Chapter 5

Coulomb Gap for Vortex-Vortex Interaction

When the two-dimensional disordered Josephson junction arrays at low temperature are in insulating phase, the vortices can move through the junction due to the hopping of the localized vortices. We can obtain the conductivity for this case via the variable range hopping (VRH) argument (Efros and Shklovskii, 1975). Through this argument we can study the transport property of vortices at zero temperature arising from the competition between the disorder and the logarithmic repulsive interaction among the vortices. In Section 5.1 we will first review the approach of Efros's model concerning the hopping conductivity of the localized correlated fermionic system at low temperature. The computer simulation result will be given in Section 5.2. And finally in Section 5.3 we modify Efros' approach to tackle the localized vortex model.

5.1 Coulomb Gap Problem

The Coulomb gap, a vanishing of DOS at zero excitation energy, was first pointed out by Efros (Efros, 1975) based on the interplay between disorder and the long-ranged $\frac{1}{r}$ Coulomb interaction. These two competition interactions cause a depletion of the single-particle density of states (DOS) near Fermi energy. At zero temperature this DOS vanishes at the Fermi energy but is nonzero elsewhere, resulting in the "soft" gap which is well-known as the Coulomb gap.

The brief conclusion above come from the detail that we consider a disordered system. The electronic states of electrons in the disordered system are localized close to the Fermi level. (For example the systems could be an amorphous or a doped crystalline semiconductor.) The derivation of the Mott law $\ln\sigma \propto T^{-1/4}$ for the DC conductivity of such a system is based upon the assumption that the DOS near the Fermi level is constant. However Efros and Shklovskii (Efros and Shklovskii, 1975) have pointed out that under the influence of Coulomb interaction DOS vanishes at Fermi energy in both two and three dimensional cases. They begin by assuming that the quantum localization length is much smaller than the distance between the centres and the overlap between the wave functions is negligible. So the energy of the system can be written in the form

$$H = \sum_i \phi_i n_i + \frac{1}{2}\sum_{i\neq j} e_{ij} n_i n_j \tag{5.1}$$

where ϕ_i is the energy of the electronic state i not taking into account the con-

tribution of electron-electron interaction, $e_{ij} = e^2/\kappa r_{ij}$ is the energy of electron-electron interaction with $r_{ij} = |r_i - r_j|$ being the distance between the states i and j, κ is the dielectric constant and n_i is the occupation number ($n_i = 0, 1$). Let us introduce the energies of one-particle excitations

$$E_i = \phi_i + \sum_j e_{ij} n_j. \tag{5.2}$$

At temperature $T = 0$, $n_i = 1$ for $E_i < \mu$ and $n_i = 0$ for $E_i > \mu$, where μ is the Fermi level. The ground state of the system should also satisfy another condition. Let us consider two states i and j, which in the ground state are occupied and vacant respectively. The transfer of an electron from state i to state j should in crease the energy of the system. Using (5.1) we find that the energy increase is

$$\Delta H(i \to j) = E_j - E_i - e_{ij} > 0 \tag{5.3}$$

The last term in eq.(5.3) describes 'the exitonic effect', i.e., the Coulomb interaction of the created electron-hole pair. So in the ground state any two energies E_i and E_j separated by the Fermi level should satisfy the inequality eq.(5.3). We can show that the density of state $g(E)$ should vanish at the Fermi level. We assume $g(\mu) = g$ and consider an energy interval of small width ϵ contred at the Fermi level. For this interval a mean distance R between the states is determined by the condition $g_0\epsilon^3 \simeq 1$ and equals $(g_0\epsilon)^{-1/3}$. If $\epsilon \ll \Delta \equiv e^3 {g_0}^{1/2}/\kappa^{3/2}$ the interaction energy of the states $e^2/\kappa R = (e^2/\kappa)(g_0\epsilon)^{1/3}$ exceeds ϵ and the inequality eq.(5.3) inevitably breaks down. Thus a constant density of states contradicts the inequality eq.(5.3) and $g(E)$ at $|E-\mu| < \Delta$ decreases with $|E-\mu|$ and should

vanish at the Fermi level. A self-consistent density of states near the Fermi level may be found from the condition that for any $\epsilon < \Delta$ the mean interaction energy e_{ij} of the states within the ϵ interval is of the order of ϵ. In other words the mean distance between the states in the ϵ interval has to be of the order of $e^2/\kappa\epsilon$, i.e.

$$g(\epsilon)(e^2/\kappa\epsilon)^3\epsilon \simeq 1\,,\; g(\epsilon) = \alpha\kappa^3\epsilon^2/e^6\;(\epsilon = E - \mu) \tag{5.4}$$

Here α is an unknown numerical coefficient. The assumption that $g(\epsilon) \propto \epsilon^\nu$, where $\nu < 2$, contradicts the inequality (5.3). If we assume that $\nu > 2$ then the mean distance between the states in the ϵ interval would be so large that interaction between the states may be neglected and the physical reason for the rapid decrease of $g(\epsilon)$ disappears. That is only $\nu = 2$. For the two-dimension case the same arguments give

$$g(\epsilon) = \alpha' \frac{|\epsilon|\kappa^2}{e^4}. \tag{5.5}$$

The Coulomb gap plays an important role in the low temperature DC conductivity. For the three-dimensional case the energy interval of width $\epsilon_M = T^{3/4}/a^{3/4}{g_0}^{1/4}$ is responsible for the hopping conductivity, which obeys the Mott law (here a is the lacalization length). The influence of the gap can be neglected if $\epsilon_M \gg \Delta$ i.e. $T \gg T_c = e^4 a g_0/\kappa^2$, at such temperatures the Mott law is valid. If $T \ll T_c$ the states within the Coulomb gap are particularly important. Using eq.(5.4) and by analogy with the Mott law derivation we obtain (see appendix A)

$$\sigma(T) \propto \exp[-(T_0/T)^{1/2}] \tag{5.6}$$

where $T_0 = e^2/\kappa a$. The same result is valid for the two-dimensional case.

5.2 Simulation of Coulomb Gap Problem

To study the character of DOS close to the Fermi level at zero-temperature using the Monte-Carlo computer simulation, we use the model of eq.(5.1) with some modifications (Efros, 1979). The electrons in this model can occupy the sites of a regular lattice. The charge of a site is taken to be $1/2$ if the site is empty and $-1/2$ if it is occupied by an electron, each site being occupied at most by one electron. The total number of electrons is half the number of sites, and so the system is neutral. The energy ϵ_i of site i consists of the initial random energy ϕ_i and the potential which is created at site i by all other sites:

$$\epsilon_i = \phi_i + \sum_{j \neq i} n_j / r_{ij}. \tag{5.7}$$

The energies ϕ_i are uniformly distributed in the range from $-A$ to A, and there is no correlation between ϕ_i values corresponding to different sites. The occupation number n_i of site i is equal to $1/2$ if site i is occupied, and to $-1/2$ of it is empty. r_{ij} is the distance between sites i and j in the units of lattice constant a. We take the electronic charge e as equal to unity, therefore the energy is measured in the units of e^2/a. The total energy of the system is

$$H = \sum_i \phi_i (n_i + \frac{1}{2}) + \frac{1}{2} \sum_{i \neq j} n_i n_j (1/r_{ij}) \tag{5.8}$$

The problem is to find the DOS $g(\epsilon)$ corresponding to the set $\{n_i\}$ which minimizes H for the given set $\{\phi_i\}$.

The conditions of the minimum are as follows: (i) There is the boundary

energy μ between the empty and occupied states. This means that for all sites

$$\begin{aligned} \epsilon_i < \mu \qquad \text{if} \qquad n_i = \frac{1}{2} \\ \epsilon_i > \mu \qquad \text{if} \qquad n_i = -\frac{1}{2} \end{aligned} \tag{5.9}$$

where μ is the Fermi level. It follows from the symmetry of the system that

$$g(\epsilon) = g(-\epsilon) \text{ and } \mu = 0. \tag{5.10}$$

(ii) The other conditions of the minimum of the energy can be formulated in terms of inequalities for energies, ϵ_i, which have the form

$$\Delta_i^j > 0. \tag{5.11}$$

Here Δ_i^j is the change of the total energy H due to the transitions of one eletron from occupied site i to empty site j. It must be positive in the ground state.

The inequality corresponding to the transfer of one electron is

$$\Delta_i^j = \epsilon_j - \epsilon_i - \frac{1}{r_{ij}} > 0 \tag{5.12}$$

Computations were made for square lattices $N \times N$. A pseudo-random number generator gave values ϕ_i uniformly distributed in the range from $-A$ to A. The initial occupation numbers n_i, were random as well, but obeyed the equation $\sum_i n_i = 0$ so that the electroneutrality was fulfilled. The energies ϵ_i for each site and the totall energy H were calculated using eq.(5.7) and eq.(5.8). Then a subroutine was called up to satisfy condition (5.9) for all lattice sites μ-Sub. It operated as follows. The site p with maximum energy ϵ_p was selected among

empty sites. The occupation numbers n_p and n_q were reversed if it was found out that $\epsilon_p > \epsilon_q$. Then all ϵ_i and H were re-computed using eq.(5.7) and eq.(5.8). This corresponded to the electron transition from occupied site p to empty site q. New values ϵ_p and ϵ_q were found. The procedure was repeated until the inequality $\epsilon_p < \epsilon_q$ was achieved. This means that the energy of any occupied site was smaller than the energy of any empty site. This was the end of μ-Sub. After the process of subroutine was finished the inquality eq.(5.12) was checked for all pairs consisting of occupied site i and empty site j. If a pair did not obey the inequality, an electron was transfered from i to j, all energies were re-computed and μ-Sub was called up. Then the program returned to checking inequality (5.12) and so on. The total energy H decreased due to any electron transition which was made in the course of the program. The minimization procedure was considered to be completed if all energies ϵ_i obeyed conditions (5.9) and (5.12), Finally under the two conditions we get the ground state by knowing the set $\{\epsilon_i\}$ associated with it.

We find DOS by defining

$$g(\epsilon) = P(\epsilon)/2\delta N^2 \tag{5.13}$$

where $P(\epsilon)$ is the number of states in the energy range $\epsilon - \frac{1}{2}\delta \leq |\epsilon_i| \leq \epsilon + \frac{1}{2}\delta$; δ was usually equal to $\Delta/20$. The values of DOS obtained were averaged over a few hundred different sets $\{\phi_i\}$. The DOS $g_s(\epsilon)$ obtained by it for a 16×16 array at $A = 1$ is shown in fig 5.1.

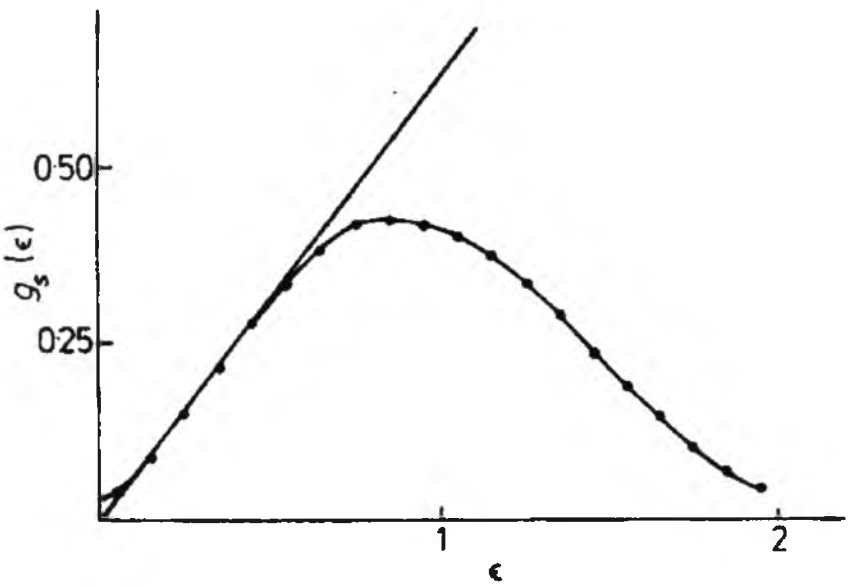

Figure 5.1: The DOS obtained by simple averaging for the 16×16 arrays at $A = 1$. A straight line is the low-energy solution of SCE.

5.3 Simulation of Bosons under Vortex-Vortex Interaction

We modify eq.(5.1) for the fermion particles by changing the possibility of the occupation number n_i to be 0, 1, 2, ... and changing the interaction, Coulomb interaction, $\frac{1}{r_{ij}}$ to vortex-vortex interaction, $\ln|r_{ij}|$. In addition to these modifications, we must also take into account the on-site repulsive interaction between bosons. Thus the Hamiltonian for the system of vortices becomes,

$$H = \sum_i \phi_i n_i + \frac{1}{2}\sum_{i\neq j} n_i n_j \ln r_{ij} + \frac{U}{2}\sum_i n_i(n_i - 1). \tag{5.14}$$

The strength of disorder is represented by the value of A, and the strength of on-site repulsive interaction is represented by U. In granular supercondutor, U represents the charging energy associated with the grain and is inversely proportional to the grain size. The one-particle excitation energy in this case is

$$E_i = \phi_i + \sum_j n_j \ln r_{ij} + U n_i, \tag{5.15}$$

and the energy change after the transfer of one vortex from site i to site j now has an additional factor U. And for the ground state this energy must be greater than zero;

$$\Delta H(i \to j) = E_j - E_i - \ln r_{ij} + U > 0. \tag{5.16}$$

First consider the large U limit (small grain) $U > A$. In this limit the occupation number is either 0 or 1 and Coulomb interaction exists in this case. While in

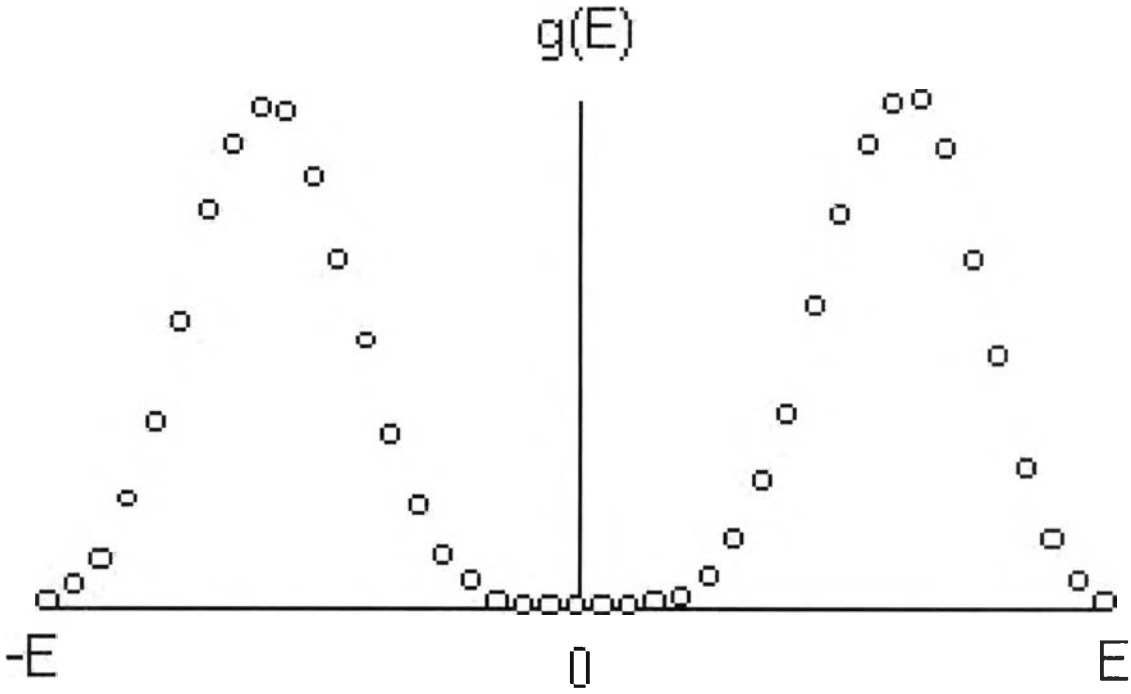

Figure 5.2: Density of states in the limit of $U > A$. The set of parameters are lattice size N=8, A=1 and U=3.

small U limit (large grain), $U < A$, the vortex-pairs begin to form on each grain and screen out the intra site interaction. Thus, the gap disappears.

The computer simulation results are in agreement with this analytical argument. Those results are shown in Figs. 5.2-5.7 by performing the Monte Carlo simulation on the 2D square lattice size 8×8, with 32 vorties.

From Fig. 5.2 and Fig. 5.3 we can see that, in the limit of $U > A$, there exists the depletion of single-particle DOS at the Fermi level. In this limit, our

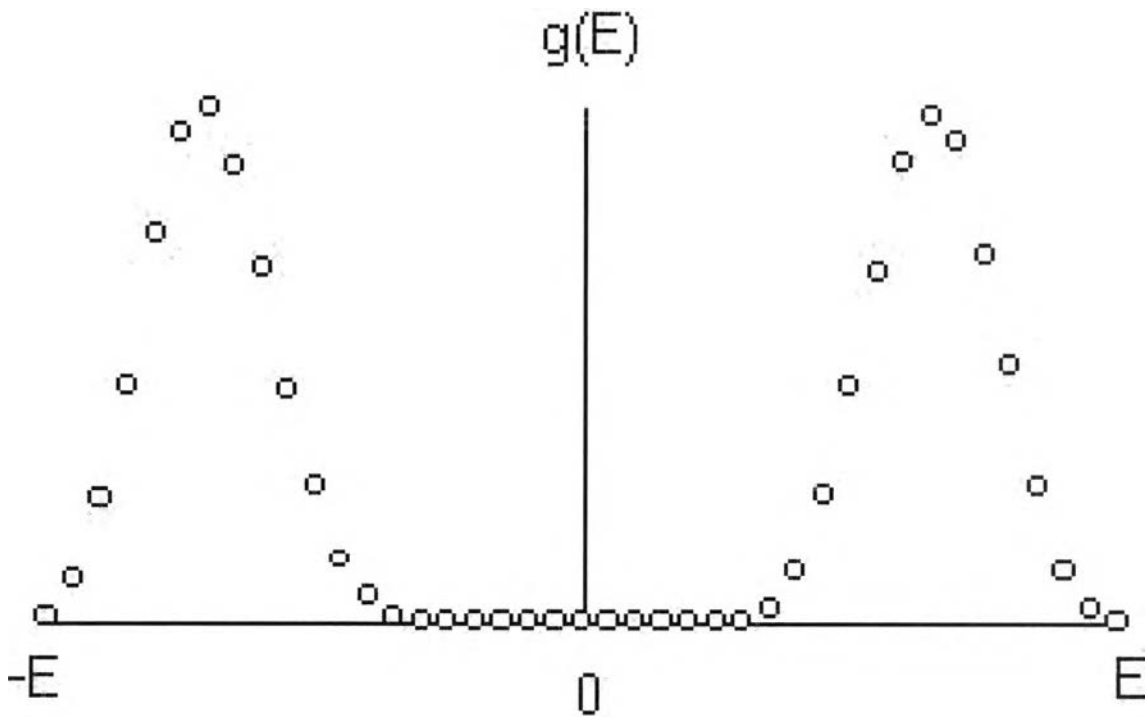

Figure 5.3: Density of states in the limit of $U \gg A$. The set of parameters are lattice size N=8, A=1 and U=5.

system is in analogy with the electrons in the disordered system (Coulomb gap problem). Because at the high value of U the bosons have repulsed each other, it is hard to occupied at a site by $n_i = 2$. That is, its behavior is similar to that of fermion, as we have seen in the problem of Coulomb gap. The influence of vortex-vortex interaction ($\ln r$) is analogous with the influence of Coulomb interaction ($\frac{1}{r}$). We can see the gap in the figure of density of states; the gap begins from the left edge of DOS, at energy of DOS is zero, to the energy which begin to be nonzero at the right of Fermi's level.

Fig. 5.4 and Fig. 5.5 show the results in the case of $U < A$, i.e., the disorder is stronger than the on-site repulsive interaction. In this limit DOS is constant at Fermi level, thus, the temperature dependence of conductivity is in the form of Mott's law (see appendix A).

Fig. 5.6 and Fig. 5.7 show the density of states in the case where U equals A, in the different size scale.

Therefore we can see the influence of the disorder by varying the value A. The result shows that the disorder makes the system localized, and destroys the gap at Fermi level. The charging energy which corresponds to the on-site repulsive interaction is controlled by varying U. We learn about the transport properties of vortices by looking the density of states, in particular, we know the conductivity by investigating the density of states of single particle in the two cases, $U > A$ and $U < A$.

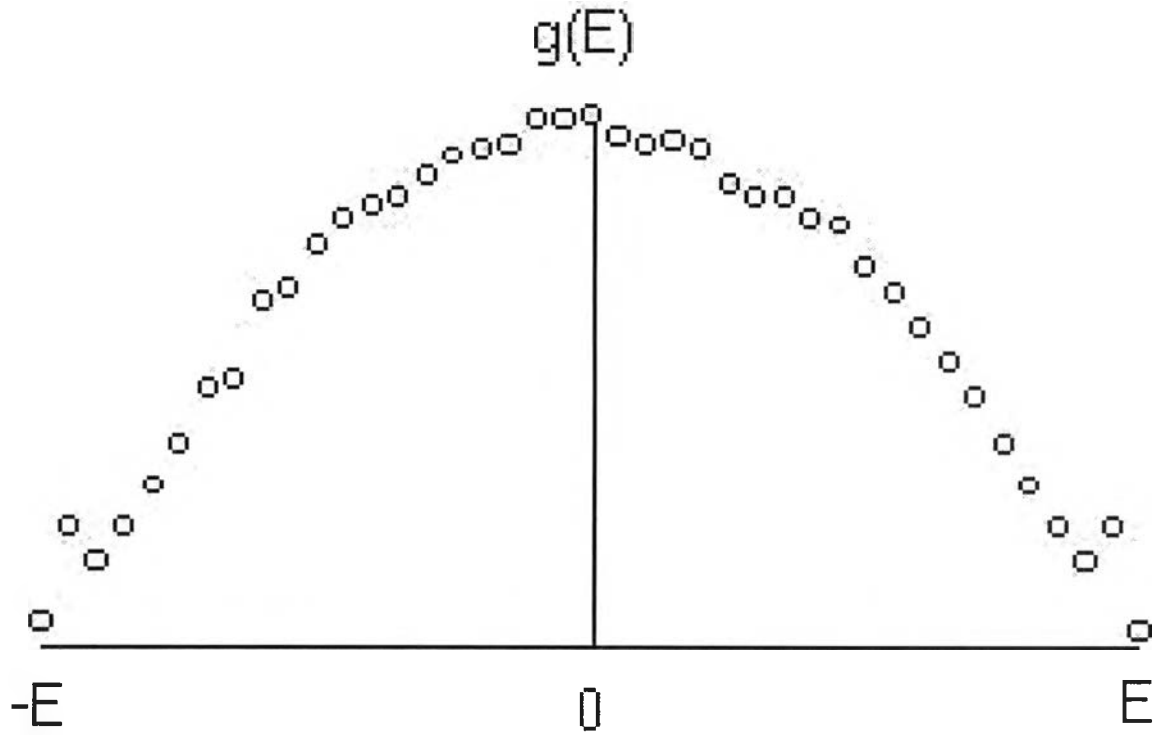

Figure 5.4: Density of states in the case of $U < A$. The parameters are lattice size N=8, A=2 and U=1.

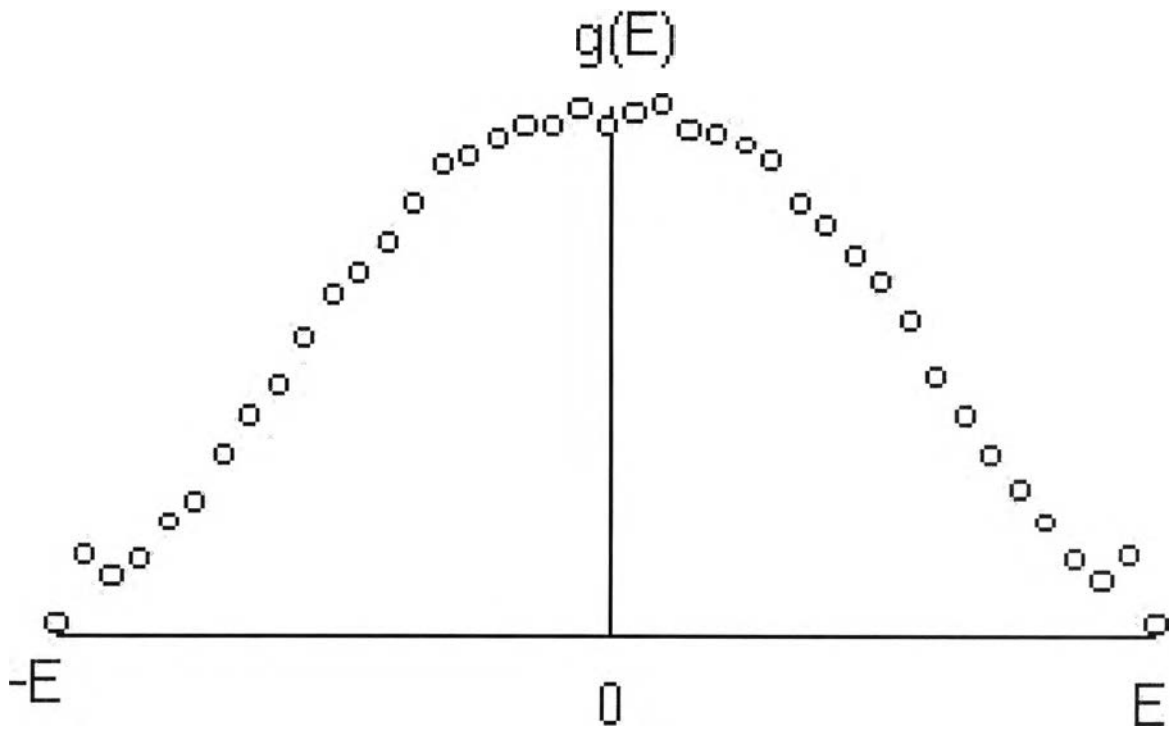

Figure 5.5: Density of states in the limit $U \ll A$. The parameters are lattice size N=8, A=3 and U=1.

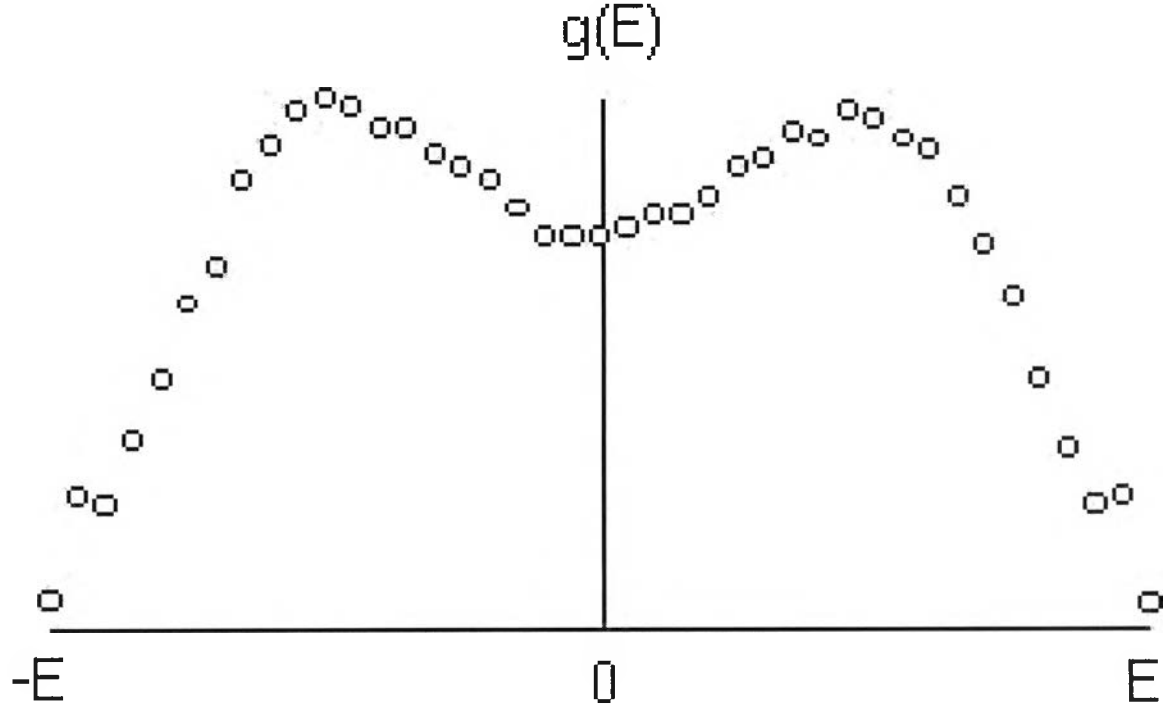

Figure 5.6: Density of states in the case of $U \sim A$. The parameters are lattice size N=8, A=2 and U=2.

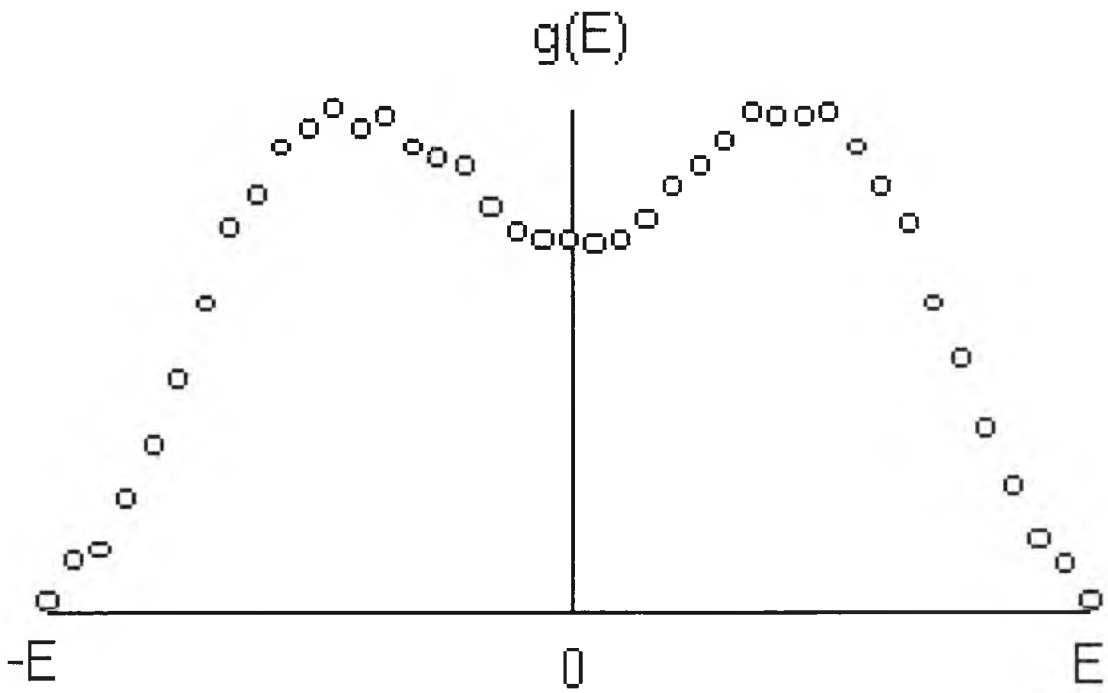

Figure 5.7: Density of states in the case of $U \sim A$. The parameters are lattice size N=10, A=2 and U=2.