Band-center Anomaly in a One-dimensional Anderson Model

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Abstract

We numerically investigate the band-center anomaly in a non-interacting one-dimensional Anderson model at zero temperature. We report on the kernel polynomial simulations of density of states and localization length, which has an $O(N)$ computational complexity. At the band center, the density of states show a cusp-like behavior in the perturbative regime. We argue that this cusp-like behavior of the density of states may be the reason of the anomalous behavior of the localization length. In addition, we find an excellent agreement of the kernel polynomial estimates of localization length with the analytical result obtained by Izrailev et. al., Phys. Rep. 512, 125 (2012).

Keywords: Anderson model, Band-center anomaly, Kernel polynomial method

1. Introduction

The density of states \cite{1, 2} of a quantum system is one of the main observable quantities of interest in solid-state physics. It describes the number of states that are available in a quantum system and is essential for determining the particle concentrations and the energy distributions of particles.

The density of states of a clean one-dimensional tight-binding chain is symmetric around the band center and exhibit van Hove singularities of the form of a square root divergence at the band edges \cite{1}. However, introducing disorder in the system \cite{3}, results the breaking of translational periodicity due to scattering effects in the lattice system. As a consequence, the singularities at the band edges are progressively broadened with disorder strength, and its weight is redistributed to energies throughout and beyond the crystal band.

All the eigenstates of a one-dimensional Anderson model are restricted to a finite region of space at the absolute zero of temperature \cite{4, 5}. These localized wavefunctions typically have

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an envelope with an exponential tail, \( \exp(-|\vec{x} - \vec{x}_0|/\xi) \), where \( \xi \) quantifies the localization of wavefunctions and is referred as the localization length \([2, 6]\). Many theoretical works \([7, 8]\) have been made for the calculations of localization length for the disordered model. The famous Thouless formula \([9]\), relates the localization length of a one-dimensional disordered electronic system in terms of the density of states:

\[
\frac{1}{\xi(E)} = \int \rho(\epsilon) \ln|E - \epsilon| d\epsilon - \ln|t|.
\]

where \( \rho(\epsilon) \) is the density of states at energy \( \epsilon \) and \( t \) is a hopping matrix element. For the Anderson model, the localization length at energy \( E \) in the perturbative regime can easily be obtained as (see Appendix A for detail),

\[
\xi(E) = \frac{96t^2}{W^2} \left( 1 - \left( \frac{E}{2t} \right)^2 \right).
\]

where \( W \) is the disorder controlling parameter. This formula allows us to determine the localization distance for a known energy spectrum.

It was found numerically \([5]\) that the Thouless expression Eq. 1, fails to produce the correct localization length for the Anderson model at the band center \( E = 0 \), known as “band-center anomaly”. Kappus and Wegner \([10]\) showed that this band-center anomaly is a resonance effect that reflects the failure of the Born approximation. In addition, Derrida and Gardner \([11]\) verified the band-center anomaly and suggested that other anomalies should appear for resonant energies \( E = 2 \cos(\alpha \pi) \), where \( \alpha \) is a rational number.

The band center and band edges anomalies was analytically investigated by Izrailev et. al., \([12]\). These calculations are based on Hamiltonian map approach \([13]\), and was found to be \( 105.2/W^2 \) at \( E = 0 \) for the Anderson model, and is in good agreement with the numerical results \([5, 10, 11]\). Furthermore, the band-center anomaly in a one-dimensional model with weak correlated disorder has also been investigated \([14]\). It is shown that the disorder correlations can augment the band-center anomaly.

In this paper we study the band-center anomaly in a non-interacting one-dimensional electronic system with diagonal disorder at absolute zero temperature. We report numerical simulations of the density of states and the localization length of the Anderson model based on the Kernel Polynomial Method (KPM). The density of states is peaked (cusp-like singularity) at the band center in the perturbative regime, and smooths out with increasing disorder. We argue that the anomalous behavior of the localization length at the band center or its neighborhood is due to this small cusp in the density of states. To complete the picture, we calculate the KPM estimates of the localization length and find a very good agreement with the analytical value \([12]\) in the perturbative regime.

The structure of the paper is as follows. In section II, we introduce the one-dimensional Anderson model and discuss the kernel polynomial approximations of the density of states and the Thouless expression. In section III, we discuss our numerical results and explore the band-center anomaly from the perspective of density of states. We discuss the origin of the band-center anomaly and show that the kernel polynomial approximation of the
Thouless formula gives a very good estimates of the data. In the last section, we sum up our conclusions.

2. Model and Computational Method

2.1. Anderson Model

The lattice model under observation is a non-interacting tight-binding system with nearest neighbor hopping and random site energies. The Hamiltonian in second quantization has the following general form,

\[ \hat{H} = - \sum_{\langle ij \rangle} t_{ij} (c_i^\dagger c_j + h.c.) + \sum_i \varepsilon_i c_i^\dagger c_i \]  

The essential parameters in the model are the transfer integrals \( t \) and the diagonal disorder potentials \( \varepsilon_i \). The transfer integrals \( t_{ij} = t = 1 \), are restricted to nearest neighbors. All energy scales are measured in unit of \( t \). For Anderson’s model, the on-site energies \( \varepsilon_i \) are the independent random variables uniformly distributed in the interval \([-\frac{W}{2}, \frac{W}{2}]\), where \( W \) is the width of distributions which controls the strength of disorder.

2.2. Kernel Polynomial Method

The kernel polynomial method (KPM) [15, 16] is a polynomial expansion-based technique and can efficiently compute the spectral function of a large disordered quantum system. It has been successfully applied to condensed matter problems [17, 18], for underpinning the Anderson transitions in non-interacting disordered systems. In the KPM technique, the Hamiltonian and all energy scales need to be normalized into the standard domain of orthogonality of the Chebyshev polynomials \([-1, 1]\). Moreover, the numerical convergence and accuracy of the KPM estimates strongly depends on Gibbs damping factor and coefficients of Chebyshev polynomials [15]. The first kind of \( m \)th degree Chebyshev polynomials \( T_m(x) \) are defined as

\[ T_m(x) = \cos(m \arccos(x)), \quad m \in \mathbb{N} \]  

Moreover, the \( T_m(x) \)'s obey the following three-term recurrence relation

\[ T_m(x) = 2xT_{m-1}(x) - T_{m-2}(x), \quad m > 1 \]  

starting with \( T_0(x) = 1 \) and \( T_1(x) = x \); moreover it satisfy the orthogonality relation

\[ \int_{-1}^{1} T_n(x)T_m(x)(1-x^2)^{-1/2}dx = \frac{\pi}{2}\delta_{n,m}(\delta_{n,0} + 1). \]  

The KPM estimate of the density of states [15] is,

\[ \rho(E) = \frac{2}{\pi\sqrt{1-E^2}} \sum_{m=0}^{M-1} \frac{g_m \mu_m}{(1 + \delta_{m,0})} T_m(E), \]
where the expansion coefficients $\mu_m$ are determined as,

$$\mu_m = \int_{-1}^{1} T_m(E) \rho(E) dE,$$

$$= \frac{1}{N} \text{Tr}[T_m(\hat{H})].$$

The trace in Eq. 8 can also be evaluated by the stochastic evaluation method of traces (see Ref. [15] for the detail).

The expression Eq. 7 represents the truncated sum over $m$ Chebyshev series. This abrupt truncation of the series can introduce unwanted oscillations namely Gibbs oscillations, that can be filtered out by employing an optimized damping factor. The most favorable filter is the so-called Jackson Kernel $g_m$ [15] defined as follows

$$g_m = \frac{1}{M + 1} ((M - m + 1) \cos\left(\frac{m\pi}{M + 1}\right) + \sin\left(\frac{m\pi}{M + 1}\right) \cot\left(\frac{\pi}{M + 1}\right)).$$

The localization length of the model can be numerically calculated by employing the kernel polynomial approximation of Thouless expression Eq. 1. As a result, the KPM estimates of the localization length is

$$\frac{1}{\xi(E)} = \frac{2}{\pi} \sum_{m=0}^{M-1} \frac{\mu_m g_m}{1 + \delta_{m,0}} \mathcal{F}_m(E),$$
where the function $\mathcal{F}_m(E)$, is given by

$$\mathcal{F}_m(E) = \int_{-1}^{1} T_m(\epsilon) \ln |E - \epsilon| \frac{d\epsilon}{\sqrt{1 - \epsilon^2}},$$  \hspace{1cm} (11)

The final expression of the localization length is 19

$$\frac{1}{\xi(E)} = - \ln 2 - 2 \sum_{m=1}^{M-1} \frac{\mu_m g_m}{m} T_m(E).$$  \hspace{1cm} (12)

Eq. (12) can be used to compute the localization length of the disordered systems for a given energy $E$. Here, we are focusing on the KPM implementations of $\xi(E)$ at the band center.

3. Numerical Results

To address the band-center anomaly, we demonstrate the KPM estimates of the density of states for the non-interacting Anderson model restricted to nearest neighbor interactions as illustrated in Fig. [1]. The data are computed for a system of size $N = 131072$ with 1024 Chebyshev moments. In the limit of clean system, the density of states is symmetric around the band center and exhibit van Hove singularities of the form of a square root divergence at the band edges (black bold curve).
The singularities at the band edges of the density of states progressively broadened with disorder strength and has been numerously investigated \[2\] [10]. By zooming the density of states at the band center Fig. 1(inset), we obtain a sharp peak of the density of states at the band center in the presence of small disorder. Increasing disorder will progressively broaden the central part of the density of states, and consequently, the peak becomes flat in the limit of strong disorder. In fact, the peak has a constant fixed value for a variety of disorder strengths. It is basically the density of states of the neighborhood of \(E = 0\), that starts to increase with disorder strength, and eventually the sharp peak disappear in the strong disorder limit.

To explore the band-center anomaly in detail, we compute the localization length of the model as depicted in Fig. 2. The computations are carried out for a system of size \(N = 131072\) with \(M = 2048\) Chebyshev moments at the band center for a fixed estimated error 1%. The estimated error is determined by the fluctuations in the localization length. For small system size \(N = 2^{12}\), a small deviation of the estimated localization length is observed from the perturbative results \(105.2/W^2\) [12], in the limit of small disorder strength, which disappear in the large system limit. In fact, one need to use larger system than the localization length for better numerical convergence. Most importantly, our numerical finding show an excellent agreement with the perturbative results in the large system limit.

4. Conclusions

We numerically investigated the band-center anomaly in the non-interacting one-dimensional Anderson model. We computed the density of states and the localization length for the model by using kernel polynomial method, which has \(O(N)\) numerical complexity. We found a sharp peak of the density of states at the band center in the small disorder limit, which smoothed out with disorder strength. We proposed that this sharp peak of the density of states is the reason of anomalous behavior of the localization length at \(E = 0\).

Furthermore, the famous Thouless expression of localization length is approximated by the kernel polynomial method and found an excellent agreement of the numerical data with the analytical perturbative result.

Appendix A. Localization Length of the 1D Anderson Model

We focus on the localization length of the Anderson model in the perturbative regime. The expression Eq. 1 in the thermodynamic limit can be written as (see Eq. 6.10 in Ref. [6]),

\[
\frac{1}{\xi(E)} = \text{Re} \int_{-\infty}^{E} G_{ii}(\epsilon) d\epsilon,
\] (A.1)

This is a basic equation and will be used to calculate the \(\xi(E)\) in units of lattice spacing. Using perturbation, the averaged Green’s function \(G_{ii}(\epsilon)\) has the following form:

\[
G_{ii}(\epsilon) = \sum_x \sum_y G_{0x}(\epsilon) G_{xy}(\epsilon) G_{y0}(\epsilon) \delta_{x,y},
\] (A.2)
The variance of the uniformly distributed random potentials with disorder strength $W$ is
\[ \varepsilon_x \varepsilon_y := \varepsilon^2 \delta_{xy} = \frac{W^2}{12} \delta_{xy}. \]  
(A.3)

Substitution of this into Eq. A.1 gives the localization length as
\[
\frac{1}{\xi(E)} = \frac{W^2}{12} \int_{-\infty}^{E} \sum_{xy} G_{0x}^0(\epsilon)G_{xy}^0(\epsilon)G_{y0}^0(\epsilon) \delta_{xy} d\epsilon,
\]
\[= \frac{W^2}{12} \int_{-\infty}^{E} \sum_{x} G_{0x}^0(\epsilon)G_{xx}^0(\epsilon)G_{x0}^0(\epsilon) d\epsilon,
\]
\[= \frac{W^2}{12} \int_{-\infty}^{E} \mathcal{G}(\epsilon) d\epsilon,
\]  
(A.4)

where
\[ \mathcal{G}(\epsilon) = \sum_{x} G_{0x}^0(\epsilon)G_{xx}^0(\epsilon)G_{x0}^0(\epsilon), \]  
(A.5)

The lattice Green’s function $G_{pq}^0(\epsilon)$, at energy $\epsilon$ has the form
\[ G_{pq}^0(\epsilon) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{dk}{\epsilon - 2t \cos k} e^{ik(p-q)}. \]  
(A.6)

Inserting into Eq. A.5 gives
\[ \mathcal{G}(\epsilon) = \frac{1}{(2\pi)^3} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \sum_{x} e^{i(x-k_3-k_1)} dk_1 dk_2 dk_3 \frac{\delta(k_3 - k_1)}{\epsilon - 2t \cos k_1(\epsilon - 2t \cos k_2)(\epsilon - 2t \cos k_3)}. \]

The sum term gives
\[ \sum_{x} e^{i(x-k_3-k_1)} = \sum_{x=-\infty}^{\infty} e^{i(x-k_3-k_1)} = 2\pi \delta(k_3 - k_1). \]  
(A.7)

The $\mathcal{G}(\epsilon)$ becomes
\[ \mathcal{G}(\epsilon) = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{\delta(k_3 - k_1) dk_1 dk_2 dk_3}{\epsilon - 2t \cos k_1(\epsilon - 2t \cos k_2)(\epsilon - 2t \cos k_3)}, \]
\[= \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{dk_1 dk_2}{\epsilon - 2t \cos k_1(\epsilon - 2t \cos k_2)^2(\epsilon - 2t \cos k_2)}, \]
\[= \frac{1}{(\epsilon^2 - 4t^2)^2}. \]  
(A.8)

Inserting into Eq. A.4 the final expression is
\[ \frac{1}{\xi(E)} = \frac{W^2}{24} \frac{1}{4t^2 - E^2}. \]  
(A.9)

This formula allows us to determine the localization distance for known energy spectrum. The localization length shows a power-law divergence in the limit of vanishing disorder.
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