Disordered systems in phase space

Dietmar Weinmann[1], Sigmund Kohler[1,2], Gert-Ludwig Ingold[1],
and Peter Hänggi[1]

[1]Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany
[2]Faculdad de Ciencias, Universidad Autonoma de Madrid, 28049 Madrid, Spain
Gert.Ingold@Physik.Uni-Augsburg.DE

Abstract. As a function of the disorder strength in a mesoscopic system, the electron dynamics crosses over from the ballistic through the diffusive towards the localized regime. The ballistic and the localized situation correspond to integrable or regular behavior while diffusive conductors correspond to chaotic behavior. The chaotic or regular character of single wave functions can be inferred from phase space concepts like the Husimi distribution and the Wehrl entropy. These quantities provide useful information about the structure of states in disordered systems. We investigate the phase space structure of one dimensional (1d) and 2d disordered systems within the Anderson model. The Wehrl entropy of the eigenstates allows to detect the crossover between the ballistic, diffusive and localized regime.

The presence of a disordered potential in mesoscopic systems strongly affects the structure of the quantum states and thereby the electronic properties of the sample. The disorder results in a finite elastic mean free path l and can lead to exponential localization of the wave functions with localization length ξ [1]. The electronic properties of the sample can be classified according to the ratios l/L and ξ/L of these length scales to the system size L. When $l > L$, the dynamics is ballistic, the wave functions being close to the plain waves with fixed momentum value found in clean systems. In contrast, the regime $\xi < L$ is called localized since the wave functions are restricted to a finite domain in real space. This implies delocalization in momentum space. A crossover between wave function structures localized in momentum space and localized in real space occurs as a function of the disorder strength. In the intermediate regime, when $l < L < \xi$, the dynamics of the particles in the disordered potential is diffusive. The particles are scattered several times while traversing the system, but the localization of the wave function is not relevant on the scale L, leading to a complex structure of the wave function. The crossover between the different regimes is accompanied by a change of not only the structure of wave functions, but also the energy level statistics. This suggests that disordered systems in the diffusive regime exhibit chaos in contrast to the ballistic and the localized regime which are both classified as integrable.

In order to investigate the changes of the structure of the wave functions throughout all regimes, it is desirable to use a concept which allows to detect both, changes in real space and in momentum space structure. A quantum state $|\psi\rangle$ is completely determined by its wave function in real space representation $\psi(x) = \langle x|\psi\rangle$ or by its

momentum space representation. It is nevertheless possible to construct quantities which depend on both, position and momentum $p = \hbar k$, and to study the structure of the wave functions in phase space (x, k). The Husimi density characterizing a given state $|\psi\rangle$,

$$\rho_{\mathrm{H}}(x_0, k_0) = |\langle x_0, k_0 | \psi \rangle|^2 , \tag{1}$$

is given by the projection of $|\psi\rangle$ on minimal uncertainty states $|x_0, k_0\rangle$. We use Gaussian wave packets with variance σ^2, centered around position x_0 and wave number k_0. In real space representation, these states are given by

$$\langle x | x_0, k_0 \rangle = \left(\frac{1}{2\pi\sigma^2} \right)^{1/4} \exp \left(-\frac{(x - x_0)^2}{4\sigma^2} + \mathrm{i}k_0 x \right) . \tag{2}$$

This definition of ρ_{H} yields the normalization $\int \frac{\mathrm{d}x\mathrm{d}k}{2\pi} \rho_{\mathrm{H}}(x, k) = 1$. The resulting Husimi-distribution can be used to visualize the phase space structure of quantum states. Its analysis allows to detect structures in wave functions which correspond to the classical dynamics in phase space [2]. Since ρ_{H} is always nonnegative, the Wehrl entropy

$$S_{\mathrm{H}} = -\int \frac{\mathrm{d}x\mathrm{d}k}{2\pi} \rho_{\mathrm{H}}(x, k) \ln [\rho_{\mathrm{H}}(x, k)] \tag{3}$$

can be defined [3, 4]. S_{H} is a measure of the phase space volume occupied by the quantum state. It has been shown for the driven rotor that the Wehrl entropy of individual states is connected to the energy level statistics. Both quantities can be used to distinguish between the chaotic and the integrable regime [5]. A very similar system, the kicked rotor, can be mapped onto the Anderson model [6], suggesting that the Wehrl entropy is a useful quantity for the characterization of the eigenstates of the Anderson model.

The Anderson Hamiltonian [1] describes a particle on a lattice. Its 1d version reads

$$H_{\mathrm{A}} = -t \sum_n (|n\rangle\langle n+1| + |n+1\rangle\langle n|) + W \sum_n v_n |n\rangle\langle n| \tag{4}$$

with Wannier states $|n\rangle$ localized at sites n. In units of the lattice spacing, the position of a site is $x_n = n$. The hopping matrix elements $t = 1$ between neighboring sites define the energy scale. The on-site disorder v_n is drawn from a box distribution inside the interval $[-1/2; 1/2]$, and W denotes the disorder strength.

We have evaluated the Husimi distributions for 1d rings containing $L = 100$ sites with periodic boundary conditions $|n\rangle \equiv |n + L\rangle$. In order to adapt the minimum uncertainty states to the lattice structure and the ring geometry of our model, we use the form (2) in the interval $x_0 - L/2 \le x \le x_0 + L/2$ such that the tails of the Gaussian in real space are cut opposite to the position of the maximum x_0. The lattice determines the possible values of the wave numbers $k_0 = 2\pi j/L$, with $j = \{-L/2 + 1, -L/2 + 2, \ldots, L/2\}$ (L even) for the first Brillouin zone. The phase space (x, k) is then represented by a $L \times L$ lattice. The choice $\sigma = \Delta x = \sqrt{L/4\pi}$ in (2) ensures that the minimum uncertainty states with $\Delta x \Delta k = 1/2$ are extended in x and in k direction over the same number of allowed discrete values.
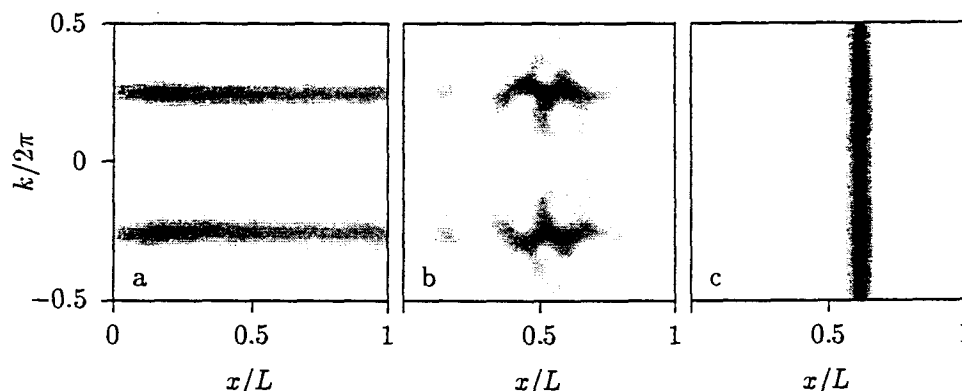
Fig. 1 Husimi distribution of an eigenstate of the 1d Anderson model of length $L = 100$ at $W = 0.5$ (a), 3 (b), and 300 (c).

The eigenstates of (4) at $W = 0$ are plain waves. This means complete delocalization in real space and maximum localization in momentum space. Obeying the symmetry $\rho_H(x,k) = \rho_H(x,-k)$, the corresponding Husimi density, presented in Fig. 1a, reflects this structure by exhibiting two lines parallel to the x-axis. In the limit of very strong disorder, the wave functions are completely localized in real space but delocalized in momentum space. Then, the Husimi density (Fig. 1c) is given by a line parallel to the k-axis. These phase space structures are typical for the ballistic ($l \gg L$) and the localized ($\xi \ll L$) regime, respectively. Since $l \approx \xi$ in 1d, no diffusive regime with chaotic wave functions appears. In the crossover regime, when L equals a few ξ, the Husimi density is subject to strong fluctuations. The typical situation is intermediate between the scenarios described above, and the density is more or less extended in both variables, position and wave number, as can be seen in Fig. 1b.

Fig. 2a shows the Wehrl entropies of 60 eigenstates around the band center for a ring of size $L = 100$ as a function of the disorder. While the average of the Wehrl entropy in 1d decreases when the disorder is increased (ρ_H exhibits two stripes when $W \to 0$, while for $W \to \infty$, only one is present, see Fig. 1), its variance clearly exhibits a maximum in the crossover region around $W \approx 3$. The entropies for states at the band edge, where the two stripes at k and $-k$ in the ballistic regime overlap are not shown, leading to well-defined values in both limits $W \to 0$ and $W \to \infty$.

Using a straightforward extension of the above concepts to 2d systems, we have also investigated the phase space structure of the eigenstates of the 2d Anderson model. The phase space $(x_1, x_2; k_1, k_2)$ is now four-dimensional and the corresponding minimum uncertainty states are given by products of two terms of the form (2). While it becomes difficult to visualize the Husimi density, the Wehrl entropy, now being obtained from a four-dimensional integral, still provides a measure for the phase space occupation of the state. In Fig. 2b, we plot the entropies for a few states below the band center in order to avoid artifacts arising at low disorder from the singularity of the density of states. In contrast to the 1d situation, the localization length is always larger than the mean free path in 2d, and the diffusive regime appears when $l < L < \xi$
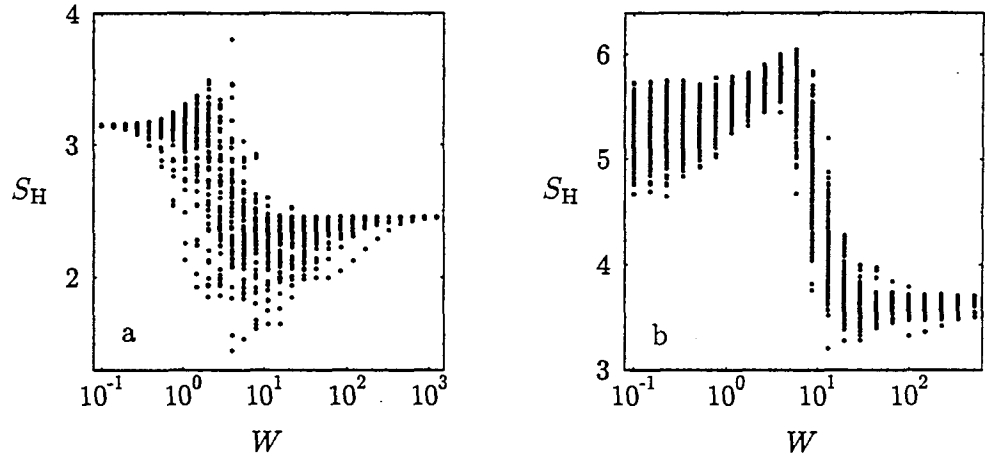
Fig. 2 a: Wehrl entropies for the states of the 1d Anderson model of length $L = 100$. Data for 60 states around the band center are shown. b: Wehrl entropies for states 180-359 on a 2d lattice of 30×30 sites.

(for our case $L = 30$, using data from [7], this corresponds to the disorder interval between $W \approx 1.5$ and $W \approx 6$). This situation is accompanied by an enhancement of the Wehrl entropy, confirming the expected chaotic character of the wave functions. The ballistic and localized limits remain regular, being characterized by smaller values of the Wehrl entropy. While all entropies converge towards the same value when $W \rightarrow \infty$, a certain variance of entropies remains in the limit $W \rightarrow 0$. In contrast to the 1d case, this cannot be avoided because it is not possible to exclude the few states with overlapping stripes in the ballistic regime by selecting a certain energy interval.

In conclusion, we have shown that phase space concepts indeed provide useful information about the states of disordered systems. In particular, they allow to distinguish the different transport regimes. It will be interesting to use this new method for detailed investigations of the Anderson metal-insulator transition, as well as for correlations in many-body problems.

References

[1] P.W. Anderson, Phys. Rev. 109 (1958) 1492
[2] K. Takahashi and N. Saitô, Phys. Rev. Lett. 55 (1985) 645
[3] A. Wehrl, Rep. Math. Phys. 16 (1979) 353
[4] B. Mirbach and H.J. Korsch, Phys. Rev. Lett. 75 (1995) 362
[5] T. Gorin, H.J. Korsch, and B. Mirbach, Chem. Phys. 217 (1997) 145
[6] S. Fishman, D.R. Grempel, and R.E. Prange, Phys. Rev. Lett. 49 (1982) 509
[7] B. Kramer and A. MacKinnon, Rep. Prog. Phys. 56 (1993) 1469