Density of states of disordered systems with a finite correlation length

J. C. Flores\textsuperscript{a,b} and M. Hilke\textsuperscript{c}

\textsuperscript{a} Departamento de Física, Universidad de Tarapacá, Casilla 7-D, Arica, Chile
\textsuperscript{b}CHIDE, Universidad de Tarapacá, Casilla 7-D, Arica, Chile
\textsuperscript{c}Physics Department, McGill University, 3600 rue University, Montréal (Québec) H3A 2T8, Canada

We consider a semiclassical formulation for the density of states (DOS) of disordered systems in any dimension. We show that this formulation becomes very accurate when the correlation length of the disorder potential is large. The disorder potential does not need to be smooth and is not limited to the perturbative regime, where the disorder is small. The DOS is expressed in terms of a convolution of the disorder distribution function and the non-disordered DOS. We apply this formalism to evaluate the broadening of Landau levels and to calculate the specific heat in disordered systems.

PACS numbers: 72.15.Rn,65.60.+a
Keywords: Disordered systems, Anderson localization, Glasses

Strong disorder plays an important role, particularly in amorphous systems such as semiconductors or glasses. In electronic systems and in waves in general, localization due to disorder is common and has been studied for many years \cite{1,2,3}. It was shown that localization can strongly affect transport properties, such as inducing metal-insulator transitions. By contrast, thermodynamical properties like the specific heat only depends on the DOS and not on the physics of localization.

Evaluating the DOS for disordered systems is usually very difficult and is often done with weak disorder expansion techniques. However, some exact results exist and include the smoothing out of band edges or singularities \cite{4} and the existence of Litshitz tails \cite{5}. In general, the DOS decays exponentially close to the band edge for most disorder distributions \cite{6}. However, there are no general results valid for the entire DOS in the case of strong disorder and particularly in dimensions larger than one. Furthermore, most of the results are based on the assumption of an uncorrelated disorder potential. Indeed, when a non-zero correlation length $\xi$ is introduced in the disorder potential the situation is not well understood. This is nonetheless important for the understanding of many physical systems, since the correlation length is often non-zero. For example, in quenched disordered systems like amorphous metals the nature of the disorder is largely dependent on the cooling rate and subsequent annealing procedure \cite{7}. In amorphous semiconductors the correlation length depends on deposition conditions \cite{8}, whereas in GaAs/AlGaAs heterostructures the correlation length can be modified by bias cooling \cite{9}.

In this letter we reformulate the semiclassical derivation of the DOS and show that it is a very good approximation to the exact result in the limit where the correlation length $\xi$ of the disorder potential is large. Our approach is based on a semiclassical formulation, which originated with Kane \cite{10} and was further developed by Ziman \cite{11}. More recently, a semiclassical approach was used in the context of amorphous semiconductors \cite{12} and in 1D \cite{13}. Here we introduce a more general situation, where we consider systems, where the volume $\tau(E)$ of energy $E$ in the phase-space can be partitioned for any given realization like:

$$\tau(E) = \sum_i \tau_i^f (E - V_i), \quad (1)$$

where $\tau_i^f (E - V_i)$ is a volume of energy $E - V_i$ of the partition $i$ of the total volume $\tau(E)$. Here $\tau_i^f$ corresponds to the volume free of disorder, since in this partition $V_i$ is assumed approximately constant for a given realization of disorder.

While the assumption in (1) is quite general and can be applied to a number of systems, we will focus our attention on the case of a particle with energy $E$ in a random potential. The potential is constant by pieces $V_i$ over a constant size $d$, which represents the correlation length, $\xi$, of the disorder potential. The Schrödinger equation in any dimension is then simply $E\psi = H_f \psi + \psi \sum_i V_i (\vec{x} - \vec{a}_i)$, where $H_f$ is the Hamiltonian of the disorder free system and the functions $V_i$ are random independent functions with a given probability distribution centered at $\vec{a}_i$. The potential energy $V_i$ is approximately constant for a given realization. In this case, the total volume $\tau(E)$ can be written as a function of the sub-volume like in eq. (1).

Semiclassically, the total number of states $N(E)$ is then proportional to the volume $\tau(E)$ in phase space. Namely, $N(E) = \tau(E)/h$. This is our main starting point to obtain an expression for the DOS of disordered systems. Further below, we will then analyze under which conditions \cite{14} holds. We assume that $\{V_i\}$ is an ensemble of random independent variables with known probability distribution $P_{tot} = \prod_i P(V_i)$. The disorder average $\langle \cdot \rangle$ of (1) is given by $\langle \tau(E) \rangle = \sum_i \langle \tau_i^f (E - V_i) \rangle$ and since the distribution of the random independent variables $V_i$ is the same, we have $\langle \tau(E) \rangle = \sum_i \int dV P(V) \left\{ \tau_i^f (E - V) \right\}$.
and \(\langle \tau(E) \rangle = \int dV P(V) \left\{ \sum_i \tau_i^f (E - V) \right\} \). Because the summation \(\sum_i \tau_i^f (E - V)\) corresponds to the volume of the disorder-free system, namely, \(\tau_i^f (E - V) = \sum_i \tau_i^f (E - V)\), the expression for the integrated DOS \(N(E) = \tau(E)/h\) becomes

\[
\langle N(E) \rangle = \int dV P(V) N(E - V)
\]

and for the DOS \(g(E) = \partial N/\partial E\) we have

\[
\langle g(E) \rangle = \int dV P(V) g^f(E - V).
\]

The disorder-free case corresponds to Dirac’s distribution \(P(V) = \delta(V)\), which leads to \(\langle g(E) \rangle = g^f(E)\) as expected. This expression can also be obtained by using the summation of local density of states following Kane’s original work \(^{10}\). In what follows we analyze under what conditions expressions (2,3) can be used and when they are accurate. We will start by considering the Anderson model \(^{1}\), i.e., a discretized version of the Schrödinger equation, which is \(\sum_j T_{ij} \psi_j = (E - V_i) \psi_i\), where \(T_{ij} = -1\) for nearest neighbors and 0 otherwise and \(V_i\) is our random potential. The DOS of the non-disordered cubic case is then simply given by

\[
g(E) \sim \int \delta(E + 2 \sum_{i=1}^D \cos(k_i)) d^D k,
\]

where \(D\) is the dimension. While evaluating the integral \(^4\) gives no simple expression for \(g(E)\) for higher dimensions, \(g(E)\) is nonetheless a symmetric function of \(E\) and the DOS near the band edges \(E_0 = \pm 2D\) scales simply as \(g(E) \sim |E - E_0|^{(D-2)/2}\) like in the continuous case. When introducing disorder, the DOS broadens.

We first considered the case of uncorrelated disorder, i.e., \(\langle V_i V_j \rangle \sim \delta_{i,j}\), and where the \(V_i\)’s are uniformly distributed between \(-\sigma\) and \(\sigma\). For this case (\(D=3\)) there exists no analytical result for the entire shape of the DOS. Hence, we evaluated the DOS numerically and show the result in figure \(^1\) for different strengths of disorder. In the same figure we also show the DOS evaluated with \(^3\). Clearly the agreement is not good. This is not too surprising and will be discussed below.

The situation changes quite dramatically, when we include the condition for the derivation of our semiclassical expression \(^3\). Indeed, when we impose that the potential is constant by pieces, we obtain a much better agreement between expression \(^3\) and the exact diagonalization (see figure \(^2\)). In figure \(^2\) we show the 3D DOS for the case where \(V_i\) is constant over a fixed interval, ranging from 1 to 4. The larger the interval the better the agreement. It is important to note that increasing the interval \(d\) does not reduce the strength of the disorder \(\langle V^2 \rangle\), but it only increases the disorder correlation length, where \(\xi = d\). While the overall quality of the fit is quite remarkable as soon as \(d\) exceeds 2, the band tails, however, are only accurate for \(|E - E_{\min}| > \delta E\), where \(E_{\min}\) corresponds to the band edge of expression \(^3\). \(\delta E\) can be estimated from the cut-off of the wavelength due to \(d\), hence \(\delta E \sim E(k_{\min} + 2\pi/d) - E(k_{\min})\), where \(E(k)\) is the dispersion relation of the disorder free system. We checked this by evaluating the 1D case, which is shown in the inset of figure \(^2\) where the accuracy of the band tail DOS is improving drastically for \(d\) increasing from 4 to 50. It is also interesting to note that the sharp structures

\[
\begin{align*}
\text{FIG. 1: Dotted lines: average density of states calculated for a 3D system of size 16^3 and averaged over 20 configurations for the Anderson model with a uniform distribution of width } \\
\sigma = 4, 8, 16. \text{ The bandwidth of the non-disordered case is 12 in these units. The solid lines are the expressions obtained from } \ ^3.
\end{align*}
\]

\[
\begin{align*}
\text{FIG. 2: Average density of states calculated for a system of size 16^3 and averaged over 30 configurations for the Anderson tight binding model } \ ^1\text{ with a uniform distribution of width } \\
\sigma = 16 \text{ and } d = 1, 2, 4. \text{ The black line is the expression obtained from } \ ^3. \text{ In the inset the 1D density of states is shown for } d=4, 16, 50 \text{ and the black line is obtained from } \ ^3.
\end{align*}
\]
close to the band center are accurately described by \( E \) for \( d \) large enough.

The disorder potential considered above, while long range in nature, is different from the often considered "smooth" disorder case. For comparison, we considered a smooth potential of the form: 
\[
 W_i = \left( d \sqrt{\pi/2} \right)^{1/2} \sum_j V_j e^{-((x-j)^2)/d^2}, 
\]
where \( \langle V^2 \rangle = \langle V^2 \rangle \) and the correlation length (FWHM) is given by \( \xi = 2.35d \). The distribution function for this potential at large \( d \) is simply given by 
\[
 P(W) = \frac{2\pi}{V} e^{-W^2/(2\langle V^2 \rangle)}. 
\]

We evaluated numerically the exact DOS in 1D and compared it to expression \( E \) for different values of \( d \) using the exact numerical distribution function. The results are shown in figure 3. Here again, expression \( E \) is in excellent agreement with the exact result when \( d \) is large.

For smooth disorder this is not too surprising, since the semiclassical approximation is accurate for a very smooth potential. Indeed, a recent perturbative calculation in 1D shows that the semiclassical approximation is exact in the limit, where \( \langle (\nabla V)^2 \rangle / \langle V^2 \rangle^{3/2} \ll 1 \). They also obtained the first order correction of the DOS to the semiclassical result. In this letter, however, we push the argument much further and show that for a disordered system the semiclassical expression \( E \) is accurate in the limit where the correlation length is large, independently of the smoothness and dimension of the system under consideration. Therefore, we have an expression, which provides a simple form for the DOS of disordered systems with a large correlation length. This is the main result of this letter. In localization physics, disorder correlations can also have a dramatic effect on the extent of the wave functions and even lead to the existence of extended states in 1D \( E \) and 2D \( E \). Without correlations, Lloyd showed that for \( P(V) \) a Lorentz distribution, the exact DOS is also given by expression \( E \).

We now turn to some important consequences of expression \( E \). We start with the singularities in the disorder-free system, which will be smoothed out if the disorder distribution is continuous. An interesting example of this is the situation of a perpendicular magnetic field in two dimensions, where the spectrum is discrete and the density of states is given by a sum of \( \delta \) functions centered at the Landau levels, i.e.,
\[
 g(E) \sim \sum_n \delta(E - (n + 1/2)h\omega_c), 
\]
where \( \omega_c \) is the cyclotron frequency. Using expression \( E \) to obtain the average DOS in the presence of disorder immediately gives a broadening of the Landau levels only related to the disorder strength and the disorder distribution. Hence,
\[
 (g(E)) \sim \sum_n P(E - (n + 1/2)h\omega_c) 
\]

It is interesting to note that this Landau level broadening does not depend on the Landau level index. While the exact shape of the Landau level broadening is still under debate, experiments on GaAs/AlGaAs heterostructures, which have long range disorder, indicate that the broadening is magnetic field dependent at low fields, where the Landau level overlap is significant. At higher fields the broadening becomes independent of the field and of the Landau level index and the shape is found to be best fitted by a Lorentzian \( E \). Hence, expression \( E \) is consistent with experimental findings for large fields in systems with long range disorder.

Another interesting consequence of expression \( E \) is the widening of the bands. Indeed, if \( P(V) \) has a finite support, namely, \(-\sigma < V < +\sigma\), then the bands will be extended by \( \sigma \) on each side. This can lead to the decrease of gaps in disordered materials. The band edges will acquire tails. Expression \( E \) leads to tails, which depend on the disorder distribution. For continuous systems the disorder free band edge is given by 
\[
 (g(E)) \sim \sqrt{E} \quad \text{in } D = 3. 
\]
Introducing disorder will modify this dependence. It is quite straightforward to see that, for a square distribution 
\[
 P(V) = 1/2\sigma \quad \text{for } -\sigma < V < +\sigma \quad \text{and } P(V) = 0 \quad \text{otherwise}, 
\]
we obtain in any dimension
\[
 (g(E)) = \frac{1}{2\sigma} \left\{ N^f(E + \sigma) - N^f(E - \sigma) \right\}, 
\]
where \( N^f \) is the integrated DOS of the disorder-free system. Therefore, \( (g(E)) \sim (E + \sigma)^{3/2} \) at the band edge and the band tail is not exponential for this distribution. Numerically, we see that this is indeed the case for the correlated case \( d = 50 \) shown in the inset of figure 2. For other disorder distributions, \( P(V) \), such as Gaussian or Poisson, we do recover an exponential band tail. Fundamentally, the disorder distribution will govern the dependence of the band tails. In the high disorder limit \( E/\sigma \ll 1 \), \( (g(E)) \approx \frac{1}{2\sigma} N^f(\sigma) \) is independent of energy.

We now turn to the specific heat of disordered systems. The internal energy \( U_F \) and the particle number \( N_F \)
for fermions is given by $U_F = \int \frac{1}{e^{(E-E_F)/k_B T}+1} g(E) dE$ and $N_F = \int \frac{1}{e^{(E-E_F)/k_B T}+1} (g(E)) dE$. As above we consider the disorder-free DOS $g(E) = \alpha D E^{\frac{D-6}{2}}$, where $\alpha$ is a constant. In the high temperature limit (Boltzmann distribution) and using (6) leads to a specific heat $C_{Boltz} = \frac{\partial}{\partial T} \left( \frac{U_{Boltz} \times N_{Boltz}}{N_{Boltz}} \right)$ or

$$C_{Boltz} = K \left\{ \frac{D+2}{2} - \left( \frac{\sigma}{KT \sinh \sigma / KT} \right)^2 \right\}. \quad (7)$$

For the case $D = 1$ we recover the results found in reference [13]. For all dimensions, the limit $\sigma \to 0$ gives $C_{Boltz} = KD/2$ in agreement with the Dunlap-Petit law. The case $\sigma \to \infty$ leads to $C_{Boltz} = K(D+2)/2$, which represents an enhancement of the specific heat due to disorder.

In the opposite limit of low temperatures, where we can use the Sommerfeld expansion, the difference between the specific heat of the disordered system and the ordered system (for the same electronic density) is given by

$$C_D - C_V \simeq \left( \frac{\pi K}{3} \right) T \frac{\alpha E_D^{\frac{D-6}{2}} \sigma^2}{12} (2-D) D, \quad (8)$$

where $E_D$ is the Fermi level of the disordered system and we further assumed that $\sigma \ll E_D$. Clearly this expression shows that the disorder decreases the specific heat in 3D but enhances it in 1D. The 3D case is simple to understand, since at low temperatures the specific heat is mainly determined by the tail of the DOS. Hence, for a given energy bandwidth, the DOS of the disordered case is smaller than the DOS of the ordered case, which leads to a smaller specific heat in the disordered case. The 1D result is more surprising, but can be understood by looking at all relative disorder strengths presented in figure 4. Indeed, at high disorder strength, (i.e. $E_D$ small), where the low energy DOS is dominated by the tails, we do recover that the specific heat is smaller in the disordered case than in the ordered case. In the opposite limit of small relative disorder the situation is reversed because the disorder-free DOS in 1D decreases with energy, leading to a comparatively larger specific heat for the disordered case.

In conclusion, we have shown that the average DOS of disordered systems can be derived in a semiclassical way to represent an accurate DOS for a disorder potential when the correlation length is large. We further, evaluated a few physical quantities such as the broadening of the Landau levels, the characterization of band edges and tails and finally, discussed the electronic specific heat in these systems.

M.H. would like to acknowledge support from RQMP, FQRNT and NSERC.

[1] P.W. Anderson, Phys. Rev. 109, 1492 (1958).
[2] P.A. Lee and T.V. Ramakrishnan, Rev. Mod. Phys. 57, 287 (1985).
[3] C.M. Soukoulis and E.N. Economou, Wave Random Media 9, 255 (1999).
[4] F.J. Wegner, Phys. Rev. B 19, 783 (1979).
[5] I.M. Lifshitz, Sov. Phys. Usp. 7, 549 (1965).
[6] L. Pastur and A Figotin, Spectra of Random and Almost periodic operators, Springer Verlag, (1992).
[7] S.R. Elliott, Physics of amorphous materials, John Wiley & Sons (1989).
[8] D. Quicker and J. Kakalios, Phys. Rev. B 60, 2449 (1999).
[9] P.T. Coleridge, Semicond. Sci. Technol. 12, 22 (1997).
[10] E. O. Kane, Phys. Rev. 131, 79 (1963).
[11] J. M. Ziman, Models of Disorder (Cambridge University Press, 1979).
[12] S.K. O’Leary, S. Zukotynski and J.M. Perz, Phys. Rev. B 51, 4143 (1995).
[13] J. C. Flores, Phys. Stat. Sol. (b) 239, 168 (2003).
[14] D.N. Quang and N.H. Tung, Phys. Rev. B 60, (1999) 13648.
[15] J.C. Flores, J. Phys. Condens. Matter 1, 8471 (1989) and D.H. Dunlap, H.-L. Wu, and P.W. Phillips, Phys. Rev. Lett. 65, 88 (1990).
[16] M. Hilke, J. Phys. A: Math. Gen. 27, 4773 (1994) and M. Hilke, Phys. Rev. Lett. 91, 226403 (2003).
[17] P. Lloyd, J. of Phys. C 2, 1717 (1969).
[18] A. Potts et al., J. of Phys.: Condens. Matter 8, 5189(1996).