potential, is

$$\rho(E) = \frac{Q^3}{E_Q(\xi')^2}\, a(\nu)\, e^{-\frac{b(\nu)}{2\xi'}}. \tag{5.11}$$

Here

$$\xi' \equiv \frac{\xi}{E_Q^2} = \frac{n\ 8\pi m^{*2} Z^2 e^4}{\hbar^4 Q^5 \varepsilon^2} \tag{5.12}$$

is the variance expressed in units of E_Q and $a(\nu)$ and $b(\nu)$ are "universal dimensionless functions" that Halperin and Lax calculated numerically.

The Halperin and Lax $\rho(E)$ in (5.11) is sketched in Fig. 3. We see there that (5.11) is much smaller than the Kane value for a given E. This is because including the kinetic energy increases the electron energy states so there are fewer low energy states in the" band tail" region. Hence the density of states in the low energy "band tail" region is reduced. Detailed values of the Halperin and Lax $\rho(E)$ are shown in Fig. 7–10 for different values of ξ'.

From (5.11) we see that $\rho(E)$ also decays exponentially in a quantum treatment. The exponent of $b(\nu)$ in $\rho(E)$ is

$$n(\nu) = \frac{\partial \ln b(\nu)}{\partial \ln \nu} \tag{5.13}$$

Halperin and Lax found that n varies from between $\frac{1}{2}$ for short range potential (Q^{-1} small) to 2 for long range potentials (Q^{-1} large). The last value agrees with the Kane theory result which is valid for long range potentials only. The Halperin and Lax density of states agreed much better with experiment, particularly $n(\nu)$. However, an overall adjustment of 1.5 to $\rho(E)$ is apparently needed to get agreement for the optical absorption coefficient[1].

The Sa-yakanit Theory

Although the Halperin and Lax $\rho(E)$ agreed well with experiment in the low energy band tail region and is a substantial improvement over Kane's $\rho(E)$, it has two limitations. Firstly, it requires numerical solution. Secondly, it cannot be extended to higher energy E. For these reasons Sa-yakanit[21] developed a new theory based on the Feynman formulation of quantum mechanics. The Feynman formulation is useful since, although a full quantum theory, it expresses the electron propagation as a sum of classical like paths. This is especially useful in disordered systems for then the density of states can be calculated in much the same way as in the Kane theory. Once the Feynman method is mastered this is much simpler than the Schrödinger picture of quantum mechanics for disordered systems. The Feynman path integral approach was first applied to disordered systems by Edwards[27,28] and has subsequently been explored by others[29-33]. However, Sa-yakanit[21] succeeded in evaluating the path integrals explicitly and obtained an expression for $\rho(E)$ valid at all energies E. In the low energy limit the $\rho(E)$ reduces to a relatively simple analytic expression. At high E it reduces to the usual free electron value (3.4)

The path integral formulation begins with the full expression (5.1) for $\rho(E)$,

$$\rho(E) = \frac{1}{\Omega}\sum_i <\delta(E - E_i(V))>_V . \tag{6.1}$$

Next the retarded propagator $G(\vec{r}_2, \vec{r}_1, t)$ is introduced which describes the propagation of an electron from point $\vec{r}_1$, to $\vec{r}_2$. (This $G(\vec{r}_2, \vec{r}_1, t)$ is $(-i\hbar)$ times the usual retarded Green function.) The $\sum_i \delta(E - E_i)$ can be expressed in terms of the Diagonal element $(\vec{r}_1 = \vec{r}_2)$ of G giving

$$\rho(E) = \frac{1}{\pi\hbar} \mathrm{Re}\int_0^\infty dt\, e^{iEt/\hbar} <G(\vec{r}_1, \vec{r}_1, t)>_V \tag{6.2}$$

The G is then written as a path integral over all the possible paths between $\vec{r}_1$ and $\vec{r}_2$,

$$G(\vec{r}_1, \vec{r}_2, t) = \int D(\vec{r}(\tau))\, e^{i/\hbar\, S_\ell} \tag{6.3}$$

where S_ℓ is the action

$$S_\ell = \int_0^t d\tau \left[\frac{m^*}{2}\dot{\vec{r}}^2(\tau) - V(\vec{r}(\tau))\right]$$

Here $V(\vec{r}(\tau))$ is the potential given by (2.1). The average $< >_V$ over G can be performed exactly as in the Kane theory, giving

$$\begin{aligned}\overline{G} \equiv <G(\vec{r}_2, \vec{r}_1, t)>_V &= \int\frac{d\vec{R}_1}{\Omega} \cdots \int\frac{d\vec{R}_N}{\Omega} G(\vec{r}_2, \vec{r}_1, t)\\ &= \int D(\vec{r}(\tau))\, e^{i/\hbar\, S}\end{aligned} \tag{6.4}$$

where

$$S = \int_0^t d\tau\left\{\frac{m^*}{2}\dot{\vec{r}}^2(\tau) - V_o + \frac{i}{2\hbar}\int_0^t d\tau'\, W(\vec{r}(\tau) - \vec{r}(\tau'))\right\} \tag{6.5}$$

Note the similarity between the exponent of P(V) in (4.5) and this averaged S. Essentially in S the kinetic energy is included and ξ is replaced by $W(\vec{r} - \vec{r}')$, the correlation function of v.

To proceed in calculating $\overline{G}$, the full action S is modeled by a non-local harmonic "trial" action

$$S_o = \int d\tau\left\{\frac{m^*}{2}\dot{\vec{r}}^2(\tau) - V_o - \frac{\omega^2}{2t}\int_0^t d\tau'\, \left|\vec{r}(\tau) - \vec{r}'(\tau')\right|^2\right\} \tag{6.6}$$

Essentially $W(\vec{r} - \vec{r})$ is modeled by a single harmonic well. With S replaced by S_o, $\overline{G}$ in (6.4) can be evaluated exactly. In S_o, ω^2 measures the steepness of the harmonic well and ω^2 is treated as a variational parameter. With S replaced by

S_o the resulting $\bar{G}$ constitutes the zero order approximation $\bar{G}_o$ to $\bar{G}$. The full $\bar{G}$ can also be re-arranged as

$$\bar{G} = \int D(\vec{r}(\tau))\ e^{i/\hbar\, S} = \int D\ e^{i/\hbar\, S_o} \frac{\int D\ e^{i/\hbar\,[S_o + (S - S_o)]}}{\int D\ e^{i/\hbar\, S_o}} \tag{6.7}$$

or in short form

$$\bar{G} = \bar{G}_o < e^{i/\hbar\,(S - S_o)} >_o \tag{6.8}$$

where $< >_o$ denotes the average with respect to the trial action. The $< >_o$ may be expanded in cumulants and keeping only the first order cumulant we obtain

$$\bar{G}_1 = \bar{G}_o \exp\left[\frac{i}{\hbar} < S - S_o >\right] \tag{6.9}$$

For a screened Coulomb $v(\vec{r})$ for which $W(\vec{r} - \vec{r}\,')$ is given by (2.8) the diagonal part of $\bar{G}_1$ may also be evaluated exactly and gives the density of states, when substituted into (6.2), of

$$\begin{aligned} \rho_1(E) &= \frac{1}{\pi\hbar} \mathrm{Re} \int_0^\infty dt \left[\left(\frac{m^*}{2\pi i \hbar t}\right)^{\frac{1}{2}} \left(\frac{\omega t}{2\sin(\frac{1}{2}\omega t)}\right)\right]^3 \\ &x \exp\left[-\frac{i}{\hbar}(V_o - E)\,t - \frac{1}{2\hbar^2}\,\xi\, \frac{Qt}{\sqrt{\pi}} \int_0^t dx \int_0^\infty dy\ y e^{-Q^2 y} j\,(x, y)^{-3/2} \right. \\ &\left. + \frac{3}{2}\left(\frac{\omega t}{2} \cot \frac{\omega t}{2} - 1\right)\right] \end{aligned} \tag{6.10}$$

where

$$j(x, y) = \left[y + \frac{\hbar i}{m^*\omega}\left(\sin\frac{\omega x}{2} \sin\frac{\omega(t - x)}{2} \Big/ \sin\frac{\omega t}{2}\right]\right.$$

Here the term in the square bracket is $G_o(0, 0, t)$ while the exponential term is the first cumulant correction, aside from $e^{iEt/\hbar}$.

To obtain the limit of $\rho(E)$ valid in the tail region where E is large and negative we first take the $t \to \infty$ limit of the integrand in (6.10). This means only in the ground states[22], the lowest energy states, will be retained in $\rho_1(E)$. The integrals (6.10) can then be performed exactly and, in the reduced units $\nu = -(E - V_o)/E_Q$, the result is

$$\rho_1(\nu, z) = \frac{Q^3}{E_Q\ \xi'^{5/4}} \frac{a(\nu, z)}{b(\nu, z)^{3/4}}\, e^{-\frac{b(\nu, z)}{4\xi'}} \cdot D_{3/2}\left(\sqrt{\frac{b(\nu, z)}{\xi'}}\right) \tag{6.11}$$

Here $E_Q = \hbar^2 Q^2/2m^*$ is again, as in the Halperin and Lax result (5.11), the energy associated with the impurity potential and all energies are expressed in units of E_Q. For example, $\nu = (V_o - E)/E_Q$ is, as in (5.11), the electron energy measured away from the mean potential V_o in units of E_Q and $z = (2E_Q/\hbar\omega)^{\frac{1}{2}}$ is a convenient reduced variational parameter, replacing ω. In the harmonic model the kinetic (zero point) energy of electron localization is just 3/4 $\hbar\omega$ and in reduced units is $T = (3/4)\hbar\omega/E_Q = 3/2\ z^{-2}$. The $a(\nu, z)$ and $b(\nu, z)$ are again the "universal", dimensionless functions but now we have relatively simple analytic expressions for them,

$$a(\nu, z) = (T + \nu)^{3/2} \ / \ 8\pi\sqrt{2}\ z^{6} \exp\left(\frac{z^2}{2}\right) D^{2}_{-3}(z) \tag{6.12}$$

$$b(\nu, z) = (T + \nu)^{2} \sqrt{\pi} \ / \ 2\sqrt{2} \exp\left(\frac{z^2}{4}\right) D_{-3}(z) \tag{6-13}$$

where $D_p(z)$ is the parabolic cylinder function[16].

The subscript l or $\rho_l(E)$ means that the first order cumulant correction for the difference between W and the harmonic model has been evaluated exactly. Higher order cumulants which correspond approximately to the higher order corrections con sidered by Halperin and Lax[17] have been ignored.

In the limit of large $b(\nu, z)/\xi'$ the asymptotic expression for the parabolic cylinder function is

$$D_p(x) = e^{-x^2/4}\ x^{p}\left(1 - \frac{p(p-1}{2}\ \frac{1}{x^2} + \ldots\right) \tag{6.14}$$

If we neglect the term in x^{-2} in (23) we obtain for $\rho_l(\nu, z)$,

$$\rho_l(\nu, z) = \frac{Q^3}{E_Q\,\xi'^2}\ a(\nu, z)\ e^{-\frac{b(\nu, z)}{2\xi'}} \tag{6.15}$$

Now we recover deep tail $\rho_l(\nu, z)$ in exactly the form (5.11) proposed by Halperin and Lax with $a(\nu, z)$ and $b(\nu, z)$ given analytically in (6.12) and (6.13).

We may also obtain the semiclassical limit of $\rho_l(E)$ from the full $\rho_l(E)$ in (6.10). This is obtained by letting t → 0 in the integrand of (6.10) which corresponds to retaining only high electron energy states in $\rho_l(E)$. The integrals in (6.10) can again be performed giving

$$\rho_l^{SC}(E) = \frac{f}{2\sqrt{2}}\ \xi^{\frac{1}{4}}\ e^{-\frac{1}{4}\frac{(E - V_o)^2}{\xi}}\ D_{-3/2}\left(\frac{V_o - E}{\sqrt{\xi}}\right) \tag{6.16}$$

which is the result (4.12) derived by Kane[18]. In the limit $|E - V_o| \rightarrow \infty$ this becomes

$$\rho_l^{SC}(E) = \begin{cases} \dfrac{f}{2\sqrt{2}}\ \xi\,(V_o - E)^{-3/2} e^{-\frac{1}{2}\frac{(E - V_o)^2}{\xi}} & \dfrac{E - V_o}{\sqrt{\xi}} \ll -\ 1 \quad (6.17) \\[2ex] f\sqrt{E - V_o} & \dfrac{E - V_o}{\sqrt{\xi}} \gg 1 \quad (6.18) \end{cases}$$

Here (6.17) is Kane's well known band tail $\rho_l(E)$ while (6.18) is the free electron or parabolic band value valid for positive $E - V_o$ only. Note that (6.16) is independent of the variational parameter. This is because at $t \rightarrow 0$ only the free particle $\overline{G}_0$ survives in (6.10) and the semiclassical $\rho_1(E)$ is independent of the harmonic model action selected here. It is for this reason that (6.16) agrees exactly with Kane's density of states.

The density of states $\rho_1(\nu, z)$ of (6.15) in the band tail region (with the universal dimensionless functions $a(\nu, z)$ and $b(\nu, z)$ given by (6.12) and (6.13) clearly depends on the variational parameter z. The value of z determines the curvature of the optimum harmonic well which models $W(\vec{r} - \vec{r}')$. To evaluate $\rho_1(\nu, z)$ explicitly we need some variational principle to determine this optimum curvature z.

In 1975 Lloyd and Best[34] showed that the density of states $\rho_1(E)$ at energy E should maximize the pressure

$$\rho(E, z) = \int_{-\infty}^{E} dE' \int_{-\infty}^{E'} dE'' \rho(E'', z) \qquad (6.19)$$

of a hypothetical free Fermion system. This may be used here to determine the free parameter z in a band tail expression for $\rho(E, z)$, since values of $\rho(E'', z)$ up to energy E only are needed. To simplify (6.19) we do an integration by parts,

$$P(E, z) = E' \int_{-\infty}^{E'} dE'' \rho(E'', z) \Big|_{-\infty}^{E} - \int_{-\infty}^{E} E' \rho(E', z) dE' \qquad (6.20)$$

and use $\rho(-\infty, z) = 0$ to writes (6.20) as

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

In terms of the reduced energy $\nu = (V_0 - E)/E_Q$, this is

$$P(\nu, z) = - E_Q^2 \int_{\nu}^{\infty} (\nu - \nu') \rho(\nu', z) d\nu'. \qquad (6.21)$$

On substituting (6.15) for $\rho(\nu', z)$ in (6.21) and maximizing $P(\nu, z)$ with respect to z ($dP(\nu, z)/dz = 0$) we obtain the variational equation for z,

$$\int_{\nu}^{\infty} d\nu' (\nu - \nu') a(\nu', z) e^{-b(\nu', z)/2\xi'}$$
$$x \left\{ \left[+ \frac{2D_{-4}(z)}{D_{-3}(z)} - \frac{1}{z} \left(\frac{T}{T + \nu'} + 2 \right) \right] - \frac{b(\nu', z)}{2\xi'} \left[\frac{D_{-4}(z)}{D_{-3}(z)} - \frac{2z^{-3}}{(T + \nu')} \right] \right\} = 0 \qquad (6.22)$$

The $\rho_1(E)$ with z determined from (6.22) is denoted case 1. Since this is a lengthy expression we investigate two approximations. If we determine z by maximizing $\rho_1(E)$ itself, the equation for z is obtained by setting the curly bracket in (6.22) equal to zero. The $\rho_1(E)$ with z determined in this way is denoted as case 2. Finally, since $\rho_1(E)$ will be dominated in the low energy tail region by the exponent, we can follow Halperin and Lax and obtain z by minimizing $b(\nu, z)/2\xi'$. This corresponds to their equation (5.9) used to obtain the optimum wave function f. It is an approximation to maximizing $\rho_1(E)$. Here the equation for z in this case (denoted case 3) is obtained by setting the last square bracket in (6.22) equal to zero. The accuracy of the two approximations (cases 2 and 3) can be tested by comparing with case 1.

The expression (6.15) plus one of the three methods (case 1, case 2 or case 3) for determining z completely determines the density of states $\rho_1(E)$ in the band tail region. The $\rho_1(E)$ obtained in the three cases are shown in Figs. 7–10 for values of the dimensionless fluctuation parameter $\xi' = 50, 5, 0.5, 0.05$. These graphs represent the central results of the Sa-yakanit theory[35].

To discuss the band tail density of states in Figs. 7–10, we note first that case 3, with z determined by minimizing the exponent only of $\rho_1(E)$, agrees numerically with Halperin and Lax's $\rho_1(E)$, who also minimized the exponent of $\rho_1(E)$. This provides an excellent point of contact with previous work. For this reason, case 3 is denoted the Halperin and Lax limit in Figs. 7–10.

Next we note that case 1 and 2 are almost identical. This means that $\rho_1(E)$ with z obtained by minimizing $\rho_1(E)$ itself is almost identical to $\rho_1(E)$ obtained using the rigorous Lloyd-Best variational principle. It is only case 1 with z determined using the Lloyd-Best variational principle that has a rigorous foundation. However, case 2 is clearly a good approximation and we denote cases 1 and 2 as the present theory. The case 3, however, is not such a good approximation and particularly shows an unphysical down turn in $\rho_1(E)$ in the range $\nu \sim 0$ to 5.

The band tail limit of $\rho_1(E)$ in (6.15) is valid only for low (negative) energy E in the band tail region (large $\nu = -(E - V_o)/E_Q$). Since $\rho_1(E)$ crosses the Kane theory, $\rho^{SC}(E)$, which is valid at higher E, an interpolation scheme is suggested. At low E we should use the band tail limit $\rho_1(E)$ given by (6.15) with z determined from (6.22) up to the point where $\rho_1(E)$ crosses $\rho^{SC}(E)$. Thereafter higher energy use Kane's $\rho_1^{SC}(E)$ in (6.17). This provides a density of states over the whole energy range. An examination of corrections to $\rho_1(E)$ due to excited state contributions and to use of the asymptotic expansion (6.14) shows that the present band tail $\rho_1(E)$ is exact within 5% for low E up to the point it crosses the $\rho^{SC}(E)$[35].

In future work it would be interesting to check this interpolation scheme by evaluating the full density of states in (6.10) and by evaluating optical properties of heavily doped semi-conductors, such as the optical absorption coefficient, for comparison with experiment.

Conclusions

In this article we have reviewed the theories and calculations of the density of states of electrons in disordered systems. The specific example considered was disorder created by impurities substituted at random in a solid. The electrons interact with the impurities via the screened Coulomb potential (2.6). For this case we find the band tail $\rho_1(E)$ derived by Sa-yakanit using the Feynman Path Integral

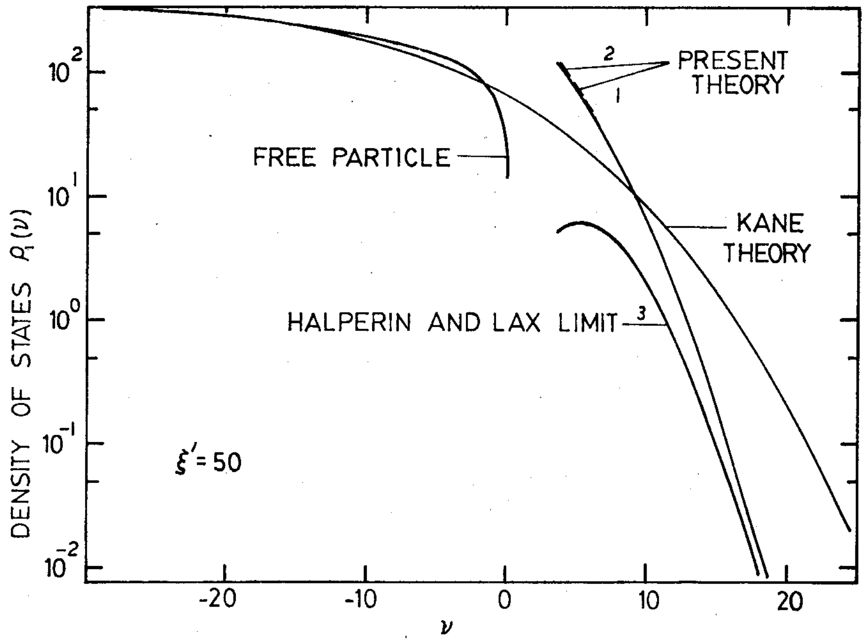


Fig. 7. The density of states

$$\rho_1(\nu, z) = \frac{Q^3}{E_Q \xi'^2} a(\nu, z)\, e^{-\frac{b(\nu, z)}{2\xi'}}$$

in units of $(Q^3/E_Q\,\xi'^2)$ for $\xi' = 8\pi m^{*2} Z^2 e^4 n / Q^5 \hbar^4 \varepsilon_0^2 = 50$.

THE PRESENT THEORY is the band-tail value $\rho_1(E)$ with the variational parameter z determined by (Case 1) the Lloyd-Best variational principle Eq. (6.22), and by (Case 2) maximizing $\rho_1(E)$ only. Case 1 and Case 2 are indistinguishable at $\xi' = 50$. The HALPERIN AND LAX LIMIT IS $\rho_1(E)$ with z determined by minimizing the exponent in $\rho_1(E)$ (Case 3). The KANE AND FREE PARTICLE values are Kane's semiclassical result (6.17) and (6.18) respectively.

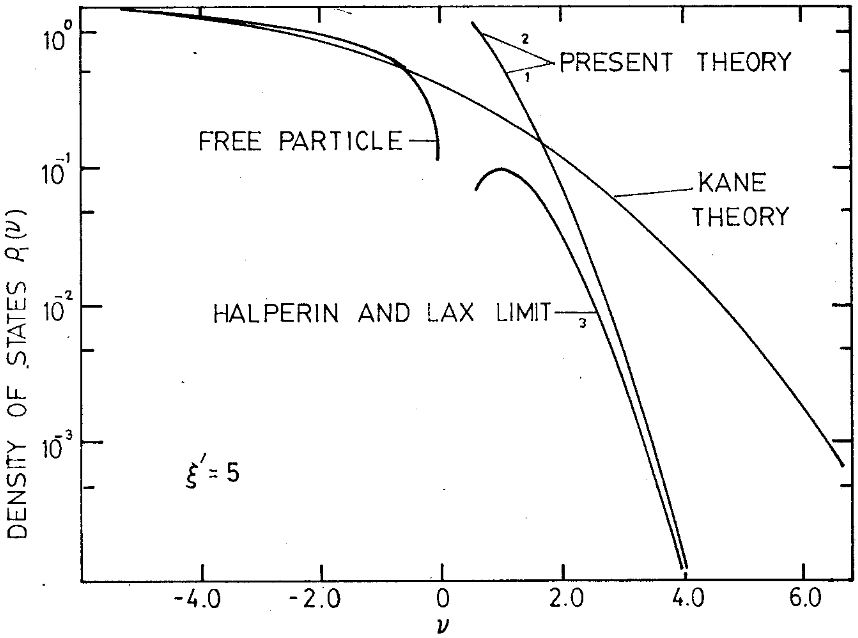


Fig. 8. As Fig. 7 for $\xi' = 5$.

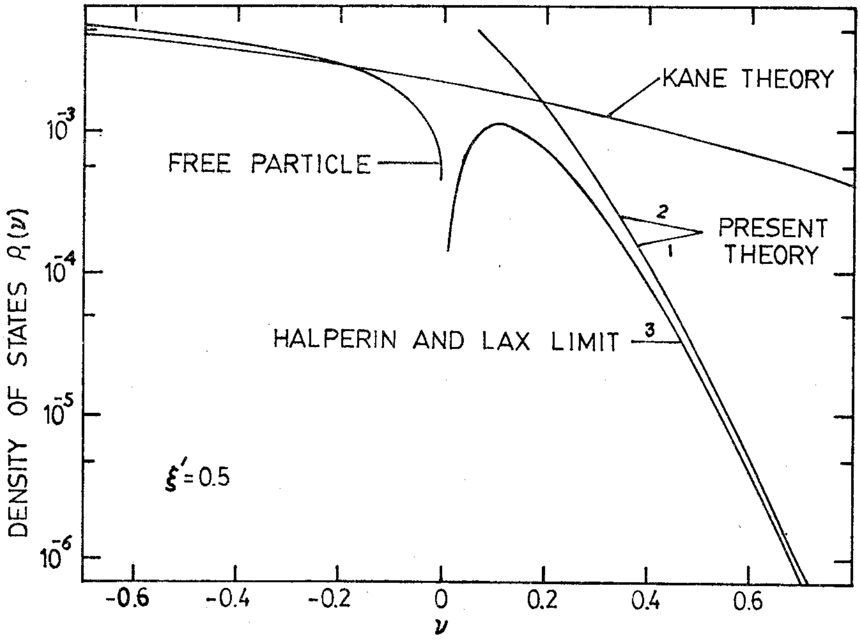


Fig. 9. As Fig. 7 for $\xi' = 0.5$.

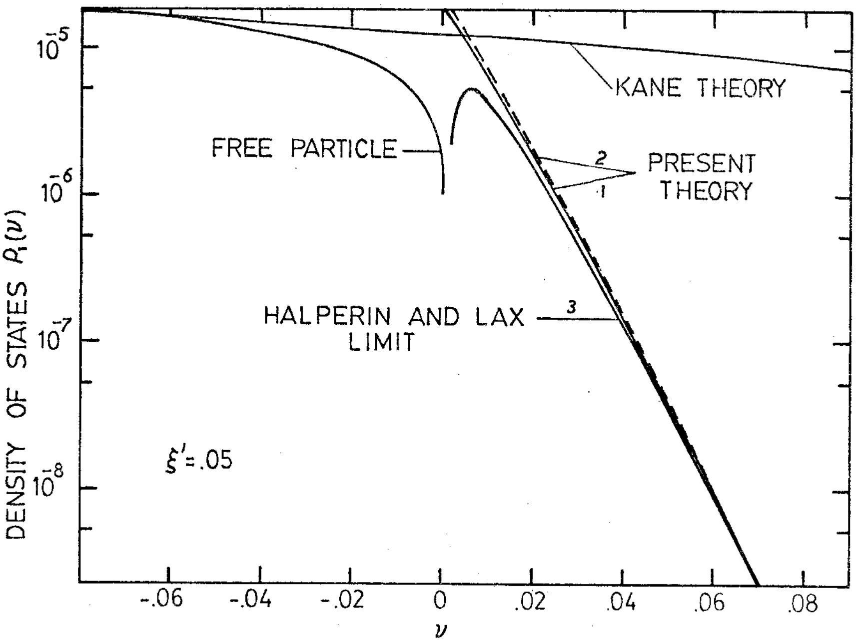


Fig. 10. As Fig. 7 for $\xi' = 0.05$.

method and the Lloyd-Best variational principle a substantial improvement over the original work of Halperin and Lax and of Kane. This band tail $\rho_1(E)$ and the higher energy semi-classical Kane result can be used to obtain $\rho(E)$ at all energies.

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บทคัดย่อ

บทความนี้กล่าวถึงอิเลกตรอนเคลื่อนที่ในสิ่งแวดล้อมที่ไร้ระเบียบ อิเลกตรอนเหล่านี้เป็นอิเลกตรอนอิสระที่ปราศจากอันตรกิริยาซึ่งกันและกัน สิ่งแวดล้อมที่ไร้ระเบียบนี้อาจจะเกิดจากการเรียงตัวของอิออนในของแข็งอย่างไม่มีระเบียบ หรือเกิดจากตัวอสุทธิแทนที่อะตอมในของแข็งอย่างไร้ระเบียบ บทความนี้กล่าวถึงเฉพาะความหนาแน่นของสถานะของระบบที่ไร้ระเบียบ ตัวอย่างที่นำมาพิจารณา คือ สารกึ่งตัวที่ถูกโดปอย่างหนัก การเสนอจะมุ่งกล่าวถึงวิธีการต่าง ๆ ที่ใช้ในการคำนวณความหนาแน่นของสถาณะบริเวณส่วนสำคัญของแถบพลังงานและส่วนหางของแถบพลังงาน วิธีการที่กล่าวถึงเป็นพิเศษ คือวิธีที่เสนอโดย วิรุฬห์ สายคณิต ท้ายสุดได้เสนอวิธีการเชื่อมโยงแถบพลังงานบริเวณส่วนสูงและส่วนต่ำเข้าด้วยกัน จนสามารถคำนวณหาความหนาแน่นของสถานะได้ตลอดช่วงพลังงาน