Band tails in disordered systems

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Introduction

We study the quartic random Schrödinger equation

$$\left[\beta_4 \alpha \nabla^4 - \beta_2 \frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right]\varphi_n = E_n \varphi_n, \qquad (1)$$

where α is a dimensional parameter, β_2 and β_4 are adimensional and control the relative strength of the dispersion terms, and $V(\vec{x})$ is a Gaussian white noise.

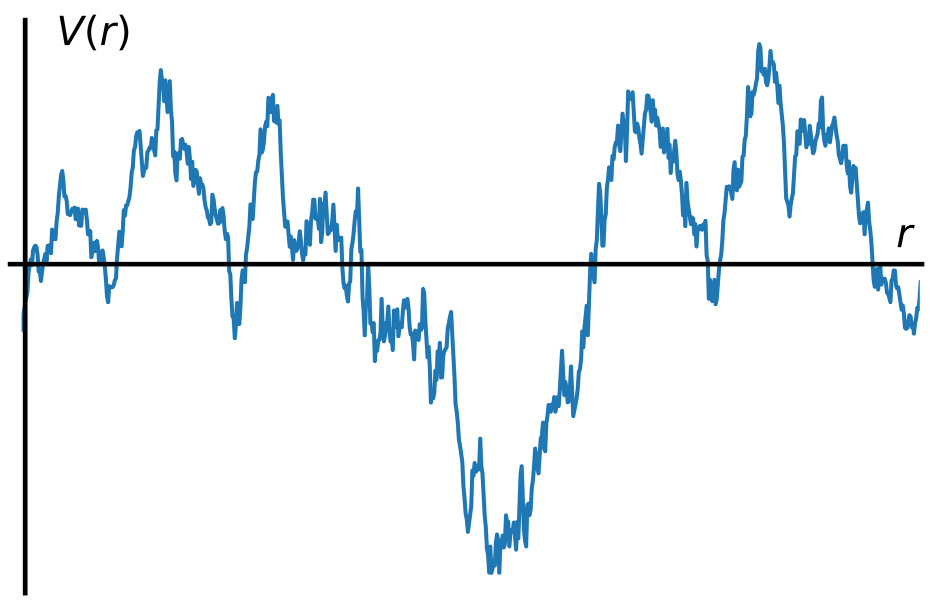

Fig 1. Representation of a random potential.

In the free case ($V = 0$) only unbounded states are possible and the calculation of the DOS is straightforward. When we introduce the random potential, we can have fluctuations to energies low enough to allow new bound states to appear. The calculation of the DOS is then the calculation of a potential fluctuation of the required magnitude.

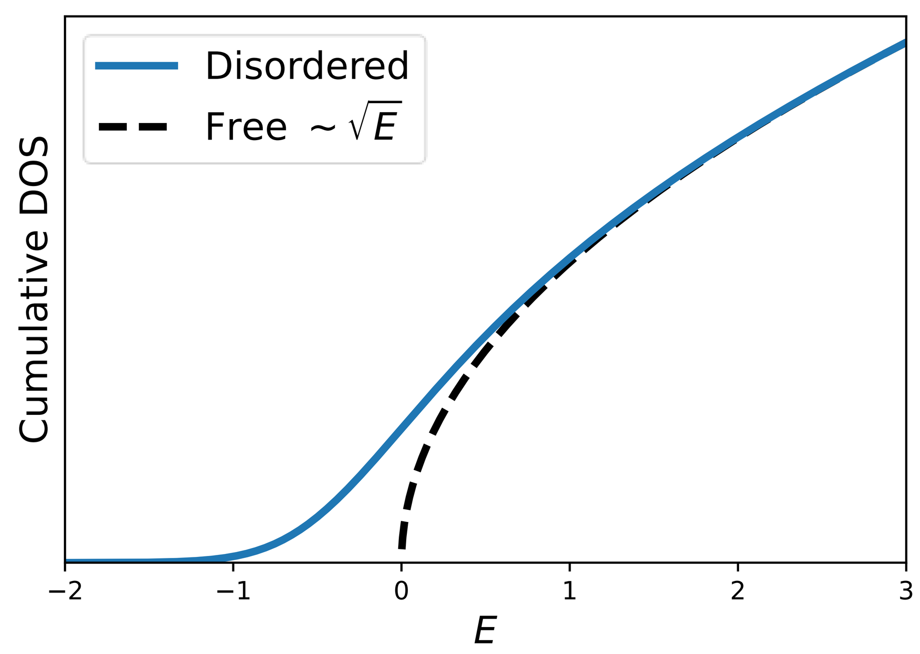

Fig 2. Tailing in 1d for $\beta_4 = 0$. Adapted from [1].

Our objective is to compute the disordered-averaged DOS, which is related to the systems partition function $\mathcal{Z}$ by

$$\rho(E) = \left\langle \frac{1}{V_0}\sum_n \delta(E - E_n) \right\rangle = \frac{2}{\pi V_0} Im\left[\frac{\partial}{\partial E}\langle \ln \mathcal{Z}\rangle\right]. \qquad (2)$$

The average in (2) is evaluated using the replica trick. This results on a field integral with action

$$-\frac{1}{\tilde{g}}\sum_{j=1}^{n}\int d\vec{x}\;\phi_j\left\{\frac{1}{2}\nabla^4 - \frac{\tilde{\beta}_2}{2}\nabla^2 + \frac{1}{2} - \frac{1}{4}\left(\sum_{j=1}^{n}\phi_j{}^2\right)\right\}\phi_j, \qquad (3)$$

where $\tilde{g}^{-1}\sim|E|^{2-\frac{d}{4}}$ and $\tilde{\beta}_2$ are rescaled adimensional parameters. We will approximate the DOS in the low energy regime by using the steepest descent method.

References

[1] Van Mieghem, Piet. "Theory of band tails in heavily doped semiconductors." Reviews of modern physics 64.3 (1992).

[2] Brezin, E., and G. Parisi. "Exponential tail of the electronic density of levels in a random potential." Journal of Physics C: Solid State Physics 13.12 (1980): L307.

[3] Ablowitz, Mark J., and Ziad H. Musslimani. "Spectral renormalization method for computing self-localized solutions to nonlinear systems." Optics letters 30.16 (2005): 2140-2142.

[4] Ng, B. S., and W. H. Reid. "The compound matrix method for ordinary differential systems." Journal of Computational Physics 58.2 (1985): 209-228.

Soliton equation

The field configuration with the largest action contribution is called a soliton [2]. By taking the variance of Eq.(3) they can be shown to be given by

$$-\nabla^2\nabla^2\,\phi(r) + \tilde{\beta}_2\nabla^2\,\phi(r) = \phi(r) - \phi^3(r), \qquad (4)$$

which we solve numerically using spectral renormalization [3].

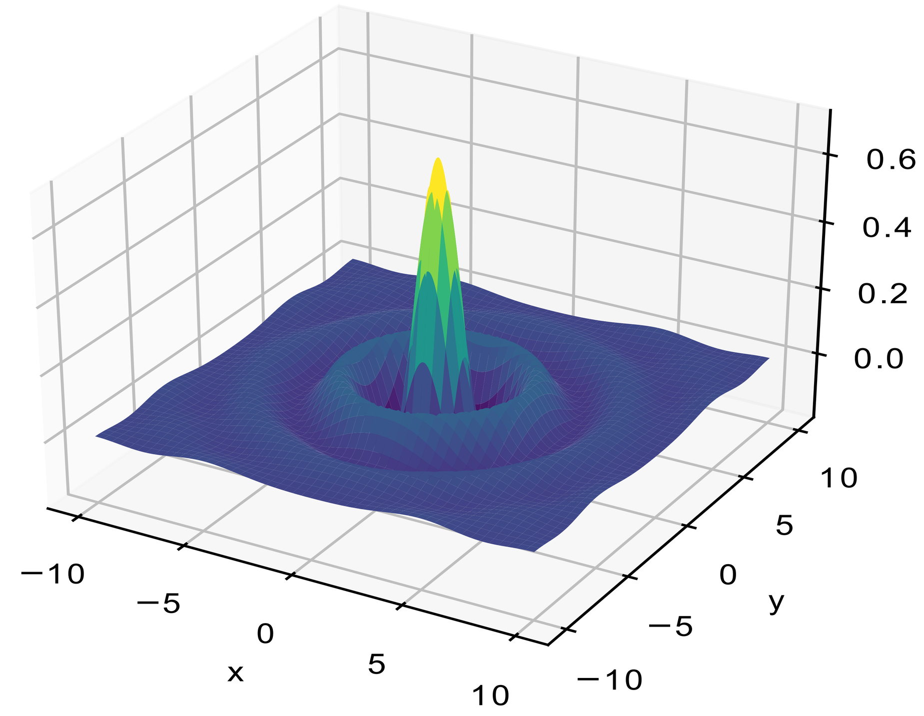

Fig 3. Two-dimensional soliton for $\tilde{\beta}_2 = -1.9$

Since solitons are localized solutions, far from the origin we can neglect the nonlinearity in Eq.(4) and solve the decaying behavior analytically. We then find that for $\tilde{\beta}_2 < -2$ the soliton solution stops existing, so we expect no tailing.

Fluctuations about the soliton

The soliton gives the leading functional dependency of the partition function. The next order of approximation is to consider fluctuations about the soliton. Making use of the spherical symmetry we separate into radial and normal components

$$\phi(\vec{x}) = [\phi(r) + \delta\phi_{\perp}(\vec{x})]\hat{r} + \delta\phi_{\parallel}(\vec{x})\hat{n}. \qquad (5)$$

It is well-known that such fluctuations result in a Gaussian integral evaluable in terms of functional determinants. Following [2] we parametrize the resulting determinants as

$$D(z) = \prod_n \left(1 - \frac{z}{\lambda_n}\right), \qquad (6)$$

where z is used to label the radial and normal cases. The eigenvalues λ_n are determined by

$$\left[\nabla^2\nabla^2 - \tilde{\beta}_2\nabla^2 + 1 - 3\lambda_n\phi^2(r)\right]f(r) = 0, \qquad (7)$$

which we obtain numerically using compound matrix methods [4]. They are shown below for the 1d case.

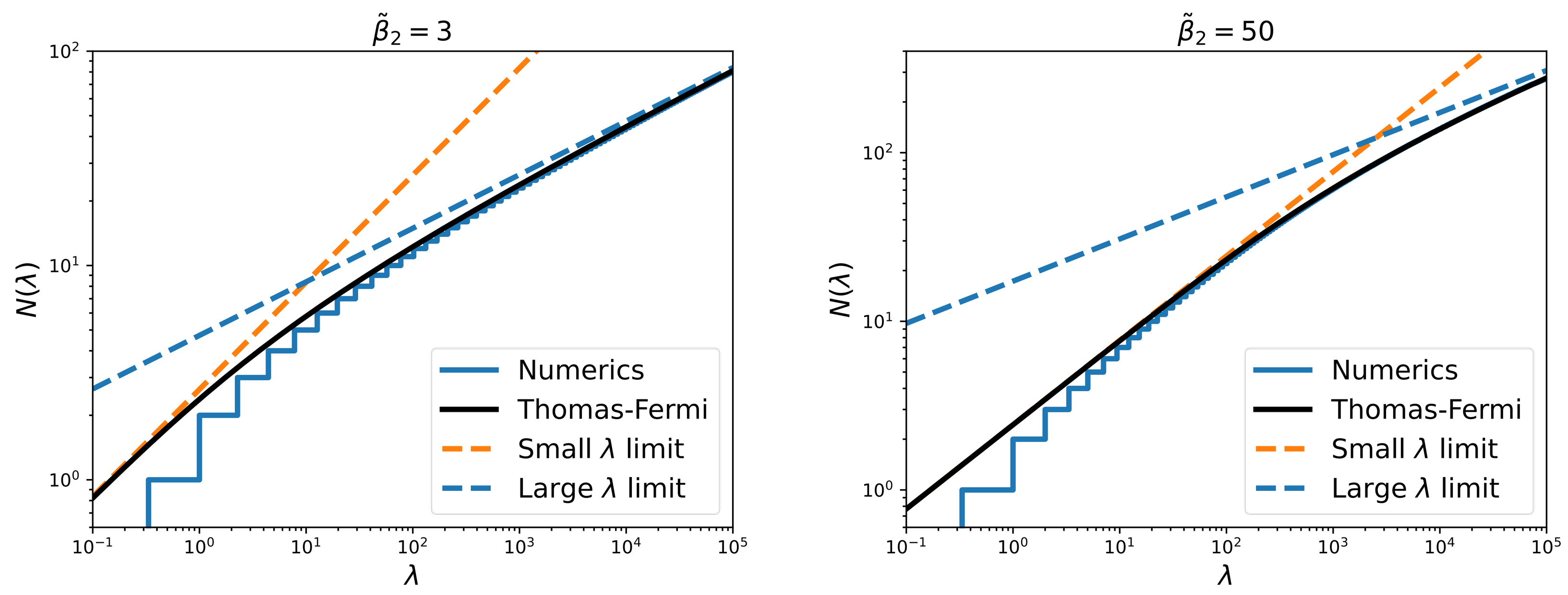

Fig 4. The asymptotic behavior of the eigenvalues can be determined using the Thomas-Fermi approximation.