Delocalization and Heisenberg's uncertainty relation

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Abstract. In the one-dimensional Anderson model the eigenstates are localized for arbitrarily small amounts of disorder. In contrast, the Aubry-André model with its quasiperiodic potential shows a transition from extended to localized states. The difference between the two models becomes particularly apparent in phase space where Heisenberg's uncertainty relation imposes a finite resolution. Our analysis points to the relevance of the coupling between momentum eigenstates at weak potential strength for the delocalization of a quantum particle.

1 Introduction

The behaviour of a quantum particle in a one-dimensional extended potential depends strongly on the nature of the potential as well as on the potential strength. While in the absence of a potential, the particle moves ballistically and is described by a plane wave, disordered potentials or certain quasiperiodic potentials of sufficient strength will lead to localized states. For a disordered potential, the transition from ballistic to localized states is smooth and the crossover shifts to ever smaller potential strength as the system size is increased [1]. In contrast, there exist quasiperiodic potentials like in the Aubry-André model where one observes a localization transition in the limit of large system sizes [2,3]. It is this qualitative difference between the Anderson model and the Aubry-André model which has stimulated the following study.

As an example for disordered systems, the analysis of the wave functions of the Anderson model either in real or in momentum space shows that position and momentum interchange their role as the potential strength is inverted [4]. In the Aubry-André model with its quasiperiodic potential, there even exists a strict duality between weak and strong potential connected with an interchange of position and momentum [2]. Therefore, one would not expect qualitative differences between the two models quite in contrast to the existence of a phase transition in the Aubry-André model.

In this paper, we will demonstrate that it is only a phase space analysis which reveals the significant differences between a disordered and a quasiperiodic potential. The existence of a localization transition in the Aubry-André model will be traced back to the nature of the coupling between plane waves by a weak potential, thereby giving insight into the mechanism of this transition. Furthermore, we will point out why phase space studies of quantum systems allow to extract more information than considerations of real or momentum space alone.

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2 Random and quasiperiodic potential

The Hamiltonian of the Anderson model is given by [5]

$$H = -\sum_n \left(|n\rangle\langle n+1| + |n+1\rangle\langle n|\right) + W\sum_n v_n |n\rangle\langle n| \tag{1}$$

where the Wannier states $|n\rangle$ are localized at the sites $n = 1,\ldots,L$ of a ring with periodic boundary conditions. The first term on the right-hand side describes the kinetic energy which defines the energy scale. The random potential of strength W is expressed by the second term. The distribution of on-site energies is determined by the coefficients v_n distributed uniformly on the interval $[-1/2;1/2]$. In the limit $L\to\infty$ the eigenstates of the Anderson model are known to localize for any nonvanishing potential strength W [5,6].

The second model of interest, the Aubry-André model, is defined by the Hamiltonian [2,7]

$$H = \sum_n \left(|n\rangle\langle n+1| + |n+1\rangle\langle n|\right) + \lambda\sum_n \cos\left(2\pi\beta n\right)|n\rangle\langle n| \tag{2}$$

where the random potential in (1) has been replaced by a quasiperiodic potential if the parameter β assumes an irrational value in the limit $L\to\infty$. This model was originally considered by Harper [7] with $\lambda = 2$ and variable β.

In the present context, we are interested in the version due to Aubry and André where a transition from extended to localized states occurs with increasing potential strength at $\lambda = 2$ for a so-called diophantic irrational β [3] which is kept fixed.

For finite size systems, it is convenient to choose $\beta = F_{i-1}/F_i$ where F_{i-1} and F_i are two successive Fibonacci numbers [8]. In the limit of large systems, β approaches the inverse of the golden mean, $(\sqrt{5}-1)/2$. With this choice of β the system contains $L = F_i$ lattice sites with F_{i-1} periods of the potential.

The Aubry-André model possesses an interesting duality property [2] which becomes evident by transforming Wannier states $|n\rangle$ into new states

$$|k\rangle = L^{-1/2} \sum_n \exp(\mathrm{i}2\pi k\beta n)|n\rangle$$
$$= L^{-1/2} \sum_n \exp\left(\mathrm{i}2\pi \frac{kF_{i-1}}{L} n\right)|n\rangle \cdot \qquad (3)$$

These are eigenstates of the momentum operator to eigenvalues $kF_{i-1} \bmod F_i$. Neighbouring values of k therefore do not imply neighbouring momentum eigenvalues.

With the transformation (3) one obtains the dual Hamiltonian

$$H = \frac{\lambda}{2}\left[\sum_k \left(|k\rangle\langle k+1| + |k+1\rangle\langle k|\right) + \frac{4}{\lambda}\sum_k \cos\left(2\pi\beta k\right)|k\rangle\langle k|\right] . \qquad (4)$$

By this transformation real and momentum space are interchanged and the original potential strength λ becomes inverted into $4/\lambda$. Comparison of (2) and (4) yields the self-dual point $\lambda = 2$ which separates the parameter regimes of extended and localized states. In contrast to the nearest neighbour coupling in real space in (2), the new Hamiltonian does not couple nearest neighbour momenta. The physical reason is that scattering by the incommensurate potential may change the momentum by a large amount. This coupling to quite different momentum values will be of central importance for our reasoning below.

3 Real and momentum space

After this discussion, the question arises why these two archetypical models behave so differently. In particular, what is the physical reason which allows a localization transition at finite value $\lambda = 2$ in the Aubry-André model? In order to answer this question, we first take a look at the structure of the wave function $|\psi\rangle = \sum_n c_n|n\rangle$ expressed in terms of the Wannier states $|n\rangle$, which will provide information about the spatial extension of the state. An often used quantity is the inverse participation ratio in real space [9–12]

$$P_x = \sum_n |c_n|^4 . \qquad (5)$$

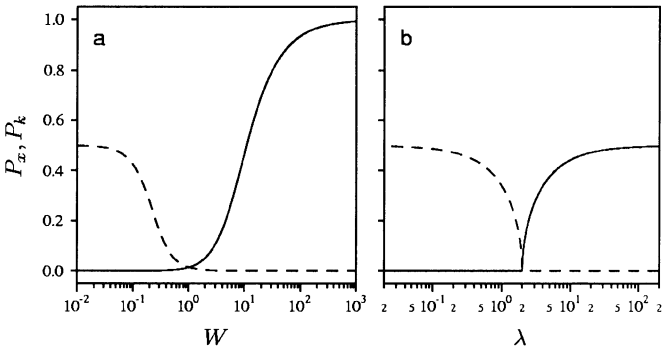

Fig. 1. The inverse participation ratio in real space (full line) and momentum space (dashed line) is shown (a) for the Anderson model with $L = 2048$ and (b) for the Aubry-André model with $L = 10946$. The curves represent averages over an ensemble of eigenstates of the respective Hamiltonian as explained in the text.

Provided that $\sum_n |c_n|^2 = 1$, the inverse of this quantity indicates the number of lattice sites over which the wave function is distributed. A corresponding quantity

$$P_k = \sum_n |d_n|^4 \qquad (6)$$

can be defined in momentum space, where

$$d_n = L^{-1/2} \sum_l \exp\left(\mathrm{i}2\pi \frac{nl}{L}\right) c_l \, . \qquad (7)$$

The two quantities are depicted as full lines (real space) and dashed lines (momentum space) in Figure 1a for the Anderson model of length $L = 2048$ and Figure 1b for the Aubry-André model of length $L = 10\,946$. For the Anderson model, the curves represent an average over 50 disorder realizations with $L/2$ states around the band center each. For the Aubry-André model, an average over all symmetric eigenstates has been taken [13].

For both models one observes a monotonically increasing inverse participation ratio in real space which corresponds to an increasing localization of the eigenfunctions as the potential strength is increased. Correspondingly, the inverse participation ratio in momentum space decreases with increasing potential strength, indicating a delocalization in momentum. The different limiting values of P_x for strong potential reflect the fact that in the Anderson model the eigenfunctions localize at one site while in the Aubry-André model two sites are occupied because we consider here symmetric eigenstates.

While the overall picture is qualitatively the same for both models, we note an important difference which becomes apparent when the system size is changed. In the Anderson model, the transition from extended to localized states is smooth and notably shifts to lower values of W as L is increased. As a consequence, in the limit of infinite system size all states are localized if finite disorder

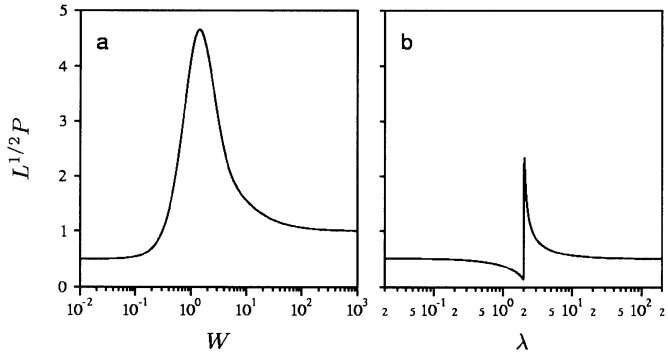

Fig. 2. The inverse participation ratio in phase space is shown (a) for the Anderson model with $L = 2048$ and (b) for the Aubry-André model with $L = 10946$. The averages have been taken with respect to the same states as in Figure 1.

is present. In contrast, for the Aubry-André model one observes a sharp transition at $\lambda = 2$ for sufficiently large system sizes.

4 Phase space approach

The differences between the two models become much more distinct in phase space. This approach has the advantage of providing a consistent description for arbitrary potential strength [14]. The inverse participation ratio in phase space [4,15,16]

$$P = \int \frac{\mathrm{d}x\mathrm{d}k}{2\pi} [\varrho(x,k)]^2 \tag{8}$$

is based on the positive definite phase space density provided by the Husimi function [17] or Q function [18]

$$\varrho(x_0,k_0) = |\langle x_0,k_0|\psi\rangle|^2. \tag{9}$$

Here, the state $|\psi\rangle$ is projected onto a minimal uncertainty state centered around position x_0 and momentum k_0. In order to ensure equal resolution in the two directions of phase space, we choose the width of the Gaussian as $\sigma = \Delta x = \sqrt{L/4\pi} = 1/2\Delta k$.

In Figure 2 we present the inverse participation ratio in phase space scaled with $L^{1/2}$ which is appropriate in the absence of a potential as well as for very strong potentials [4]. For the Anderson model (Fig. 2a), one obtains an increased inverse participation ratio at intermediate potential strengths implying that the eigenstates contract in phase space. As we will demonstrate below, the behaviour to the left of the peak is dominated by a contraction in real space corresponding to the increase of P_x (*cf.* Fig. 1a) while to the right of the peak the decrease is dominated by the decrease of P_k.

The qualitative agreement between the inverse participation ratios in real and momentum space for the Anderson and Aubry-André models suggests that the same should hold true for the inverse participation ratio in phase space. This is even more so since the scenario just described for the Anderson model is consistent with the duality property of the Aubry-André model where an inversion of the potential strength is accompanied by a transformation between real and momentum space. However, the results depicted in Figure 2b tell a different story.

In contrast to the Anderson model, the inverse participation ratio P shown in Figure 2b initially decreases with increasing potential strength up to $\lambda = 2$. In this regime, the eigenstates therefore become more and more delocalized in phase space. Then, at $\lambda = 2$, the phase space distribution contracts and starts to become delocalized in momentum as λ is increased further. Therefore, for almost all values of λ, the phase space behaviour is dominated by the momentum component except for the transition which is dominated by the real space behaviour.

The two curves shown in Figure 2 result from the same averaging procedure as was employed to obtain the Figures 1a and b. It is important to note that the variance of the inverse participation ratio at a given potential strength is so small that the peak in Figure 2a and the jump in Figure 2b represent genuine features. In particular, for the Anderson model the inverse participation ratio for a given state displays a maximum at intermediate disorder strength [4]. On the other hand, in the Aubry-André model the jump of the inverse participation ratio at $\lambda = 2$ is found for all states. Furthermore, the dependence on system size shows the expected behavior. In the Anderson model, the curves scale to smaller disorder with increasing system size [19], while in the Aubry-André model, the jump remains at the critical value of $\lambda = 2$ [20].

The question now arises, why for weak potential the Anderson and Aubry-André models behave so differently while for strong potentials they behave in the same way. The mechanism at work for weak potential can be considered to be responsible for the localization transition in the Aubry-André models because the jump found in Figure 2b can only occur if the phase space distribution broadens as λ is increased from zero.

5 Uncertainty in phase space

Before addressing this question in detail, we recall the Gaussian smearing arising from the projection onto minimal uncertainty states which is inevitable if a positive definite phase space density is required. As a consequence, the Husimi function only provides limited resolution which, as discussed above, we have chosen to be equal for the spatial and momentum components. The resolution is of the order of $\sqrt{L}$ sites which in the thermodynamic limit becomes small compared to the number L of sites in real as well as momentum space. It should be kept in mind, however, that for large L a phenomenon occurring on a fixed and finite number of sites cannot be resolved. These considerations would still hold, if we chose Δx and $1/\Delta k$ to scale according to L^α with $0 < \alpha < 1$. In contrast, an entirely different situation arises, if we keep the resolution fixed in one of the two phase space directions as is the case for the inverse participation ratios in real and momentum space, (5) and (6). Then, even in the thermodynamic limit no effects occurring in the other direction can be resolved.

6 Limit of strong potential

We are now in a position to answer the question raised above. It is useful to start by considering the limit of strong potential where the phase space behaviour of the Anderson and the Aubry-André models agree. For infinitely strong potential, the eigenstates of the Anderson model are localized at one site while for the Aubry-André model it is sufficient to restrict the discussion to one of the two sites occupied by a symmetric eigenstate. The kinetic energy may now be considered as a perturbation coupling in lowest order to the two neighbouring sites. The dominant contribution will be due to the neighbouring site closer in energy so that the problem reduces to the solution of a two-level system [19].

The energy eigenstates at very large but finite potential strength will be delocalized over two sites. While this will reduce the inverse participation ratio P_x in real space, it will not directly affect the inverse participation ratio P in phase space which can only resolve spatial structures of size $\sqrt{L}$ and larger. We recall, that this argument is independent of our particular choice of σ since the absolute width of the minimal uncertainty state has to increase with increasing system size even though its relative width decreases to ensure a proper classical limit.

The increase in P observed in Figure 2 with decreasing potential strength therefore has to be explained in momentum space. The spatially localized states occurring for infinite potential strength are fully delocalized in momentum space. Now, a coupling of states due to the kinetic energy leads to a contraction of the momentum distribution. This can readily be verified by considering as an example the superpositions $(|n\rangle \pm |n+1\rangle)/\sqrt{2}$ which in momentum space exhibit large scale density oscillations of period L. By means of the Fourier transformation the effect of the coupling on short real space distances, too small to be resolved in phase space, is turned into a large scale phenomenon in momentum space. Therefore, in the momentum component the coupling is easily detected even with the finite resolution of the Husimi function. As a consequence, the behaviour of the inverse participation ratio in phase space is dominated by momentum which allows to understand the increase of the inverse participation ratio with decreasing potential strength depicted in Figure 2.

7 Limit of weak potential

We now apply a similar perturbative reasoning to the regime of weak potential by starting from momentum eigenstates, *i.e.* states well localized in momentum analogous to the localized states in real space considered before. In the Anderson model the random potential will lead to a coupling among all momentum eigenstates. However, as before, the coupling between states close in energy, and therefore close in momentum, will be most effective. As a consequence, the role of position and momentum are interchanged and with the same arguments as above, we find an increase of the inverse participation ratio in phase space with increasing potential strength, albeit now due to the behaviour in real space. Within this perturbative treatment, we can readily understand the behaviour of P depicted in Figure 2a.

The situation is quite different for the Aubry-André model where we may consider the dual model (4) for small λ. The perturbation is now represented by the first term on the right-hand side of (4) which couples to well-defined momentum eigenstates. However, as remarked below (4), due to the scattering by the incommensurate potential these eigenstates in general do not correspond to nearest neighbour momenta. For most of the energy eigenstates, the momentum eigenstates to which the coupling occurs are far away on the scale of the resolution of the Husimi function. The resulting broadening of the momentum distribution leads to a reduction of the inverse participation ratio. In real space, on the other hand, the coupling will lead to short scale oscillations which are not resolved because of the finite resolution σ in phase space. Therefore, the influence of the momentum component dominates and the inverse participation ratio decreases with increasing potential strength.

It follows from this discussion that, in contrast to the Anderson model, the Aubry-André model for both weak and strong potential is dominated by the momentum properties. It is only around $\lambda = 2$ that real space becomes important. From the comparison of the Anderson and the Aubry-André models we conclude, that the form of the coupling between the momentum eigenstates due to a weak potential plays a decisive role for the structure of the eigenstates in phase space and for the appearance of a delocalization-localization transition.

As a further example we briefly comment on the Anderson model in two and three dimensions where the inverse participation ratio in phase space behaves very much like in the case of the Aubry-André model (*cf.* Fig. 2b) [4]. In the marginal case of two dimensions, the tendency towards a transition is therefore clearly visible for finite system size, even though the critical disorder strength vanishes in the thermodynamic limit [19] and no true phase transition occurs. In contrast, in three dimensions the Anderson transition is recovered [21,22]. The main difference between the Anderson model in one dimension on the one hand and in two and three dimensions on the other hand lies again in the coupling of momentum eigenstates by a weak random potential. In the one-dimensional case, eigenstates close in energy are necessarily close in momentum. In contrast, in higher dimensions there may exist even energetically degenerate states far away in momentum, so that they can be resolved in phase space.

8 Conclusions

A crucial aspect of our discussion was the finite resolution available in phase space. This is in strong contrast to the ideal resolution available with the inverse participation ratio in real or momentum space, albeit only in one direction of phase space. As a consequence, there is no possibility to resolve the other direction even in the limit of large system size. Accepting Heisenberg's uncertainty relation

and thus the finite resolution in phase space allows one to analyze the structure of the eigenstates in real as well as momentum space and, as was demonstrated above, to obtain valuable information about the model of interest.

This is corroborated by a recent observation by Varga *et al.* [23], that instead of a full-fledged phase space calculation, one can alternatively make use of marginal distributions in real and momentum space. Even though the inverse participation ratios deduced from them resemble those defined in equations (5) and (6) a Gaussian smearing is again crucial.

We therefore conclude that for the understanding of the localization properties of a quantum particle, where both position and momentum are relevant, the smearing in phase space called for by the uncertainty relation is not only necessary but also represents an essential ingredient of the physical argumentation.

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