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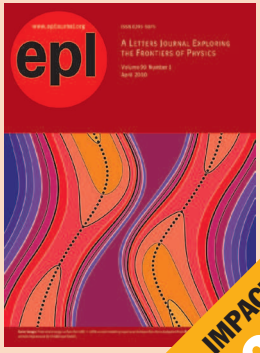

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Correlated metallic two-particle bound states in quasiperiodic chains

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Abstract – Single-particle states in a chain with quasiperiodic potential show a metal-insulator transition upon the change of the potential strength. We consider two particles with local interaction in the single-particle insulating regime. The two-particle states change from being localized to delocalized upon an increase of the interaction strength to a nonperturbative finite value. At even larger interaction strength the states become localized again. This transition of two-particle bound states into correlated metallic ones is due to a resonant mixing of the noninteracting two-particle eigenstates. In the discovered correlated metal states two particles move coherently together through the whole chain.

Introduction. – The interplay of localization and many-body interactions has been a highly active research topic since the discovery of Anderson localization [1]. While the direct theoretical study of such systems is quite complex and recently hotly debated (see, *e.g.*, [2]), another route is taken by studying few interacting particles. The potential applicability to recent experimental activities with ultracold atoms in optical lattices [3] increased the interest in corresponding theoretical studies. Localization of single-particle states in a one-dimensional lattice can be realized in spatially inhomogeneous potentials. An external dc field leads to Wannier-Stark localization and Bloch oscillations [4], random field yields Anderson localization [1], and quasiperiodic modulation evokes Aubry-Andre localization [5]. Two interacting particles (TIP) in a dc field lead to no substantial change of the localization length due to the Stark ladder structure of the single-particle eigenenergies (disregarding some resonant tunneling events which, however, are also suppressed for large distances) [6]. TIP in the random case do lead to an increase of the localization length with some controversial discussions about the quantitative outcome [7–9], but do not yield complete delocalization, For TIP in the quasiperiodic potential case few numerical results give varying predictions from incremental increase of localization length to opposite reports of decrease of localization length in the insulating regime [10–12].

In this work we consider the TIP problem in a quasiperiodic chain at finite (nonperturbative) strength of interaction, deep in the single-particle insulating regime. We find strong evidence for a complete delocalization of certain two-particle bound states, in which both particles keep a relative distance less than the one-particle localization length. The interaction renormalizes eigenenergies of different classes of localized TIP eigenstates with different strength, and leads to a resonant overlap of these energies in a certain range of the interaction constant. In this nonperturbative window the overlap between these groups of eigenstates leads finally to a complete delocalization of a finite fraction of states. This results in the novel observation of a correlated metal state built from only two interacting particles.

TIP model. – We study the TIP in the framework of the Hubbard model with Hamiltonian

$$\hat{\mathcal{H}} = \sum_j \left[\hat{b}^+_{j+1}\hat{b}_j + \hat{b}^+_j\hat{b}_{j+1} + \epsilon_j \hat{b}^+_j\hat{b}_j + \frac{U}{2}\hat{b}^+_j\hat{b}^+_j\hat{b}_j\hat{b}_j \right], \quad (1)$$

where $\hat{b}^+_j$ and $\hat{b}_j$ are creation and annihilation operators of indistinguishable bosons at lattice site j, and U measures

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the onsite interaction strength between the bosons. The potential

$$\epsilon_j = \lambda \cos(\beta + 2\pi\alpha n) \qquad (2)$$

controls the single-particle problem via its strength λ. The incommensurability parameter $\alpha = (\sqrt{5}-1)/2$ (golden mean). β is an arbitrary phase which controls wave packet dynamics and is irrelevant for the properties of extended metallic eigenstates.

For a single particle the interaction term does not contribute. Using the basis $|j\rangle \equiv \hat{b}_j^+|0\rangle$ the eigenstates $|\nu\rangle$ of Hamiltonian (1) with eigenvalues λ_ν are computed using $|\nu\rangle = \sum_j A_j^\nu b_j^+|0\rangle$, $\hat{\mathcal{H}}|\nu\rangle = \lambda_\nu|\nu\rangle$. $A_j^\nu \equiv \langle j|\nu\rangle$ are the eigenvectors. As was first shown by Aubry and Andre [5] (see also [13,14]), for $\lambda < 2$ all eigenstates are delocalized (metallic phase) and for $\lambda > 2$ all states are localized (insulating phase) with a localization length $\xi_1 = 1/\ln(\lambda/2)$. Consequently the probability distribution function (PDF) $p_l^{(\nu)} = \langle q|\hat{b}_l^+\hat{b}_l|q\rangle \sim \exp[-2|l|/\xi_1]$ is exponentially localized in the insulating regime. The bounded eigenvalue spectrum shows fractal properties (see, *e.g.*, [15]). At the value $\lambda = 2.5$ (which is the main reference parameter for computational studies in this work) the spectrum has three main minibands called SP1, SP2, and SP3 with centers around $\lambda = -2.5, 0, 2.5$ and ordered with increasing energy.

For two particles we expand the eigenstates $|q\rangle$ of the TIP problem in the local basis,

$$|q\rangle = \sum_{m,l\leqslant m}^{N} \mathcal{L}_{l,m}^{(q)}|l,m\rangle, \qquad |l,m\rangle \equiv \frac{b_l^+ b_m^+|0\rangle}{\sqrt{1+\delta_{lm}}}, \qquad (3)$$

where $\mathcal{L}_{l,m}^{(q)} = \langle l,m|q\rangle$ are the normalized eigenvectors with $l \leqslant m$. Thus, $[\mathcal{L}_{l,m}^{(q)}]^2$ is the probability to find two particles on the sites l and m. We also compute the PDF of the eigenmodes $|q\rangle$ as

$$p_l^{(q)} = \frac{\langle q|\hat{b}_l^+\hat{b}_l|q\rangle}{2} = \frac{1}{2}\left(\sum_{k,l\leqslant k}^{N} \mathcal{L}_{l,k}^{(q)2} + \sum_{m,l\geqslant m}^{N} \mathcal{L}_{m,l}^{(q)2}\right) \qquad (4)$$

and their participation numbers $P_q = 1/\sum_l^N (p_l^{(q)})^2$ that are proportional to the respective localization lengths. We note that at the noninteracting limit $U = 0$ and $\lambda = 2.5$ the spectrum decomposes into five minibands TP1, TP2, TP3, TP4, TP5 (see fig. 1). This follows from the three-miniband structure of the single-particle spectrum, such that, *e.g.*, TP1 is formed from two single-particle states SP1: TP1 = (SP1× SP1). Analogously, TP2 = (SP1 × SP2), TP3 = (SP2 × SP2) ∪ (SP1 × SP3), TP4 = (SP2 × SP3), TP5 = (SP3 × SP3), where TPp = (SPm × SPn) corresponds to a two-particle product state TPp with one of the particles being in a single-particle eigenstate in miniband SPm and another one in SPn.

Exact diagonalization studies. – To check for the selective character of a delocalization effect we present

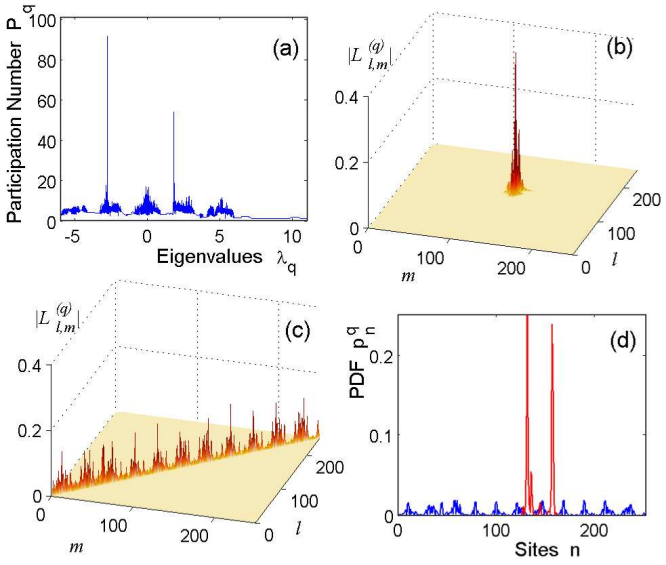

Fig. 1: (Color online) (a) Participation number of interacting particle eigenstates *vs.* their eigenenergies; (b) and (c) present typical localized and delocalized eigenfunctions $|\mathcal{L}_{l,m}^{(q)}|$ which correspond to the background and peaks in graph (a), respectively. In (d) we plot PDFs of localized (red) and delocalized (blue) eigenmodes. Here $U = 7.9$ and $\lambda = 2.5$.

participation numbers of all eigenstates *vs.* their eigenenergies for the particular choice of the interaction constant $U = 7.9$ (fig. 1(a)). The five-miniband structure of the noninteracting case is clearly seen. This follows from the fact, that most states correspond to two particles separated by a distance larger than the localization length, and, therefore, these states do not change when the interaction is increased. It is these states that also stay at a small value of the participation number of the order of $P \approx 5$. However, in the minibands TP2 and TP4 we observe candidates for metallic delocalized states with $50 < P < 100$ being one order of magnitude larger. Two characteristic eigenvectors for localized and delocalized states are shown in fig. 1(b), (c), and their corresponding PDFs are plotted in fig. 1(d). The metallic state in fig. 1(b), (d) indeed occupies the whole system. For this state both particles stay close to each other, forming a diagonal structure in fig. 1(b). Therefore, we coin these correlated metallic two-particle bound states.

Next we examine the characteristics of eigenstates for $\lambda = 2.5$ and various systems sizes and different values of U. We start with $N = 100$. For each value of U we find the state with the largest participation number and plot this number *vs.* U in fig. 2. While for $U < 4$ and $U > 10$ the number stays around 10–20, three humps up to a value of 40 are noted for $4 < U < 10$. Since the spatial size of an eigenvector is roughly 2–3 times larger than its participation number, we conclude that in the hump regions the analyzed states extend over the whole system. We increase the system size to $N = 150, 200, 250$ and repeat the above analysis. We observe that the hump

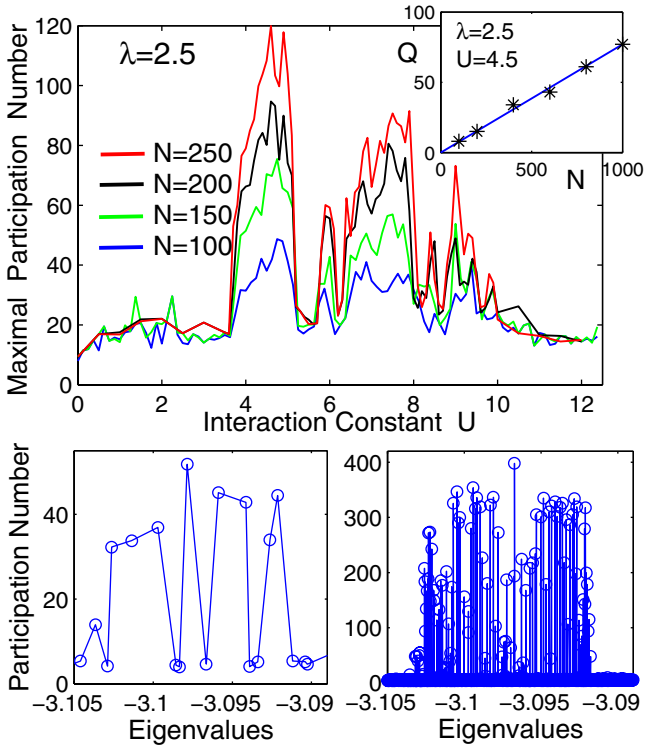

Fig. 2: (Color online) Top panel: dependence of the largest participation number (of the mostly delocalized eigenstate) on U for different lattice sizes $N = 100, 150, 200, 250$ (from bottom to top) and for $\lambda = 2.5$. Inset: the dependence of the number Q of delocalized states on the system size for the parameters $\lambda = 2.5$ and $U = 4.5$. The straight line is a fit $Q = N/13$. Bottom panel: dependence of the participation number (circles) on the energy eigenvalues in the frequency range where delocalized modes are observed for short ($N = 100$, left) and long (N = 1000, right) chains. Other parameters are $\lambda = 2.5$ and $U = 4.5$.

heights grow linearly with the system size, indicating that for all system sizes the most delocalized eigenstates in the hump regions spread over the whole system. This is a clear evidence of complete delocalization of some eigenvectors in the mentioned parameter region.

Since the eigenvalues of delocalized modes are located within a narrow frequency range which is not affected by the system size, we extend the diagonalization up to $N = 1000$ using the standard MATLAB diagonalization procedure tailored for square large sparse matrices. For such large systems we are restricted to narrow frequency ranges. We computed the dependence of the number of delocalized modes Q on N and present the result in the inset of fig. 2. We obtain $Q \approx N/13$ for $\lambda = 2.5$ and $U = 4.5$ diagonalizing in the range of eigenvalues -3.097 ± 0.01. Such a scaling is a clear evidence that the delocalized states have a nonzero measure with respect to the number of modes at the diagonal (which is also proportional to N). Obviously off-diagonal Hilbert states are not relevant in forming a wave packet since their contribution is exponentially small if one has an initial state in a form

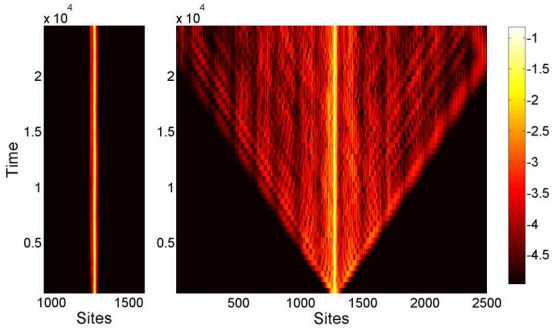

Fig. 3: (Color online) Time and space dependence of the PDF of an initial state with two particles at adjacent sites for $\lambda = 2.5$ (color maps $\log_{10}$ PDF). Left panel: isolator phase, $U = 2$, right panel: correlated metal phase, $U = 4.5$.

of closely placed particles. We also plot the locations of delocalized modes in energy space for short ($N = 100$) and long ($N = 1000$) chains. As seen from the bottom panel of fig. 2, localized and delocalized states coexist in the same frequency range. Increasing the length of the chain causes a growth of the density of delocalized states proportional to N.

Simulations on evolving wave packets. – Using exact diagonalization we are restricted to lattice sizes $N < 1000$. In order to push the limits, we compute the evolution of the Schrödinger equation in real time without diagonalization, starting with two particles located on adjacent sites. When and if the extended states exist, such initial conditions must excite them, making a part of a two-particle wave packet propagate. Typical PDFs as a function of space and time are shown in fig. 3. We find ballistic spreading over the whole system with $N = 2500$ sites for $U = 4.5$, and complete localization for $U = 2$. This extends the evidence for complete delocalization of the initial state into extended eigenstates of two interacting particles.

We perform a scan in the parameter space $\{U, \lambda\}$ in order to identify the region of correlated metallic two-particle bound states. We choose a system size $N = 610$, and place two particles at adjacent sites in the center of the chain. The Schrödinger equation is evolved up to time $t = 1.5 \times 10^4$. The square-root second moment of the wave packet PDF is then measured for 60 different original particle positions and the outcome for the fastest growing realization is plotted in color code as a function of both λ and U in fig. 4. For $\lambda \leqslant 2$ all single-particle states are metallic, therefore this region is not of interest. However, for $\lambda > 2$ single-particle states are localized. Here we find a large region of metallic bound states for $3 \lesssim U \lesssim 15$ and $\lambda \lesssim 3$. Towards larger values of λ the existence region breaks up into two main tongues, which we observed also in fig. 2. Note also two separate tongue structures at around $U \approx 1.5$ and $U \approx 15$ which stretch up to $\lambda \approx 2.4$.

The observed correlated metallic bound states have to form bands with a continuous spectrum. The width of

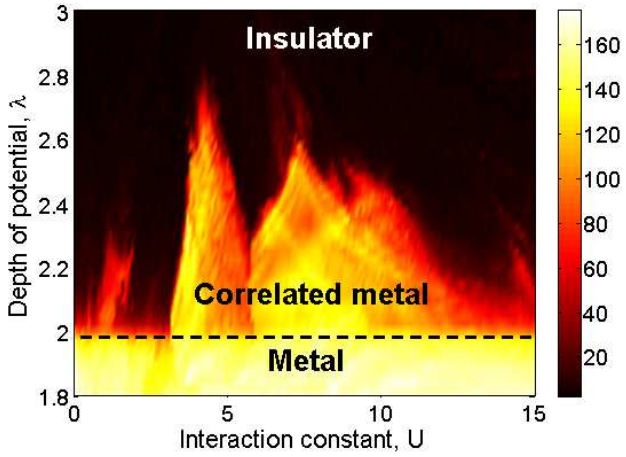

Fig. 4: (Color online) The phase diagram of the TIP in a quasiperiodic potential as suggested by the long-term wave packet evolution (the color code maps its square-root second moment, see text for further details). In light areas metallic eigenstates exist, in the dark area there exist localized eigenstates only. The dashed horizontal line marks the MIT for the noninteracting case. Below it the system is a metal. For nonzero interactions a new phase of a correlated metal is formed in the midst of the insulator region.

these bands will determine the largest group velocity of spreading fronts as in fig. 3. We found that these velocities are in general dependent on the control parameter values.

Theoretical interpretation. – In the following we will discuss a possible mechanism for the observed effect of the appearance of correlated metallic bound states in the main existence region of the correlated metal phase in fig. 4 for $\lambda = 2.5$. Let us consider the Fock space of two noninteracting particle eigenfunctions

$$|\mu,\nu\rangle = \frac{1}{\sqrt{\delta_{\mu\nu}+1}} \sum_{k,\ell} A_k^\mu A_\ell^\nu \hat{b}_k^+ \hat{b}_\ell^+ |0\rangle, \qquad (5)$$

where $\mu \leqslant \nu$ are the indices of the single-particle eigenstates, sorted according to their position along the chain. For nonzero interactions we expand an eigenstate as

$$|\Psi(t)\rangle = \sum_{\mu\leqslant\nu} \sum_{\nu} \phi_{\mu\nu}(t)|\mu,\nu\rangle. \qquad (6)$$

and the evolution equation for the coefficients $\phi_{\mu\nu}$ reads

$$i\dot{\phi}_{\mu\nu} = \mathcal{E}_{\mu\nu}\phi_{\mu\nu} + \sum_{\mu'\leqslant\nu',\nu'} U \cdot I_{\mu\nu,\mu'\nu'}\phi_{\mu'\nu'}. \qquad (7)$$

The renormalized energies $\mathcal{E}_{\mu\nu}$ and the overlap integrals $I_{\mu\nu,\mu'\nu'}$ responsible for hopping between the modes $|\mu,\nu\rangle$ and $|\mu',\nu'\rangle$, are obtained from

$$\mathcal{E}_{\mu\nu} = (\lambda_\mu + \lambda_\nu) + U I^0_{\mu\nu}, \quad I^0_{\mu\nu} = \frac{2}{\delta_{\mu\nu}+1} \sum_j \left(A_j^\mu A_j^\nu\right)^2,$$

$$I_{\mu\nu,\mu'\nu'} = \frac{2}{\sqrt{(\delta_{\mu\nu}+1)(\delta_{\mu'\nu'}+1)}} \sum_j A_j^\mu A_j^\nu A_j^{\mu'} A_j^{\nu'}. \qquad (8)$$

We are interested only in bound states where the two particles are within a localization length distance from each other, since these are observed to yield a transition to a correlated metal. The renormalization in each miniband depends on the strength of the overlap integrals $I^0_{\mu\nu}$. We compute them numerically and find that the average overlap integrals $I^0 \approx 0.5$ from TP1 and $I^0 \approx 0.3$ from TP3. Note that the values for I^0 for states from TP2 and TP4 are much smaller, since the Fock states are made of products of *different* single-particle states. TP5 yields again large values of I^0 but is irrelevant for reasons given below. We also obtain that the average overlap integrals $I_{\mu\nu,\mu'\nu'} \approx 0.1$. Let us consider only states from TP1. The increase in U leads to a *broadening* of TP1 width, since some energies get strongly renormalized and some less. In the Fock space we therefore observe an increase of an effective potential strength (which is similar to λ for the noninteracting case) as $0.5U$. At the same time the different Fock states from TP1 increase their overlap (which is similar to the hopping strength of a single particle) as $0.1U$. Therefore, the increase of the potential strength wins, and these states do not cross over into a delocalized regime, when no further Fock states are considered. The same is essentially true for all TIP minibands. However, at some value of U some renormalized states from TP1 will resonate with weakly renormalized states from TP2. This group of states is characterized by a zero potential strength (since they are resonant) and any finite overlap will therefore lead to a complete delocalization. The expected value of U follows from the distance between the minibands which is around 2, and with $I^0 = 0.5$ we predict the delocalization to start around $U = 4$ as observed in the numerics. This is the rough location of the left large tongue in fig. 4.

Using the same reasoning we predict that a resonant mixing of renormalized states from TP3 with some from TP4 is expected at around $U = 6.7$, as follows from the miniband distance around 2 and the TP3 value $I^0 = 0.3$. Again this is indeed the observed location of the right large tongue in fig. 4. It is a challenging task to extend the above arguments to the whole phase diagram in fig. 4.

The novel state of a correlated metal formed from two interacting particles should be easily measured using interacting pairs of ultracold Rb atoms in optical lattices [3], due to the recent advances in single-atom control [16]. Also the effect is expected to show up in optical beam patterns in 2D waveguide arrays which is a classical analogy [17] of the considered model.

Conclusions. – To summarize, we observed a nonperturbative delocalization of two interacting particles in a quasiperiodic potential deep in the insulator phase of the noninteracting problem. The corresponding correlated metallic bound states keep both interacting particles at a distance less than the single-particle localization length. This happens because the interacting particles may

redistribute their total energy into different Fock states which are coupled due to the interaction. We gave estimates for the appearance of the correlated metallic phase in the parameter space, which agree well with the numerical data. It is a challenging task to extend the theory to the whole parameter space, to make it quantitative, and to explore the effect of a further increase of the particle number. The spectral entanglement of localized and delocalized states appears to be rather intricate. We do not observe a classical conduction band separated by mobility edges from localized states. At the same time the spectrum of the single-particle problem is already highly complex, and far from having a simple one-band structure. The spectral properties of the TIP remain therefore a highly interesting and important open issue for future studies. Another very intriguing issue concerns the fate of delocalized TIP states in the presence of more particles, up to finite particle densities.

* * *

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