ELECTRONIC PROPERTIES OF DISORDERED SYSTEMS

By

Shama Afroz

Under the Guidance of

Prof. Biplab Ganguli

Department Of Physics

National Institute of Technology, Rourkela

CERTIFICATE

This is to certify that the project thesis entitled, ELECTRONIC PROPERTIES OF DISORDERED SYSTEMS being submitted by Shama Afroz in partial fulfilments for the requirements of the one-year project course PH 592 of M.Sc. Degree in Physics at National Institute of Technology, Rourkela has been carried out under my supervision and guidance.

The result incorporated in the thesis has been produced by developing her own computer code.

Prof. Biplab Ganguli

Dept. of Physics

National Institute of Technology

Rourkela-769008

ACKNOWLEDGEMENT

I would like to acknowledge my guide Prof. Biplab Ganguli for his help and guidance in the completion of my one-year project and also for his enormous motivation and encouragement. I am also very much thankful to PhD scholars of computational physics lab whose encouragement and support helped me to complete my project.

ABSTRACT

In this thesis we have calculated the density of state for an ordered and disordered model system using the Green's function technique and the recursion method. We have considered a model of binary disordered system. The recursion parameters are calculated by transforming the Hamiltonian into a tridiagonal Hamiltonian. The infinite continued fraction size is truncated after 8th step.

Contents

1 INTRODUCTION TO DISORDERED SYSTEM

1.1 ORDER AND DISORDER [1]

Order and disorder are rather complex concepts with various and sometimes contrary exceptions and shades and this makes it somewhat difficult to give them a generally valid definition. The dictionary defines order as the arrangement of objects in position, or of events in time or, more generally, the manner in which one thing succeeds another .

Rather than the general definition of order we are more interested in a series of criteria that can be used in Physics and in particular in analysing the structure of condensed matter, and that can possibly include objects in Nature and in art that give the observer the feeling of order.

First of all it is common to consider order and regularity as equivalent, namely that they belong to the same category and refer to objects in that category. In actual fact the idea that something is regular is geometric and is based on the idea that one or more geometric elements are repeated, whereas order is probabilistic and hinges on the idea of singleness in that a given macroscopic structure corresponds to a single microscopic configuration. Structures may be ordered but not necessarily regular.

An example is Eschers covering of a flat surface in his xylography called Path of Life II another example is given by the proteins which have a single configuration (ordered) with an irregular structure.

Crystals are ordered and regular since they can be obtained by periodical translation of an elementary (geometric) cell in space. Excluding the trivial case of a vacuum, crystals constitute the highest degree of three-dimensional order that can be achieved. In a crystal an assembly of innumerable particles (atoms or molecules) is packed in a regular structure along lines in space and on planes in a geometric lattice in order to obtain the highest density possible. With exception to vibrational motion the atoms have a fixed position and are temporarily invariable. As such, from a rheological point of view a crystal is a solid. Crystal structures do not change when they undergo lattice translations, rotations about axes of different order or reflections in various planes and combinations of reflections and rotations. The concept of disorder is intuitive and, to some extent, primitive. As such, since it is closely connected to the concept of casual it may be defined independently only in a specific context. It is easier to define disorder as a state of absence of, or departure from, the condition of order. The immediate consequence of this approach is that we have to give a better definition of perfect order. From this we have to be able to recognise how much more or less departure from the condition of order is achievable.

1.2 TYPES OF DISORDERED SYSTEMS

In general, there are various types of disorderedness in a system. But the most widespread sort of disorder is short-range disorder due to localised defects (point and line defects) such as vacancies, di-vacancies, interstitials, substitutional impurity atoms, F centres, dislocations. Apart from the atoms in the core of the defect, the first neighbour atoms of the defect, too, are not to be found on their ideal lattice sites. Many properties of materials with a technological interest are the outcome of the presence and mutual interaction of these kinds of imperfection.

At a temperature T = 0 K, in those systems with chemical or orientational disorder, both molecular and involving atomic spins, perfect order sets, whereas disorder is prevalent at temperatures above the pertinent critical temperature, T_c.

Disorderedness in a system can be broadly classified into two categories

1. Cellular disorder [1]

2. Topological disorder [1]

CELLULAR DISORDER

Cellular disorder is the kind of disorder can be described with reference to a particle placed on an ideal lattice site of a solid. The properties involved are intrinsic, as in the case of spin direction and chemical composition, or pertain to the presence or absence of defects at low or moderate concentration or, as in the case of thermal motion.

TOPOLOGICAL DISORDER

Unlike a crystal with some degree of disorder, a microscopic sample of an amorphous liquid, or a solid with no defined crystal lattice, is characterized by topological disorder. This is the outcome of a relevant property in a liquid, such as the absence of translational atomic motion. In these kinds of system we must consider the distribution of the relative positions of the molecules.

Furthermore, if the material is a mixture or an alloy of X and Y then it will also have chemical disorder. The preferential attraction of an X atom for atoms (Y) of the other kind leads to the formation of structural units characterised by well defined geometrical shapes, sizes and structures (often based on tetrahedral packing) with partial Chemical Short Range Order. In the very same way, topologically disordered structures may display complete order regarding the spin orientation, as can be seen in saturated amorphous ferromagnetic materials.

1.3 BINARY ALLOYS

A homogeneous mixture or solid solution of two metals is called as BINARY AL-LOY. It refers to a disordered system. Here the disorderedness is due to the chemical disorder. Hence, it is under the cellular disorderedness.

Effective cluster interactions (ECI's) are calculated from electronic tight-binding Hamiltonians of random binary systems.

The main intention here is to predict the density of state (DOS) of the Binary alloy(disordered system). Again in order to calculate the Density Of State, we need to find out the Green's function and also we should have knowledge about Recursion method to calculate density of state (DOS) of binary.

First We will discuss about Green's Function and after that we will study something about Recursion method.

2   GREEN'S FUNCTION [2]

2.1   DEFINITION AND BASIC PROPERTIES

Green's function can be defined as solution of inhomogeneous differential equation of the type

$$[Z - L(r)]G(r, r'; z) = \delta(r - r') \tag{1}$$

Z is a complex variable with $\lambda \equiv Re[Z]$
and $S \equiv Im[Z]$
$L(r)$ is a time independent, linear, hermitian differential operator that possesses a complete set of eigenvalue functions $\Phi_n(r)$, i.e.

$$L(r) = \lambda \Phi_n(r) \tag{2}$$

Φ_n can be considered as orthonormal i.e.

$$\int \Phi_n^*(r)\Phi_m(r)dr = \delta_{nm} \tag{3}$$

Again completeness of a set $\Phi_n(r)$ i.e.

$$\Sigma \Phi_n(r)\Phi_n^*(r') = \delta(r - r') \tag{4}$$

Any well behaved function ψ can be written as a linear combination of Φ_ns i.e.

$$\psi(r) = \Sigma c_n \Phi_n(r) \tag{5}$$

If $|\Phi_n\rangle$is the complete orthonormal set of eigenfunctions of L(r) and λ_n is the set of the corresponding eigenvalues, then we can have,

$$G = (z - L)^{-1} = (\Sigma |\Phi_n\rangle\langle\Phi_n|)/(z - \lambda_n) \tag{6}$$

7

Where,$z \neq \lambda_n$ Here L(r) is the time independent differential operator.

From equation (1) we can conclude that, the Green's function can be uniquely defined if and only if $z \neq \lambda_n$. If z coincides with any of the discrete eigenvalues of L(r), then the Green's function value G (z) does not exist. From the principles of complex variables we can say from equation (1) that, G (z) has simple poles at the position of the discrete eigenvalues or otherwise we can say that, the poles of G (z) give the discrete eigenvalues of L. if $z = \lambda_n$,where λ_n belongs to the continuous spectrum of L and G (z) is not well defined. So in this case we can choose the limiting procedure in order to find out the value of green's function. Since, we know that G(λ) cannot have exact value, so we can write,

$$\lim_{\delta \to 0} G(\lambda \pm i\delta) \tag{7}$$

Here the side limits, that is the values of G for $\delta \to 0^+$
are different from each other. Thus, this type of continuous spectrum produces a branch cut in G(z) along part(s) of the real z-axis.

For λ belonging to such a spectrum we define two Green's functions as follows:

$$G^+(\lambda) \equiv \lim_{\delta \to 0^+} G(\lambda + i\delta) \tag{8}$$

$$G^-(\lambda) \equiv \lim_{\delta \to 0^+} G(\lambda - i\delta) \tag{9}$$

For infinite disordered systems, part of the continuous spectrum may give rise to the so-called natural boundary, i.e., a singular line. Because L is hermitian, all its eigenvalues are real; hence, the singularities of G(z) are on the real z-axis.

with similar definitions for the corresponding operators $G^+(\lambda)$, $G^-(\lambda)$,one can easily say that

$$G^-(\lambda) = [G^+(\lambda)]^* \tag{10}$$

which suggests that one side limit is complex conjugate of the other one. From this we can explain that both the side limits have the same real values but opposite imaginary values.

$$Re[G^-(\lambda)] = Re[G^+(\lambda)] \tag{11}$$

But

$$Im[G^-(\lambda)] = -Im[G^+(\lambda)] \tag{12}$$

2.2   TYPES OF GREEN'S FUNCTION

Basically, Green's function is divided into two categories

1. Time independent

2. Time dependent

TIME INDEPENDENT GREEN'S FUNCTION

Time independent Green's function can be explained as

$$[Z - L(r)]G(r, r'; z) = \delta(r - r') \tag{13}$$

Z is a complex variable with $\lambda \equiv Re[Z]$
and $S \equiv Im[Z]$
$L(r)$ is a time independent, linear, hermitian differential operator.

TIME DEPENDENT GREEN'S FUNCTION

For Time dependent Green's function, two cases arises

1. First order time dependent Green's function

2. Second order time dependent Green's function

The Green's function $G(r, r', t - t')$ for the first order case is defined as the solution of

$$[\frac{i}{c} \frac{\partial}{\partial t} - L(r)]g(r, r', t - t') = (r - r')(t - t') \tag{14}$$

Here, L(r) is linear hermitian operator. The Green's function$G(r, r', t - t')$ for the second order case is defined as the solution of

$$[-\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - L(r)]g(r, r', t - t') = (r - r')(t - t') \tag{15}$$

Here, we will emphasize on Time independent Green's function.

2.3   USE OF TIME INDEPENDENT GREEN'S FUNCTION

Obtain information about the homogeneous equation corresponding to the equation (1), i.e., about the eigenvalues and eigenfunctions of L. Thus the position of the poles of G(z) give the discrete eigenvalues of L, and the residues at these poles provide information about the corresponding eigenfunctions. The branch cuts (or the natural boundaries, if any) give the location of the continuous spectrum, and the discontinuity across the branch cut gives the density of states

$$N(\lambda) = \mp\frac{1}{\pi}ImG^{\pm}(\lambda) \tag{16}$$

Hence, the most common and useful application of green's function is that after finding the value of green's function of a particular system, then we can easily find out the density of states of that particular system.Again from density of state we can predict the electronic behaviour of that particular system.

2.4   PHYSICAL SIGNIFICANCES OF G

The singularities of G(z) vs. z are on the real z-axis. They can be used as follows:

1. The position of the poles of G(z) coincide with the discrete eigenenergies corresponding to H, and vice versa.

2. The residue at each pole E_n of $G(r, r'; z)$ equals $\Sigma \phi_i(r)\phi_i^*(r')$, where the summation runs over the f_n degenerate eigenstates corresponding to the discrete eigenenergy E_n.

3. The degeneracy f_n can be found by integrating the residue (Res) of the diagonal matrix element $G(r, r; E_n)$ over r, i.e.,

$$f_n = \int dr\, Res[G(r, r; E_n)] = Tr(Res[G(E_n)]) \tag{17}$$

   For a non degenerate eigenstate, $f_n = 1$, and consequently

$$\phi_i(r)\phi_i^*(r') = Res[G(r, r'; E_n)] \tag{18}$$

$$\mid \phi_i(r) \mid = \sqrt{\mid Res[G(r, r; E_n)] \mid} \tag{19}$$

4. The branch cuts of $G(z)$ along the real z-axis coincide with the continuous spectrum of H(Hamiltonian operator), and vice versa. [We assume that the continuous spectrum of H(Hamiltonian operator) consists of extended (or propagating) eigenstates].

5. The density of states per unit volume $\varrho(r, E)$ is given by

$$(\varrho(r; E)) = \mp\frac{1}{\pi}Im[G^\pm(r, r; E)] \tag{20}$$

6. The density of states $N(E)$ is given by integrating $(\varrho(r; E))$ over r, i.e.,

$$N(E) = \int dr(\varrho(r; E)) = \mp\frac{1}{\pi}TrIm[G^\pm(r, r; E)]. \tag{21}$$

Knowledge of $G(z) \equiv (z - H)^{-1}$ permits us to obtain the discrete eigenenergies, the corresponding eigenfunctions, and the density of states in the continuous parts of the spectrum of H. Knowledge of Green's function allows us to calculate the time development of the wave function.

For the simple case where $H = H_0 \equiv p^2/2m$, we obtain the density of states per unit volume (area or length) as follows:

$$
\begin{aligned}
\varrho_0(E) &= \theta(E)\frac{m^{3/2}}{\sqrt{2}\pi^2\hbar^3}\sqrt{E} & \text{For 3D} \\
&= \theta(E)\frac{m}{2\pi\hbar^2} & \text{For 2D} \\
&= \theta(E)\frac{m^{1/2}}{\sqrt{2}\pi\hbar}\frac{1}{\sqrt{E}} & \text{For 1D} \qquad (22)
\end{aligned}
$$

The behaviour of $\varrho_0(E)$ near the boundary of the spectrum (E = 0) depends strongly on the dimensionality. The behaviour of $\varrho(E)$ around an energy E_0 determines the analytical structure of $G(E)$ around E_0. Thus, continuity of $\varrho(E)$ (as in the 3-d case) implies continuity of $G(E)$; discontinuity of $\varrho(E)$ (as in the 2-d case) implies a logarithmic singularity in $G(E)$; and divergence of $\varrho(E)$ (as in the 1-d case) implies divergence of $G(E)$ with the same critical exponent.

We calculated also the density of states for a free particle of mass m obeying the KleinGordon equation. In the particular case where m = 0, we have the wave equation, which implies an energymomentum relation of the form $E = \hbar c|k|$ and for which the density of states per unit volume (area or length) is

$$
\begin{aligned}
\varrho(E) &= \theta(E)\frac{E^2}{2\pi^2\hbar^3c^3} & \text{For 3D} \\
&= \theta(E)\frac{E}{2\pi\hbar^2c^2} & \text{For 2D} \\
&= \theta(E)\frac{1}{\pi\hbar c} & \text{For 1D} \qquad (23)
\end{aligned}
$$

3   GREEN'S FUNCTION AND PERTURBATION THEORY

Here, we have to find out the eigenvalues and eigenfunctions of a Hamiltonian H, which can be decomposed as

$$H = H_0 + H_1 \qquad (24)$$

where H_0 is such that its eigenvalues and eigenfunctions can be easily determined. This problem was solved by

1. Calculating $G_0(z)$ corresponding to H_0;

2. Expressing $G(z)$ in terms of $G_0(z)$ andH_1, where $G(z)$ is the Green's function associated with H; and

3. Extracting from $G(z)$ information about the eigenvalues and eigenfunctions of H.

Information about the eigenvalues and eigenfunctions of H are extracted as follows:

1. The poles of T (z) and G(z) give the discrete eigenenergies of H.

2. The residue of G(z) [or T (z)] at each pole determines the corresponding eigenfunction (if it is non degenerate).

3. The eigenfunction(s) of H associated with E belonging to the continuous spectrum of H is (are) given by

$$| \psi^{\pm}(E)\rangle = | \Phi(E)\rangle + G_0^{\pm}(E)T^{\pm}(E) | \Phi(E)\rangle \qquad (25)$$

$$= | \Phi(E)\rangle + G^{\pm}(E)H_1 | \Phi(E)\rangle \qquad (26)$$

where $\Phi(E)$ is any eigenfunction of H_0 corresponding to the same eigenvalue E. In most physical applications the solution $| \psi^-(E)\rangle$ is excluded on physical grounds.

4. The discontinuity of G(z) across the branch cut gives the density of states.

Here T(z) is defined as the t-matrix,

$$T(z) = H_1 + H_1 G_0(z)H_1 + H_1 G_0(z)H_1 G_0(z)H_1 + ... \qquad (27)$$

4 RECURSION METHOD [3]

There are various calculational techniques in condensed matter theory, which are used to detect the different properties of matters.
Calculational techniques in condensed matter theory is divided into two parts

1. Universal tool

2. Precession instruments

4.1 UNIVERSAL TOOLS

These are the general methods for the calculations of observable quantities of interest in condensed matter physics. These are the general methods for the calculations of dynamic co-relation function, which is applicable to arbitrarily selected model system. It can not yield exact results on wide territory of application.

4.2 PRECESSION TOOLS

These are the collection of the special methods. These are designed for the exact solution of particular problems. Mean field theory may be required as a special method, for the solution of certain model systems with long range interaction. Spin wave theory derives its legitimacy from those special situations in which anharmonicities can be ignored in magnetic excitation. Various limitations are also there in order to solve any system using the methods described above .

These limitations are categorised into two parts

1. Extrinsic limitations

2. Intrinsic limitations

   EXTRINSIC LIMITATION

   These limitations are found in these following methods, such as

1. Computer simulations

2. Green's function methods

3. Recursion methods or finite size studies
   etc...

These limitations are set by the amount of calculational effort or computational power invested in them.

INTRINSIC LIMITATIONS

   These types of limitations are found in the following methods, such as

1. Mean field theory

2. Linear spin-wave theory

3. The random phase approximation

4. n-pole approximation(within framework of recursion method)

These limitations are in-built and can not be overcome within their own respective scopes. There are two types of simplifications, which may bring an exact solution within reach.

1. Simplification due to a spherical type of interaction between the degree's of freedom. The free-particle limit or special types of infinite-range interaction are examples.

2. Simplification due to a special state of a model system, which otherwise exhibits general behaviour. A typical example is the ordered ground state of the Heisenberg's ferromagnet.

In general this method can be written as

$$b_{n+1}u_{n+1} = Hu_n - a_nu_n - b_nu_{n+1} \qquad (28)$$

Here, H is the Hamiltonian. a_n, b_n are the recursion parameters . U_n are the states for n=1,2,3 . n is the number of shells in the chain model. Chain model of a two dimensional square lattice is taken here.

Physics (such as charge densities and magnetic moments) is contained in the local density of state. This is stable under small changes of system . Local density is related to Green's function. By integrating the local densities of states upto the Fermi-level, one can calculate the total weight on one atom and the magnetic moment in spin polarised system. It is desirable to calculate the Green's function directly without first calculating eigenfunctions using the local density of states. There are broadly two types of situations regarding the periodicity of solids, such as

1. First is where an essential lack of periodicity exists : Surfaces and interfaces, random alloys, amorphous materials, defects in solids, liquids, metals, spin glasses, molecules, clusters and micro-crystallites etc...

2. In the second type of situation one may have perfect crystal symmetry.

It is desirable to calculate the Green's function directly without first calculating the eigenfunction, using the local density of states. at a perfect surface one looses the periodicity perpendicular to the surface, retaining a two dimensional periodicity. Again that two dimensional periodicity is also lost at an adsorbed atom.
There basic principle that make recursion method very useful.

1. The structure of the method is already incorporates as much of the right physics as possible.

2. In a large system such as all solid state physics, one is always overwhelmed with too much of information, in principle an infinite amount. One does not want all the eigenstates and all the eigenvalues. Although one uses clusters with N equals to a thousands or more atoms one only recurses about 20 times to obtain a very good representation of the local density of state.

3. One has an unlimited freedom to choose the starting vector u_0 to suit one's problem.

4.3   RECURSIVE SOLUTION OF SCHROEDINGER'S EQUATION [4]

The method gives a convergent sequence of bounded approximates to the solution of Schroedinger's equation and other linear Hamiltonian equations.

In order to solve the large or infinite strong coupling case, the Recursion method is used. i n condensed system, where we want to understand the relation between various ground states and their excitations, the Recursion method is used and it gives the appropriate way to proceed.

Other approaches to infinite strong coupling has a firm mathematical basis and provides bounds for approximations to many quantities. It is harder to find cases of weak coupling. Correlation between electrons is greatest, where there are many configurations with nearly the same energy, the strong coupling case.

For atoms and molecules, the strong coupling is still finite, though involving more degrees of freedom than in the mean field approximation.

1. Firstly, the time independent Schroedinger's equation and it's solution by means of the resolvent are introduced.

2. Then, the starting state, what properties it must possess and how it relates to the physics under investigation.

3. A description of the method and it's relation to the mathematical moment problem, computational aspects of the method and termination should be discussed.

4. The various physical quantities which can be calculated from recursion method are observed.

5. Lastly, some trends in development of the method are solved.

   STARTING STATE

Each quantum problem has two parts ,

1. Hamiltonian (H) specifies the laws of motion

2. Starting state u_0 specifies that, which kind of motion are resolvent to the problem.

The choice of u_0 reduces the problem from that of calculating all of the resolvent operator i.e. $R(E)$ to that of calculating only the state $R(E)u_0$. In order to apply the recursion method u_0 must also have the property that the nth moment,

$$u_n = u_0^{\dagger} H_n u_0 \tag{29}$$

is finite for all n.

The subspace $R(E)u_0$ is called as smallest invariant subspace containing u_0. Again, being much smaller than the full space of states, this subspace has no degeneracy. This non-degeneracy is an important point in running the Recursion method to solve the problem. This non-degeneracy is an exact property of H and u_0. On symmetry grounds the space swept out by $R(E)u_0$ is compatible with semi-infinite model with a single position co-ordinate.

RECURSION

Here, the recursion method has reduced the general Hamiltonian to hopping between discrete states on a semi-infinite chain model. Now, from this Hamiltonian we can see how parameters,a_n and b_{n+1} affect the behaviour. Large b's means the system diffuses rapidly along the chain. While, large changes in a's are like barrier to this quantum diffusion.

5 MODEL IN ORDER TO FIND OUT THE DOS

Here, in the binary alloy case the atoms are arranged like a chain model in 2d square lattice. DOS of binary alloy can be calculated in two steps

Step-1

Calculation of green's function using recursion method.

Step-2

Finding DOS using the green's function.

5.1 STEP-1

Various shells and the recursion parameters of any binary alloy can be found out from the recursive equation

$$|n+1\} = H|n\} - \alpha_n|n\} - \beta_n|n-1\} \tag{30}$$

$|1\} = |1\rangle$, the first shell
$|2\} = |2\rangle + |3\rangle + |4\rangle + |5\rangle$, the second shell

and so on ....
$n = 0, 1, 2, 3......$

The Hamiltonian(H) is calculated from the tight binding model, which is given by,

$$H = \Sigma_l |l\rangle \varepsilon_l \langle l| + \Sigma_{lm} |l\rangle V_{lm} \langle m| \tag{31}$$

where each state $|l\rangle$ is an atomic like orbital centred at the site l; the sites l form a lattice. Such Hamiltonians are very important in solid-state physics. Here we calculate the Green's functions associated with the TBH for various simple lattices.

We need to take the initial state $|1\} = |1\rangle$

Assumption here is that all the states are orthonormal to each other. Hence, using the recursive formula the recursive parameters can be calculated. It has been observed that after 8th shell, the values of parameters are converged to zero.

Both the recursion parameters can be found out from the relations given below

$$\alpha_n = \frac{\{n \mid H \mid n\}}{\{n \mid n\}} \tag{32}$$

$$\beta_n^2 = \frac{\{n \mid n\}}{\{n-1 \mid n-1\}} \tag{33}$$

We can find the value of Green's function in the following form

$$G(\omega^2 + i\delta) = \cfrac{1}{(\omega^2 + i\delta) - \alpha_1 - \cfrac{\beta_2^2}{(\omega^2 + i\delta) - \alpha_2 - \cfrac{\beta_3^2}{\ddots \cfrac{}{\cfrac{\beta_r^2}{(\omega^2 + i\delta) - \alpha_r - \Sigma}}}}} \tag{34}$$

Here,

$$\Sigma = \frac{\beta_\infty^2}{(\omega^2 + i\delta) - \alpha_\infty - \Sigma} \tag{35}$$

is the terminating value of the equation that is the last term we take and δ is a very small quantity that tends to zero.
Hence, here the calculation of Green's function is done.

17

5.2 STEP-2

After the calculation of Green's function, using the following equation we can easily find out the values for the density of state(DOS).

$$N(\omega) = \lim_{\delta \to 0} \mp \frac{1}{\pi} Im \langle G^{\pm}(\omega^2 + i\delta) \rangle \tag{36}$$

6 PLOT FOR DENSITY OF STATE

6.1 CASE-I

For, the ordered system there is only one electronic energy for a particular type of atoms. The energy is given by ε and the interaction potential between the two atoms is V. Now, using the above two steps we can find out the density of state for an ordered system. Putting different values of ω , we can find different values for density of state $N(\omega)$. The behaviour is plotted below
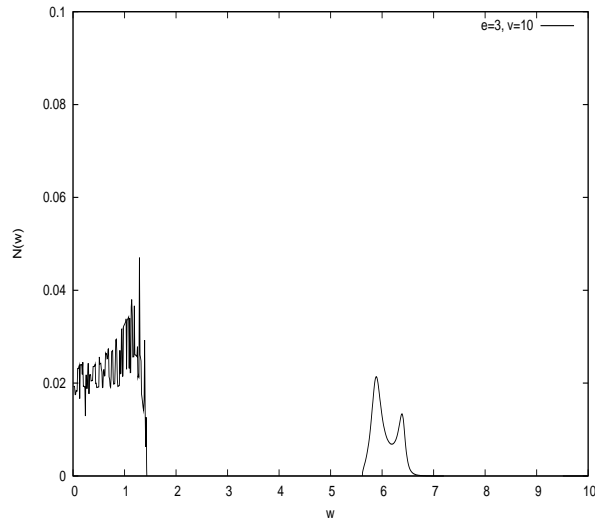

Figure 1:

6.2   CASE-II

If the binary alloy is made up of two types of atoms A and B. The electronic energy of atom A and atom B are let ε_A and ε_B respectively. The interaction potential between the two atoms is V (say), which is assumed to be as constant here. From tight binding model we can find out the Hamiltonian(H).

Again, from step 2 we can find out the density of state for a binary alloy (disordered system). Putting different values of ω , we can find different values for density of state $N(\omega)$. The behaviour is plotted below
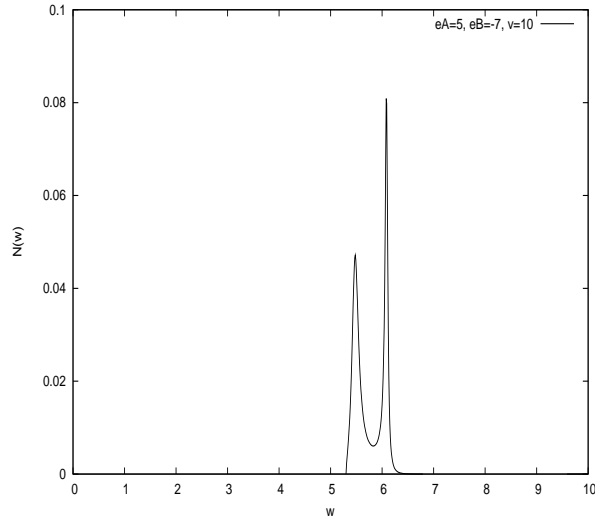

Figure 2:

7   CONCLUSION

The DOS of a system describes the number of states per interval of energy at each energy level that are available to be occupied. A high DOS at a specific energy level means that there are many states available for occupation. A DOS of zero means that no states can be occupied at that energy level. Hence, DOS calculation is necessary in order to study the electronic properties of a disorder system.

8   REFERENCE

1. Paolo M. Ossi, Disordered Materials An Introduction, Second Edition, Springer

2. Eleftherios N. Economou, Green's Functions in Quantum Physics, Third Edition, Springer

3. D.G. Pettifor and D.L. Weaire, The Recursion Method And Its Applications, Proceeding of the conference, Imperial college, London, **1984**

4. Henry Ehrenreich, Fredrick Seitz and David Turnbull, Solid State Physics, Volume-35, Academic Press,**1980**