The Aubry–André model as a hobbyhorse for understanding the localization phenomenon

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Abstract
We present a thorough pedagogical analysis of the single particle localization phenomenon in a quasiperiodic lattice in one dimension. Beginning with a detailed derivation of the Aubry–André Hamiltonian we describe the localization transition through the analysis of stationary and dynamical observables. Emphasis is placed on both the properties of the model and technical aspects of the performed calculations. In particular, the stationary properties investigated are the inverse participation ratio, the normalized participation ratio and the energy spectrum as a function of the disorder strength. Two dynamical quantities allow us to discern the localization phenomenon, being the spreading of an initially localized state and the evolution of population imbalance in even and odd sites across the lattice. The present manuscript could be useful in bringing advanced undergraduate and graduate students closer to the comprehension of localization phenomena, a topic of current interest in fields of condensed matter, ultracold atoms and complex systems.

Keywords: localization, quantum mechanics, ultracold physics

(Some figures may appear in colour only in the online journal)

1. Introduction
The understanding of electronic mobility in quasiperiodic or disordered media is one of the fundamental issues in the condensed matter domain. Structural disorder, together with the interparticle interactions, intrinsically present in every macroscopic sample, are the responsible ones of the physical behavior and response properties of solids. A material becomes an insulator as a result of either electron–electron or electron–ion interactions. While the study of
electron–electron interactions demands the use of a many-body theory and leads to identification of the Mott insulating phases \[1, 2\], electron–ion interactions can be addressed, within the single electron theory, and allow one to discern among several types of insulators. Among them are band insulators arising from periodicity in the lattice \[3\], Peierls insulators associated with lattice distortions \[4–7\] and Anderson insulators resulting from lattice imperfections or impurities, also known as lattice disorder \[8\].

The lattice imperfections referred to above, arising from a variety of sources as, for example, substitutional impurities, thermal vibrations, grain boundaries and point defects associated with the formation of the solid, among others, are crucial in determining the mobility of electrons. From a technical point of view, these irregularities translate into on-site energetic variations, which in turn determine the nature of the electronic states. Generally speaking, the wave function of the electrons can be extended or localized. While electron extended states are such that the wave functions have a significant overlap through the lattice sites, localized states are characterized, in contrast, by having negligible overlap between wave functions associated with neighboring sites. Although the localization phenomenon has been extensively investigated, it is up to now a central topic because it still has many open questions to be addressed. For example, the interplay between disorder and dimensionality, and between disorder and interactions. The purpose of this manuscript is to show how the loss of long range order in a 1D homogeneous lattice leads to localized single electrons, and thus causes the absence of its diffusion across the lattice. In other words, we shall focus our attention on the isolated effects that disorder has on producing localization; thus, interparticle interactions are not discussed in this work.

As a first step, the characterization of localization phenomena requires the election of an effective model representing the disorder, and then the use of the standard quantum mechanics techniques to analyze their effects. There are two general schemes from which localization has been envisaged: the Anderson model \[8\], in which disorder is represented by a random amplitude of the on-site energies; and the Aubry–André model \[9, 10\], where disorder arises from the superposition of two lattice potentials with incommensurate wavelengths. These models capture the metal-insulator transition in disordered lattices and allow one to characterize such a transition by tracking different properties, as we describe below. Here, we shall use the Aubry–André model as the hobbyhorse for studying and characterizing the influence that disorder has in producing localized states. This model, introduced in 1980, has been shown to be very successful in describing such transitions, not only in the single electron case but when interparticle interactions are considered \[11–15\]. Localization in a lattice can be recognized through several signatures, either of stationary or dynamical character. What it is important to stress is that localization can be identified as the result of both destructive interference associated with the multiple scattering process of the wave function traveling along the disordered medium, and the spectral properties of the Schrödinger equation \[16\]. Destruction of wave coherence or loss of mobility can be quantified in terms of several properties that can be extracted from the wave function. The first distinctive signature of localization, identified in the seminal work of Anderson, was the localization length that measures the size of the exponentially localized single particle state as a function of the disorder strength. Here, we concentrate on analyzing the properties enunciated in the following lines. First, we analyze the properties of the Aubry–André model, and then we investigate the inverse participation ratio (IPR) and its opposite, the normalized participation ratio (NPR), that quantify the fraction of sites contributing to the state along the lattice. Next, we investigate the energy spectrum that also allows monitoring the transition to localization. As we shall demonstrate, from the energy spectrum structure, signatures of localized or extended states can be discerned. In addition to these quantities characterizing localization of
the stationary states, there are dynamical parameters that also allow one to track the evolution of a given initial state in the presence of disorder. Among them, the spreading of the initial state and the imbalance between the density probability of even and odd sites in the lattice, as a function of time.

Current experiments with ultracold neutral atoms realized in the laboratory represent the ideal scenario where the spatial quasiperiodicity of the Aubry–André model can be recreated. Optical lattice potentials produced by standing waves resulting from interfering laser fields confine the atoms, and thus emulate the non-crystalline environment seen by electrons moving across the ion cores. Nowadays, such large ensembles of fermionic or bosonic atoms loaded in optical lattices offer advantages with respect to experiments performed in real solids. For example, interparticle interactions in ultracold atoms can be tuned externally from the non-interacting regime, to weakly and strongly interacting regimes. This experimental versatility allows one to observe the isolated effects of the lattice seen by the neutral atoms, thus providing insights into the consequences of the quasiperiodic confinement on the localization problem [17]. As a matter of fact, ten years ago, the Aubry–André model was experimentally set in a laboratory for the first time [18].

The aim of the present manuscript is to present a pedagogical description of the Aubry–André model, to understand and characterize the localization phenomenon in 1D. Advanced undergraduate and graduate students should be able to follow this article with no difficulty. Although this material provides the appropriate tools and techniques to address the single particle localization phenomenon only, we believe that the knowledge of this physics sets the reference to the many-body localization phenomenon.

The manuscript is organized in six sections. First, in section 2, considering an ultracold gas of Bose atoms confined in a quasiperiodic potential, we derive the Aubry–André Hamiltonian model, demonstrating how quasiperiodicity of the potential gives rise to a cosine function incommensurate with the underlying periodic tight-binding 1D lattice. Then, in section 3, the properties characterizing the Aubry–André model are delineated, placing special emphasis on the dual structure of the Hamiltonian in the coordinate and momentum representations. Sections 4 and 5 account for the analysis of time-independent and time-dependent properties that characterize the localization transition. Finally, in section 6, a summary of the results is presented.

2. Model

Our starting point is the 1D Hamiltonian operator, describing an ultracold gas of bosonic atoms with mass \( m \), confined in an external potential \( V(x) \), and interacting via a contact potential written, as usual, in terms of the \( s \)-wave scattering length \( a_s \),

\[
\hat{H} = \int dx \hat{\psi}^\dagger(x) \left( -\frac{\hbar^2}{2m} \nabla^2 + V(x) \right) \hat{\psi}(x) + \frac{1}{2} \frac{4\pi a_s \hbar^2}{m} \int dx \hat{\psi}^\dagger(x) \hat{\psi}^\dagger(x) \hat{\psi}(x) \hat{\psi}(x),
\]

(1)

\( \hat{\psi}^\dagger(x) \) and \( \hat{\psi}(x) \) are the bosonic creation and annihilation field operators satisfying the usual commutations relations for bosons, \([\hat{\psi}(x), \hat{\psi}^\dagger(x')] = \delta(x - x')\). It is important to stress here that the Hamiltonian operator \( \hat{H} \) in equation (1) has been written in the standard second quantized notation with the purpose of asserting the quantum character of the system under consideration, and, at the same time, with the aim of emphasizing that the most general
expression for the 1D Hamiltonian must include both the non-interacting case (first term of the Hamiltonian $H$), and the interacting contribution associated with particles interacting between pairs (second term of the Hamiltonian $H$). However, the purpose of the present manuscript is to deal with the non-interacting case. Thus, after derivation of the single particle energy Hamiltonian depicted in the next paragraphs, the reader can go directly to the manuscript is to deal with the non-interacting case. Thus, after derivation of the single particle

$\hat{H} = H_{x} + H_{r}$

potential, which as a matter of fact is written in the usual Dirac notation.

In the presence of disorder, $V(x)\sin(\pi x)$, which introduces an optical disorder $V_{opt}(x)$, consists of two optical lattices [19], the main lattice $V_{1}(x) = s_{1}E_{Ri}\sin^{2}(k_{i}x)$, which is used to create a tight-binding environment for the atoms, and a secondary one $V_{2}(x) = s_{2}E_{Ri}\sin^{2}(k_{2}x)$, which introduces an optical disorder [20]. Superimposing both lattices gives rise to the following bichromatic potential:

$$V_{opt}(x) = V_{1}(x) + V_{2}(x) = s_{1}E_{Ri}\sin^{2}(k_{1}x) + s_{2}E_{Ri}\sin^{2}(k_{2}x + \varphi)$$

$$= s_{1}E_{Ri}\sin^{2}(k_{1}x) + s_{2}E_{Ri}\beta^{2}\sin^{2}(\beta k_{1}x + \varphi)$$

(2)

where $k_{i} = 2\pi/\lambda_{i}$ ($i = 1, 2$) are the wave vectors, with $\lambda_{i}$ the wavelength of the lasers fields, $s_{i}$ are the heights of the lattices in units of the recoil energy $E_{Ri} = \hbar^{2}/(2m\lambda_{i}^{2})$, $\varphi$ is an arbitrary phase and $\beta = \lambda_{1}/\lambda_{2}$ is the ratio between the wavelengths. When $s_{2} \ll s_{1}$ and $\beta$ is an incommensurate number, the secondary lattice does not considerably change the positions of the potential minima generated by the main lattice [21]. Instead, as shown in figure 1(b), it has the effect of shifting the local site energy by an amount $\Delta_{i}$ only.

For single atoms and no net disorder $s_{2} = 0$, the eigenstates of equation (1) are Bloch wave functions [22]. As it is well known, an appropriate linear combination of Bloch states yields a Wannier wave function $w_{i,\nu}(x - x_{i})$, characterized by large probability amplitude around the lattice site $i$, that is a localized wave function at each site $i$. Since the atoms under study are at ultracold temperatures, the assumption that the energies involved in the system are smaller compared to the energy required to allow second and higher band populations is well justified. This consideration allows us to drop the band index $\nu$ in the Wannier functions and contemplate first band populations only. Having this assumption in mind, it is convenient to expand the field operators $\hat{\psi}(x)$ and $\hat{\psi}^{\dagger}(x)$ in the Wannier basis:
\[ \hat{\psi}(x) = \sum_i \hat{b}_i w(x - x_i), \]
\[ \hat{\psi}^\dagger(x) = \sum_i \hat{b}_i^\dagger w^*(x - x_i), \] (3)

where \( \hat{b}_i \) and \( \hat{b}_i^\dagger \) are the annihilation and creation operators for a particle in a Wannier state at the lattice site \( i \), respectively. It is worthwhile stressing that the sums in equation (3) run over all lattice sites. As mentioned above, for weak disorder \( s_2 < s_1 \) the minima of the main lattice are not remarkably affected and we can safely substitute the latter expansion of the field operators in equation (1). After some straightforward algebra, one can obtain the following expression for the Hamiltonian (1):

\[ \hat{H} = -\sum_{i,j} J_{ij} \hat{b}_i^\dagger \hat{b}_j + \sum_{i,j} \epsilon_{ij} \hat{b}_i^\dagger \hat{b}_j + \sum_{i,j,i',i''} U_{ij,i',i''} \hat{b}_i^\dagger \hat{b}_{i'} \hat{b}_{i''} \hat{b}_j, \] (4)

where we have defined the following constants:

\[ J_{ij} = -\int dx \ w^*(x - x_i) \left( -\frac{\hbar^2}{2m} \nabla^2 + s_1 E_R \sin^2(k_0 x) \right) w(x - x_j), \]
\[ \epsilon_{ij} = \int dx \ w^*(x - x_i) V_T(x) w(x - x_j), \]
\[ \Delta_{ij} = s_2 E_R \beta^2 \int dx \ w^*(x - x_i) \sin^2(\beta k_0 x + \varphi) w(x - x_j), \]
\[ U_{ij,i',i''} = \frac{4\pi\alpha_s \hbar^2}{2m} \int dx \ w^*(x - x_i) w^*(x - x_j) w(x - x_{i'}) w^*(x - x_{i''}). \] (5)

The first term in equation (4) describes the energy cost for an atom to hop from site \( i \) to site \( j \) with \( i \neq j \), see figure 2. Note that the hopping probability \( J_{ij} \) is proportional to the overlap between the Wannier functions centered at different lattice sites. Within the so-called tight-binding approximation, this overlap is essential only for the nearest neighbors \([22]\), thus we can neglect the tunneling terms between the next nearest neighbors and beyond. Also, since the main lattice potential is invariant under translations by one lattice period, \( a = \lambda/2 \), the hopping parameter \( J_{ij} \) becomes a constant \( J \) independent of the lattice site. For the case \( i = j \) the \( J_{ii} \) term represents an on-site energy shift, which is equal for all sites and thus can be dropped. Analogously to \( J_{ij} \), the second term \( \epsilon_{ii} \) represents an on-site shift of the energy and thus can be safely neglected. Regarding the contribution of \( \epsilon_{i\alpha} \), one should notice that due to the fact that the typical size of the frequencies used to confine ultracold atoms \( \omega_T \), are such that \([23]\) \( \sqrt{\hbar/(m\omega_T)} \gg \lambda/2 \), the energy variation associated with \( \epsilon_{i\alpha} \) is essentially the same as \( \epsilon_{ii} \), see figure 1(a). Therefore, at the same level of approximation, the contribution \( \epsilon_{i\alpha} \) can be neglected. The third term in equation (4) is responsible for the optical disorder in the lattice. To deal with it, we first use the trigonometric relation

\[ \text{Figure 2. A schematic representation of the hopping of a particle in a lattice.} \]
\sin^2(\beta k_1 x + \varphi) = (1 - \cos(2\beta k_1 x + \varphi')) / 2 \quad \text{with} \quad \varphi' = 2\varphi.

Inserting this relation into the third equality of equation (5) and dropping the constant term, we obtain
\begin{equation}
\Delta_{ij} = -\frac{s:\!E_{\!R}\!\beta^2}{2} \int dx \ w^*(x - x_i) \cos(2\beta k_1 x + \varphi') w(x - x_i). \tag{6}
\end{equation}

Again, for deep enough lattices, the leading contribution of equation (6) is the \( i = j \) term, which corresponds to an on-site energy shift variation. Further, we can change the variable \( y = x - x_i \), leading to
\begin{equation}
\Delta_{ii} = -\frac{s:\!E_{\!R}\!\beta^2}{2} \cos(2\pi \beta i + \varphi') \int dy \ \cos(2\beta k_1 y) |w(y)|^2. \tag{7}
\end{equation}

Where in the last equation we have identified \( x_i \to i \), we have used the subsequent trigonometric identity:
\begin{align*}
\cos(2\beta k_1 y + 2\beta k_1 x_i + \varphi') &= \cos(2\pi \beta i + \varphi') \cos(2\beta k_1 y) \\
&- \sin(2\pi \beta i + \varphi') \sin(2\beta k_1 y), \tag{8}
\end{align*}

and symmetric properties to drop the sine integral. Following the above steps we finally get the usual disorder term [19]:
\begin{equation}
\Delta_{ij} = \Delta \cos(2\pi \beta i + \phi) \delta_{ij}, \tag{9}
\end{equation}

where \( \phi = \varphi' + \pi \) and \( \Delta \) is defined as the following constant parameter:
\begin{equation}
\Delta = \frac{s:\!E_{\!R}\!\beta^2}{2} \int dy \ \cos(2\beta k_1 y) |w(y)|^2. \tag{10}
\end{equation}

The term associated with the interaction energy can also be simplified by taking into account the tight-binding approximation. The dominant term of the overlap of four Wannier functions is due to the term \( i = j = l = v \), which corresponds to an on-site interaction, where the atoms only ‘see each other’ whenever they are in the same lattice site:
\begin{equation}
U = U_{\!i,i,i,i} = \frac{4\pi a_s \hbar^2}{2m} \int |w(x)|^4 dx. \tag{11}
\end{equation}

Summarizing all the above approximations, we end with the following interacting Hamiltonian:
\begin{equation}
\hat{H} = -J \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \Delta \sum_i \cos(2\pi \beta i + \phi) \hat{n}_i + U \sum_i \hat{n}_i (\hat{n}_i - 1), \tag{12}
\end{equation}

where the notation \( \langle i, j \rangle \) indicates that the sum runs over the nearest neighbors only and \( \hat{n}_i = \hat{b}_i^\dagger \hat{b}_i \) is the number operator at site \( i \). As mentioned in the introduction, one of the most outstanding advantages of the experiments with ultracold atomic gases is the possibility of tuning the strength of the pairwise interactions between atoms, via an external magnetic field. This procedure, called Feshbach resonance [17], allows the experimentalist to prepare a gas of atoms with a zero scattering length \( a_s \), and consequently \( U = 0 \). Such a non-interacting system constitutes an experimental realization of the non-interacting Harper [10] or Aubry–André [9] model:
\begin{equation}
\hat{H} = -J \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \Delta \sum_i \cos(2\pi \beta i + \phi) \hat{n}_i. \tag{13}
\end{equation}

This model, and also the interacting version, have been realized in experiments with ultracold atoms in bichromatic optical lattice potentials [18, 24]. Written in the Dirac notation, the
above Hamiltonian takes the form
\[ \hat{H} = -J \sum_j |w_j\rangle\langle w_{j+1}| + |w_{j+1}\rangle\langle w_j| + \Delta \sum_j \cos(2\pi j \beta + \phi) |w_j\rangle \langle w_j|. \] (14)

It is important to emphasize that recent investigations \[16, 25\] pointed out that the Hamiltonian in equation (14) is strictly valid in the extreme tight-binding limit of a very deep main lattice potential.

3. Properties of the Aubry–André model

Having set the Aubry–André Hamiltonian it is worthwhile exposing some basic properties of this model. Beginning with its duality in space and momentum representations, one can transform the Hamiltonian \((14)\) written in the Wannier representation to one in the momentum representation, via the following transformation:
\[ |k_n\rangle = \sum_j e^{2\pi i j k_n} |w_j\rangle. \] (15)

After substitution and straightforward algebra, we find the dual Hamiltonian:
\[ H = -\frac{\Delta}{2} \sum_s (|k_s\rangle\langle k_{s+1}| + |k_{s+1}\rangle\langle k_s|) + 2J \sum_s \cos(2\pi j \beta) |k_s\rangle \langle k_s|, \] (16)

which resembles the Hamiltonian of equation (14), except that the tunneling rate has changed from \(J \to \Delta/2\) and the disorder strength from \(\Delta \to 2J\). Also, for simplicity we set \(\phi = 0\). One can notice that to fully recover the Hamiltonian (14) one must set \(\Delta/J = 2\). Furthermore, the localization transition is sensitive to the value of the parameter \(\beta\) \([19]\). For example, an integer value \(\beta\) would not display any localization transition. To observe such a transition, \(\beta\) must have some degree of incommensurability. One way to achieve this requirement is to choose \(\beta\) as the ratio of two adjacent Fibonacci numbers \(F_{n-1}/F_n\), with \(F_{n-1}\) and \(F_n\) being two consecutive elements of the Fibonacci sequence. Such a procedure approaches the inverse Golden ratio \(\varphi = (\sqrt{5} - 1)/2\) for large enough Fibonacci numbers. Also, one can express \(\beta\) as the ratio of two relative prime numbers \(\beta = P/Q\), with \(P\) and \(Q\) larger than the system size of simulation \([26]\). However, in experimental realizations, \(\beta\) is restricted to the available laser wavelengths. For example, recent experiments \([25]\) were performed with \(\beta = 532/738\).

Summarizing, we can state that \(\beta\) must be selected to ensure that the system remains aperiodic within the size of interest \([16]\). If these requirements are accomplished one would observe that for \(\Delta/J = 2\), the wave functions, either that associated with the ground state or those corresponding to the excited states, develop peaks around certain lattice sites; such peaks become a single peak as the disorder amplitude \(\Delta\) is increased. To complete this section we should mention the relevance of the phase \(\phi\) in equation (14). As can be seen from figure 3, different values of \(\phi\) provide distinct shapes of the confining potential in 1D. Thus, one can say that a given value of \(\phi\) leads to a particular realization of disorder. However, the main purpose of our study is to extract the dominant effects of disordered media, independently of...
how the disorder is distributed on the lattice. Hence, to circumvent this apparent difficulty, one has to average over an ensemble of realizations, namely to consider different values of $\phi$, until convergence is reached.

4. Time-independent results

In this section, we describe some of the most distinctive single particle time-independent results of the Aubry–André model. In the deep tight-binding approximation, the Wannier functions are highly localized and thus can be represented by the site basis [22], that is, $|w_i\rangle \rightarrow |x_i\rangle$, where $|x_i\rangle$ means that the particle is localized at site $i$. In this scenario, equation (14) is reduced to the Schrödinger equation $H|\psi\rangle = E|\psi\rangle$, with $|\psi\rangle$ being an eigenstate of the one particle Hamiltonian $H$:

$$
\hat{H} = -J \sum_i (|x_{i+1}\rangle \langle x_i| + |x_{i-1}\rangle \langle x_i|) + \Delta \sum_i \cos(2\pi \beta i + \phi) |x_i\rangle \langle x_i| 
$$

By expanding the wave function $|\psi\rangle$ in terms of the site basis $|\psi\rangle = \sum_i \psi_i |x_i\rangle$ and calculating the product $(x_j \hat{H}|\psi\rangle$, we obtain the following difference equation for the coefficients $\psi_i$:

$$
-(\psi_{i+1} - \psi_{i-1}) + \frac{\Delta}{J} \cos(2\pi \beta j + \phi) \psi_j = \frac{E}{J} \psi_j, 
$$

where we have divided by $J$ to have dimensionless equations and at the same time to set the energy scale. It is easy to see that equation (18) can be rewritten in a matrix form $H\vec{\psi} = \frac{E}{J} \vec{\psi}$ with $\vec{\psi} = (\psi_1, \psi_2, \cdots, \psi_\Omega)^T$ being the state vector and $H$ the Hamiltonian matrix:

$$
H = \begin{pmatrix}
\frac{\Delta}{J} \cos(2\pi \beta + \phi) & -1 & \cdots & -1 \\
-1 & \frac{\Delta}{J} \cos(4\pi \beta + \phi) & \cdots & 0 \\
\vdots & \ddots & \ddots & \vdots \\
-1 & 0 & \cdots & \frac{\Delta}{J} \cos(2\Omega \pi \beta + \phi)
\end{pmatrix},
$$

where $\Omega$ is the number of sites in the lattice. In the following calculations we consider $\Omega = 987$ sites, although similar results are found for larger lattice sizes. At this point, it is instructive to state two aspects that were considered in our numerical calculations. The first one is related to the boundary conditions of the problem. As can be seen from the Hamiltonian matrix (19), we take periodic boundary conditions, which means that the 1D
lattice closes itself. Also, for the subsequent calculations we consider $\beta = 610/987 \approx 0.618034$.

Now, we are left to find the eigenvalues and eigenvectors of the matrix $H$. In the case of vanishing disorder $\Delta/J = 0$, equation (18) is easily solved with the ansatz $\psi_i = e^{ik_0i}$, which displays the energy spectrum of a free particle in a 1D lattice $E_k = -2J \cos(ka)$ [3]. In figure 4(a) we plot the ground state density $|\psi_i|^2$ as a function of the lattice site $i$ for zero disorder $\Delta/J = 0$, and for the nonzero disorder $\Delta/J = 1.5$, shown in figure 4(b).

As one would expect, the ground state profile in the absence of disorder is a normalized constant at each site. This means that the particle is completely delocalized in the lattice. For the case $\Delta/J = 1.5$, the density profile of the ground state displays multiple peaks, which indicates the presence of different potential depths across the sites. However, the wave function is still extended over all the lattice.

With the aim of sketching the ground state density for two different values of the disorder amplitude satisfying $\Delta/J \geq 2$, in figure 5 we exhibit two cases: the left one is associated with $\Delta/J = 2$, and the right one corresponds to $\Delta/J = 4$. As can be seen from these density profiles, $\Delta/J = 2$ exhibits the transition from an extended to a localized state, while the case $\Delta/J = 4$ shows that when the disorder amplitude is increased, the localization becomes sharp.

An important quantity that arises in describing the localization transition, and is widely used in the literature, is the IPR. For a normalized state $|\psi\rangle = \sum_i \psi_i |x_i\rangle$, it is defined as
The IPR gives us the inverse of the number of sites occupied by the wave function. For example, it approaches zero as $1/\Omega$, for an extended wave function, while it goes to 1 for a localized state on a single lattice site.

The great advantage of using the IPR parameter is that instead of looking at the wave function in each realization, we just have to check a single parameter to confirm the nature of the wave function. In figure 6 we illustrate the IPR associated with the ground state as a function of the disorder strength $\Delta/J$. Each point in this figure corresponds to an average over ten realizations of the phase $\phi$, which is set randomly in the interval $\phi \in [0, 2\pi)$. As shown, the IPR parameter becomes different from zero for $\Delta/J = 2$ and it approaches unity as the disorder increases. This peculiar behavior makes the IPR a good parameter for studying the localization transition. Even though the above definition of the IPR is related to the localization in real space, one could extend the idea to momentum space or to a more exotic basis as the Floquet basis in periodic driven optical lattices [27, 28].

Another interesting quantity is the NPR, which plays the opposite role to the IPR parameter [16]. That is, the NPR parameter remains finite for spatially extended states, while approaching zero for a localized one. For a given normalized state $|\psi\rangle = \sum_i \psi_i |x_i\rangle$, the NPR parameter is defined as follows:

$$\text{NPR}(|\psi\rangle) = \frac{1}{\Omega} \frac{1}{\sum_i |\psi_i|^4}.$$  \hspace{1cm} (21)

To illustrate the utility of the NPR parameter, first, one should notice that the above definitions for the IPR and NPR parameters are related to a single eigenstate $|\psi\rangle$. However, one can calculate these two quantities for the full eigenstate spectrum, and display the average of the IPR and NPR parameters. In figure 7 we plot such averages as a function of the disorder strength $\Delta/J$. As shown in this figure, for $\Delta/J < 2$ we obtain, as expected, IPR = 0 and NPR $\neq 0$, while for $\Delta/J > 2$, IPR $\neq 0$ and NPR = 0. This indicates that the spectrum is either completely delocalized ($\Delta/J < 2$) or completely localized ($\Delta/J > 2$), but not a mixture of both localized and extended states.

We should emphasize that this peculiar behavior of the IPR and NPR curves is a direct consequence of the tight-binding approximation used in deriving the Aubry–André model [16]. Nevertheless, when hopping to the next nearest neighbors is considered, a noticeable
overlap between both curves emerges [16, 29–31]. In such a scenario extended and localized states take place in the same spectrum; the value of the energy that separates localized and delocalized eigenstates is called mobility edge energy. At the transition point $\Delta/J = 2$ all the eigenstates exhibit a multifractal structure [32], a subject which is out of the scope of this work. Summarizing, we can organize the latter result in the diagram shown in figure 8, which displays an absence of a mixture between localized and extended eigenstates in the full spectrum.

To conclude this section, in figure 9 we show the energy spectrum of the Aubry–André model as a function of the parameter $\beta$ for two different disorder strengths $\Delta/J$. In our calculations we used $\beta \in (0,1)$ such that $\beta = i/\Omega$ with $i = 1, 2, 3, \ldots, 986$. This spectrum has been studied in numerous works [33–38], since it displays a very rich structure in both the

**Figure 7.** The IPR and NPR of the full spectrum as a function of the disorder strength $\Delta/J$. Each point corresponds to the average of the full spectrum over ten realizations of the phase $\phi$.

**Figure 8.** A diagram of the Aubry–André spectrum as a function of the disorder strength $\Delta/J$.
extended and localized regimes. We should stress that strictly speaking only incommensurate values of $\beta$ lead to localized states.

For values of disorder amplitude above and below the transition point, the energy spectrum structure is completely different from that associated with $\Delta/J = 2$, where it shows the Hofstadter butterfly [35]. The case $\Delta/J = 2$ has been widely investigated, since it describes the quantum physics of an electron moving on a 2D square lattice in the presence of a transverse magnetic field [10].

5. Time-dependent results

In this section, we discuss the time evolution of a given initial condition, in the presence of disorder. This is one of the ways in which experimentalists measure how much a system is apart from an initially delocalized or extended state [18, 25]. First, we briefly summarize some basic concepts related to the evolution in time of single particle problems. According to quantum mechanics, the time evolution of a ket $|\psi\rangle$ is given by the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = H|\psi\rangle.$$  \hspace{1cm} (22)

Again, we expand the ket in the site basis $|\psi\rangle = \sum_i \psi_i(t)|i\rangle$ and after substitution in equation (22), we obtain the time-dependent equation for the coefficients $\psi_i(t)$:

$$\frac{d}{dt} \psi_i(t) = \frac{i}{\hbar} \sum_j H_{ij} \psi_j(t).$$  \hspace{1cm} (23)

where $H_{ij}$ are the matrix elements of $H$ given in equality (19). Equation (23) represents a system of $\Omega$ coupled ordinary differential equations, which can be easily solved using the Runge-Kutta 4 (RK4) method:
where we have set $\tau = \Delta t / \hbar$ as our dimensionless unit of time. The advantage of using the RK4 method resides on one side in its accuracy $(\Delta \tau)^4$, and on the other side, in the relatively simple way in which the above equations can be implemented. In our calculations, we set $\Delta \tau = 0.01$, which displays conservation of both the norm and the energy within the whole numerical time evolution.

As is well known, the time evolution of an eigenstate of $H$ would give trivial results. Nevertheless, the evolution of an arbitrary state can yield signatures of the presence of disorder. For this reason, we first study the evolution in time of an initially fully localized state in the middle of the lattice $\psi(\tau) = |0\rangle$. This initial condition mimics ‘designs’ prepared in current experiments performed with ultracold atoms [18]. In figure 10(a) and figure 10(b), we plot the initial density profile and the spreading of such an initial state in the absence of disorder for a time of $\tau = 100$, respectively.

To quantify the spreading of the initial wave function, we determine the root mean square of the displacement (RMSD) in each time step; this latter quantity is defined as

$$\sigma(\tau) = \left[ \sum_i i^2 |\psi_i(\tau)|^2 \right]^{1/2}. \tag{25}$$

The RMSD is a measure of the deviation of the position of the particle at time $\tau$ with respect to its initial position. In other words, the RMSD measures the portion of the lattice that is ‘explored’ by the particle during a time interval. In figure 11 we plot the RMSD, in logarithmic scale, as a function of the time $\tau$ for five different disorder strengths. The shaded area in each curve represents the standard error over ten realizations of random phase $\phi$. As one can observe, for zero disorder $\Delta / J = 0$ the wave packet propagates ballistically, that is $\sigma(\tau) \propto \tau$, showing that the RMSD grows linearly in time. Due to the system finite size, the RMSD reaches a maximum value and oscillates around it. For this reason, we let the system evolve until the RMSD reaches its maximum value for zero disorder.

The time dependence of the RMSD can be fitted with a power law ansatz $\sigma(\tau) \propto \tau^\gamma$. This fit must be carried out at intermediate times scales, where one neglects the contribution
of the transient behavior at short times and the maximum spreading at later ones [28]. Figure 12 shows the exponent $\gamma$ of the above fit as a function of the disorder strength $\Delta/J$. This plot allows us to identify the ballistic regime $\gamma = 1$, the superdiffusive $1/2 < \gamma < 1$, the subdiffusive $0 < \gamma < 1/2$ and the localized one $\gamma = 0$, associated with the diffusion of an initially localized wave packet.

Another interesting observable that allows us to discern between a localized and extended phase, and can also be detected in current experiments [24, 25], is the imbalance
The imbalance parameter is defined as follows:

\[
I(\tau) = \frac{n_e(\tau) - n_o(\tau)}{n_e(\tau) + n_o(\tau)},
\]

where \( n_e(\tau) = \sum_{\text{even}} |\psi(\tau)|^2 \) is the total probability density of the particle on even sites, and \( n_o(\tau) = \sum_{\text{odd}} |\psi(\tau)|^2 \) corresponds to the total probability density of the particle on odd sites of the lattice. As the name suggests, the \( I(\tau) \) parameter measures the imbalance of the population occupying odd and even sites of the lattice. To condense the whole time evolution of the imbalance, we defined \( I \) as the asymptotic value of \( I(\tau) \):

\[
I = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau \left[ \frac{n_e(\tau') - n_o(\tau')} {n_e(\tau') + n_o(\tau')} \right] d\tau'.
\]

For calculation purposes, our numerical simulations were performed until \( \tau = 1000 \), which corresponds to a real time of \( t = 1000 \hbar/J \) that is much bigger than the hopping time in the lattice.

Besides being a measurable observable, the most significant advantage of using the imbalance parameter as an order parameter for probing localization is that it can also provide signatures of many-body localization, when interactions are present. To show the dynamical behavior of \( I(\tau) \), we start by considering the evolution of a density-wave-like pattern in which only even sites are initially occupied. To obtain meaningful calculations we have to impose the same number of odd and even sites in the full lattice. Here, we consider \( \Omega = 1000 \) and the incommensurate parameter \( \beta = 987/1597 \). Then, we calculate the value of the imbalance \( I(\tau) \) at every time step until \( \tau = 1000 \), at which we observe that the imbalance oscillates around its asymptotic value. For illustration purposes in figure 13, we plot the imbalance as a function of time \( \tau \) for a disorder \( \Delta/J = 4.0 \).

In figure 14 we show the asymptotic value of the imbalance as a function of the disorder strength \( \Delta/J \). Since for \( \Delta/J < 2 \) all the states are extended, the particle can easily tunnel to nearby sites leading to a zero value of the imbalance in a few tunneling times. The vanishing of the imbalance must be interpreted as an indication of ergodicity, since the system completely loses any previous information associated with the initial state. However, for \( \Delta/J > 2 \) the imbalance reaches a finite value, which is closer to the initial value as the disorder is increased. This suggests that the system is non-ergodic as it retains certain memory of the initial configuration.
6. Final remarks

The main purpose of the manuscript is to introduce the undergraduate and graduate student to one of the most studied topics in condensed matter: the localization phenomenon. For this purpose, we have presented a comprehensive and detailed study of a single particle moving in a disordered lattice in one dimension. In particular, the disorder analyzed here corresponds to a quasiperiodic one. Considering as a starting point a quantum analog of such a condensed matter system, namely a weakly interacting ultracold Bose gas confined in a 1D quasiperiodic lattice, in section 2 we presented a straightforward derivation of the Aubry–André Hamiltonian. Then, in section 3 we proceeded to review the essential aspects regarding the 1D Aubry–André model and the localization transition. In particular, we determined the transition point by making use of the duality in space and momentum representations of the Aubry–André Hamiltonian. In section 4, we focused on the introduction and description of the stationary properties that allowed us to characterize the localization transition as a function of the disorder amplitude. Specifically, we determined the IPR and its opposite, the NPR, that provide information of how localized across the lattice a wave function is, as a function of the disorder amplitude. These parameters were calculated for both the ground state and the full energy spectrum. Our analysis concluded with the study of the time-dependent properties presented in section 5. In particular, the transition from extended to localized states was recognized by following the evolution in time of two different initial states.

All the formalism and techniques used here are at the level of an advanced undergraduate student or equivalent. We believe that this type of reading brings a student closer to the comprehension of current research on single particle and many particle localization phenomena. With the tools used in this paper, the interested reader can address the study of vanguard problems related to the central topic of this manuscript, for example, the dependence of localization on dimensionality, the effects of the next nearest neighbors in the localization phenomenon and the response of the system in the novel driven disordered lattices among others.

Finally, in this paragraph we want to briefly summarize some of the reported predictions of the Aubry–André model. These include spin–orbit coupling effects [41], closed expressions for the energy separating localized and non-localized states [42] and coexistence of localized and extended states in interacting quasiperiodic systems [43] among others. At the
many-body level, localization of the ground state is established rigorously in the weakly interacting regime for both repulsive and attractive interactions [44] and many-body localization versus thermalization and onset of equilibrium [45], which can have implications for quantum devices and quantum computation. All of these phenomena can be analyzed by means of a generalized Hamiltonian that includes the interparticle interactions. Here, we have restricted our work to the single particle localization phenomenon.

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