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Eigenfunction fluctuations and correlations at the mobility edge in a two-dimensional system with spin–orbit scattering

J T Chalker†, G J Daniell‡, S N Evangelou§ and I H Nahm¶
† Theoretical Physics, University of Oxford, 1 Keble Road, Oxford 0X1 3NP, UK
‡ Physics Department, University of Southampton, Southampton SO9 5NH, UK
§ Physics Department, University of Ioanina, Ioanina 451 10, Greece
¶ Physics Department, Sungwha University, PO box 16, Cheonan, Korea

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Abstract. The critical behaviour of wavefunctions at the Anderson metal–insulator transition is studied by numerical simulation, using as an example of a system with a mobility edge a two-dimensional tight-binding model with spin–orbit scattering. It is demonstrated that individual eigenstates have multifractal fluctuations of their probability density. The influence of these fluctuations on the two-particle correlations is examined via calculations of the wavevector and frequency dependence of the diffusion constant.

1. Introduction

This paper is concerned with the nature of single-particle eigenstates near a mobility edge in a disordered conductor. Our aim is to test numerically some current ideas about eigenstate fluctuations and correlations. Briefly, these ideas are that individual eigenstates have a multifractal amplitude distribution [1, 2, 3, 4, 5, 6, 7] and that short-distance correlations between states close in energy should reflect such fluctuations [1, 8, 9, 10]. Numerical simulations are clearly more likely to be successful in low-dimensional systems. There are two circumstances in which planar systems are known to have a mobility edge: in the presence of a magnetic field strong enough to produce the quantum Hall effect, and when spin–orbit scattering is dominant. Studies of a model for the quantum Hall effect have been described elsewhere [9, 11]. Here we present results for behaviour at the mobility edge in a two-dimensional tight-binding model with spin–orbit coupling. Related calculations for a continuum model have been reported recently [12]. Where comparison is possible, our results are in qualitative, but not quantitative agreement with those of [12]

In general terms, it is reasonable to expect eigenstates at a mobility edge to have properties intermediate between those in the insulating and conducting phases. Since localized states are point-like and extended states are space-filling, it is plausible that critical eigenstates should have a fractal amplitude distribution[2]. A range of approaches [1, 3, 5, 6, 7] indicates that the amplitude distribution is, in fact, multifractal, in the sense that the different moments of wavefunction amplitudes scale with independent powers of system size. Calculations of these generalized fractal dimensions for our model are described in section 2.

The low-frequency response of a system to an external probe is determined by correlations between eigenstates close in energy. Associated with an energy

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separation, ω, is a length scale, L_ω: the linear size of a finite system in which the mean level spacing is equal to ω. With ρ being the density of states per unit energy and volume, one has $L_\omega = (\omega\rho)^{-1/d}$ in d-dimensions. This length scale is central to the behaviour of eigenfunction correlations: over short distances compared with L_ω, correlations reflect multifractal fluctuations of individual eigenstates, whilst over long distances, correlations are controlled by relative fluctuations of different eigenstates. In section 3 we present evidence for this crossover in our model, from calculations of the frequency- and wavevector-dependent (ω and q respectively) diffusion constant, $D(q,\omega)$.

Our starting point is the tight-binding Hamiltonian for spin-1/2 particles

$$H = \sum_{i,\alpha} \epsilon_i |i\alpha\rangle\langle i\alpha| + \sum_{ij\alpha\beta} |i\alpha\rangle V_{i\alpha j\beta} \langle j\beta| \tag{1}$$

where $|i\alpha\rangle$ denotes the basis state at site i with spin component α. The random site energies, ϵ_i, are independently and uniformly distributed on $[-w/2, w/2]$. The sites are arranged on a square lattice. We take the lattice spacing as our unit of length and consider systems of size $L \times L$ with periodic boundary conditions in both directions. Non-zero hopping matrix elements, $V_{i\alpha j\beta}$, connect only nearest-neighbour pairs i, j of sites, and have the form

$$V_{i\alpha j\beta} = t^0 \mathbf{1} + \boldsymbol{t}_{ij} \cdot \boldsymbol{\sigma}$$

where 1 is a 2×2 unit matrix in the spin indices α, β and $\boldsymbol{\sigma}$ is the vector of 2×2 Pauli spin matrices. The choice $t^0 = 1$ sets the energy scale. Time-reversal invariance requires that the components of $\boldsymbol{t}_{ij}$ are real; we take them independently and uniformly distributed in $[-\mu/2, \mu/2]$, for each component and each bond i, j. Eigenstates of the model are doubly degenerate and lie in a band centred on energy $E = 0$. The phase diagram has been studied previously [13, 14] using transfer matrix techniques and finite-size scaling. For fixed μ (spin–orbit coupling), states at the band centre are extended if w is small (weak random potential) and localized if w is large (strong random potential). Thus there is a critical line in the $w - \mu$ plane, along which a mobility edge lies at the band centre. Three points on the critical line have been identified: $w = 7$, $\mu = 1$ [13]; $w = 6.0$, $\mu = 0.5$; $w = 8.5$, $\mu = 2.0$ [14]. We use these parameter values in the present work, and examine only those states sufficiently close to the band centre that the localization length at their energies is larger than the finite system size. From previous calculations of the localization length [13], we know that this requirement is satisfied for the M eigenvalues closest to $E = 0$, provided $M \leqslant 1.6L$.

2. *Fluctuations of individual eigenstates*

The amplitude distribution of individual eigenstates can be characterized by the scaling with system size of moments of the associated probability density. We obtain numerically the eigenvectors, $\psi_\alpha(r_i)$, of the Hamiltonian, equation (1), and calculate the moments

$$P_q = \left\langle \sum_{r_i} \left[\sum_\alpha |\psi_\alpha(r_i)|^2 \right]^q \right\rangle \tag{2}$$

where $\sum_\alpha$ is a sum over spin components, $\sum_{r_i}$ is a sum over sites, and the average, $\langle \ldots \rangle$ runs over states within a window (described above) around the mobility edge, and also over different realizations of the Hamiltonian with $w = 7.0$ and $\mu = 1.0$ (2000, 600, 600, 400, 400 and 50 samples, for $L = 6$, 8, 10, 12, 14 and 18, respectively).

If P_q decreases as a power of the system size, the multifractal exponent [15], D_q, is defined via $P_q \sim L^{-(q-1)D_q}$. A natural extension to the special case, $q = 1$, is to define $-D_1$ as the slope of

$$\log(P_1) \equiv \left\langle \sum_{r_i} \left[\sum_\alpha |\psi_\alpha(r_i)|^2 \right] \log \left(\sum_\alpha |\psi_\alpha(r_i)|^2 \right) \right\rangle$$

against $\log(L)$. For localized states, one expects $D_q = 0$ for all q, whilst for uniformly extended states, $D_q = d$, independent of q. Intermediate values of D_q can be interpreted as the generalized dimension of the set of sites on which resides the dominant contribution to the qth moment of the probability density.

Table 1. Values determined for the generalized fractal dimensions, D_q.

D_0	D_1	D_2	D_3	D_4
1.84	1.63	1.48	1.35	1.18

The dependence we obtain for $\log(P_q)$ on $\log(L)$ is illustrated in figure 1. The resulting exponents, D_q, are shown in figure 2 and table 1. There is a clear indication of multifractal behaviour for the q-values studied, in the sense that $d > D_q > 0$ and that D_q varies with q.

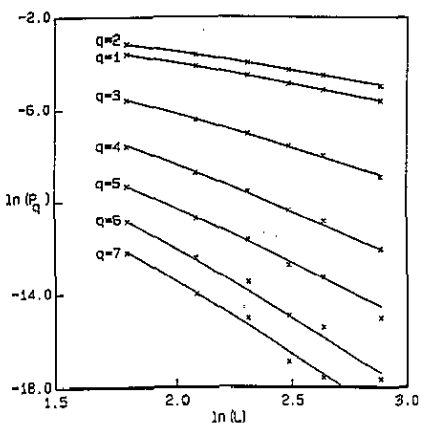

Figure 1. Dependence of P_q, the qth moment of the probability density, on system size, L.

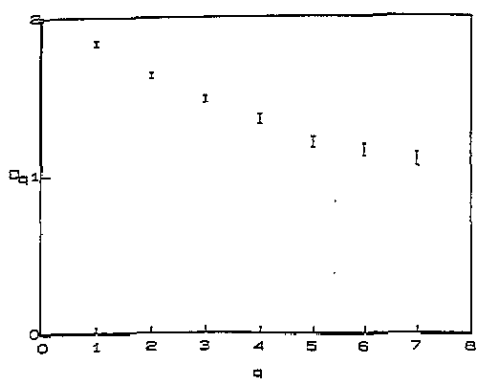

Figure 2. Dependence of D_q, the generalized fractal dimension, on q.

3. Correlations between eigenstates

The simplest measure of correlations between eigenstates at different energies is the two-particle spectral function, defined by

$$S(r;E,\omega)=\Big\langle\sum_{\alpha,\beta}\sum_{m,n}\delta(E+\omega/2-E_m)\delta(E-\omega/2-E_n)$$
$$\times\,\psi^*_{\alpha,m}(0)\psi_{\beta,m}(r)\psi^*_{\beta,n}(r)\psi_{\alpha,n}(0)\Big\rangle \tag{3}$$

where $\psi_{\alpha,m}(r)$ is the amplitude of the mth eigenstate, with energy E_m and spin component α at site r. In terms of the Fourier transform

$$S(q;E,\omega)=\sum_r e^{iqr}S(r;E,\omega)$$

the hydrodynamic (small q, ω) behaviour of the spectral function can be parameterized by a wavevector- and frequency-dependent diffusion constant, according to

$$S(q;E,\omega)\underset{q,\omega\to 0}{\sim}\frac{\rho}{\pi}\frac{D(q,\omega)q^2}{\omega^2+[D(q,\omega)q^2]^2}.$$

Scaling arguments [16, 17, 18, 10] suggest that, at a mobility edge, $D(q,\omega)$ should depend only on the variable $(q^d/\rho\omega)\equiv(qL_\omega)^d$. Its form for $qL_\omega\ll 1$ is related to the scaling with distance of the conductivity, and for $qL_\omega\gg 1$ is dominated by fluctuations of single eigenstates. In two dimensions one expects [10]: $D(q,\omega)\sim$ constant, for $qL_\omega\ll 1$; and $D(q,\omega)\sim(qL_\omega)^{-\eta}$, for $qL_\omega\gg 1$, with $\eta=1-D_2/2$.

We use eigenfunctions and eigenvalues obtained by numerical diagonalization of the Hamiltonian, equation (1), to calculate $S(q,\omega)$ at the mobility edge. One of the delta functions in the definition, equation (3), is replaced by integration over a narrow energy window and the other is replaced with a gaussian of width $\sigma=4.3L^{-2}$, comparable to the mean level spacing. The calculations span a range of wavevectors ($q=(2\pi/L)(k,l)$ with $k,l=0,1,2$) and energies ($\omega=n\sigma$ with $n=2,3\ldots 19$), and involve an average over 2000, 400, 100 and 20 samples, for $l=8,12,16$ and 20, respectively. We combine all determinations of $S(q,\omega)$ relating to a given value of the scaling variable, q^2/ω, and extrapolate $\omega S(q,\omega)$ to $\omega=0$, in order to find the hydrodynamic behaviour. Four such extrapolations are illustrated in figure 3. Finally, the diffusion constant, extracted from these values of $\omega S(q,\omega)$, is displayed as a function of the scaling variable, q^2/ω, in figure 4.

4. Discussion

Our results are much less clear-cut than those from an analogous calculation using a model for the quantum Hall effect [9, 11]. There are probably two reasons for this. First, because of the spin degree of freedom in the present case, we are restricted to spatially smaller systems. Second, because in the present case we start from a lattice

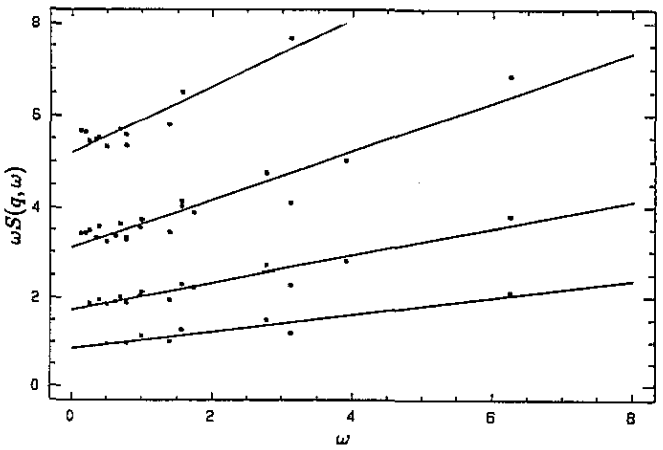

Figure 3. Extrapolations of $\omega S(q,\omega)$ to the hydrodynamic regime, for four values of the scaling variable, q^2/ω.

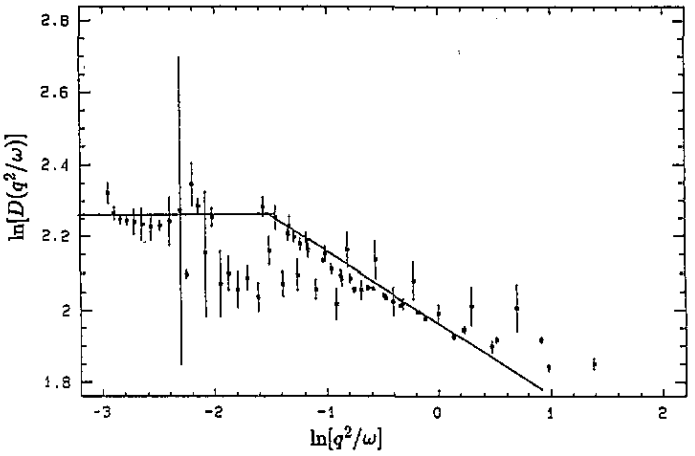

Figure 4. Dependence of the diffusion constant on the scaling variable q^2/ω. The data points are values derived from calculations of $\omega S(q,\omega)$, with error bars arising from the uncertainty in the extrapolation to the hydrodynamic regime. The lines indicate the behaviour expected theoretically in the small and large q^2/ω limits, with the slope in the latter case taken from our determination of the fractal exponent, D_q.

model, $S(q,\omega)$ has an appreciable anisotropy in q-space, except at the smallest q-values studied. This naturally complicates the extrapolation to the hydrodynamic limit.

Despite these difficulties, there is a plausible indication from the data in figure 4 that the diffusion constant decreases for large values of the scaling variable, q^2/ω. The rate of decrease is compatible with the value of the fractal exponent, $D_2 = 1.48$, determined from the properties of single eigenstates.

Acknowledgments

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