УДК 530.182

ДИФФУЗИЯ НЕСКОЛЬКИХ ВЗАИМОДЕЙСТВУЮЩИХ ЧАСТИЦ В ЛОКАЛИЗУЮЩИХ ПОТЕНЦИАЛАХ: КВАНТОВАЯ РЕГУЛЯРНАЯ И ХАОТИЧЕСКАЯ ДИНАМИКА

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В данной работе изучается динамика распространения волновых пакетов в моделях нескольких взаимодействующих квантовых частиц с разными видами пространственной модуляции. Для одной частицы или, что эквивалентно, многих невзаимодействующих частиц, известно, что в случае пространственного беспорядка все собственные состояния становятся локализованными, а в случае квазипериодической неоднородности существует порог перехода к локализации по силе неоднородности. В другом предельном случае – многих взаимодействующих частиц – задача решалась в среднеполевом приближении, в рамках нелинейного дискретного уравнения Шредингера. Здесь наблюдалось разрушение локализации за счет нелинейности, возникающего динамического хаоса. Основными наблюдаемыми свойствами были субдиффузия волновых пакетов, их самоподобие в асимптотическом пределе, зависимость показателя субдиффузии от порядка нелинейности. В настоящей работе показано, что эти свойства обнаруживаются и для нескольких квантовых частиц в решетке с беспорядком, при том, что условия среднеполевого приближения не выполнены. Тем не менее квантовый хаос обеспечивает подобную динамику. При этом показатель субдиффузии уменьшается при увеличении порядка взаимодействия, так же как и в нелинейных уравнениях. В случае квазипериодического потенциала в модели нескольких взаимодействующих частиц наблюдается квантовая регулярная динамика и почти баллистическое распространение волновых пакетов. При этом малая добавка беспорядка разрушает квантовую регулярную динамику.

Ключевые слова: Андерсоновская локализация, квантовый хаос, субдиффузия, самоподобие.

DOI: 10.18500/0869-6632-2017-25-1-52-63

Ссылка на статью: Юсипов И.И., Лаптева Т.В., Пирова А.Ю., Мееров И.Б., Иванченко М.В. Диффузия нескольких взаимодействующих частиц в локализующих потенциалах: Квантовая регулярная и хаотическая динамика // Известия вузов. Прикладная нелинейная динамика. 2017. Т. 25, № 1. С. 52–63.

FEW PARTICLE DIFFUSION IN LOCALIZING POTENTIALS: CHAOS AND REGULARITY

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In this work we study the dynamics of wave packets propagation of a few interacting quantum particles with different types of spatial inhomogeneity. Single particle or, equivalently, many noninteracting particles are localized in the case of spatial disorder, and experience localization–delocalization transition in the case of quasi-periodic inhomogeneity. In the other limiting case of many interacting particles, the problem is solved in the mean-field approximation, which leads to discrete nonlinear Schrodinger equation. There localization is destroyed due to dynamical chaos inherent to nonlinearity. It results in wave packets subdiffusion, their self-similarity in the asymptotic limit, the dependence of the subdiffusion rate from the nonlinearity order. We demonstrate that analogous features emerge in disordered lattice even for two quantum particles due to quantum chaos, much away from the validity of the mean-field approximation. The subdiffusion exponent decreases with the increasing order of interaction, as found in nonlinear equations. On the contrary, in the case of a quasi-periodic potential we find regular quantum dynamics and almost ballistic wave packets propagation. Wherein a small additive of disorder destroys the regular quantum dynamics.

Keywords: Anderson localization, quantum chaos, subdiffusion, self-similarity

DOI: 10.18500/0869-6632-2017-25-1-52-63

Paper reference: Yusipov I.I., Laptyeva T.V., Pirova A.Yu., Meyerov I.B., Ivanchenko M.V. Few particle diffusion in localizing potentials: Chaos and regularity. *Izvestiya VUZ. Applied Nonlinear Dynamics.* 2017. Vol. 25. Issue 1. P. 52–63.

Introduction

Localization of quantum particles or waves due to random (Anderson) or quasi-periodic (Aubry–Andre) spatial inhomogeneity of the lattice potential is a fundamental physical phenomenon manifested by light, sound, and matter waves [1–10]. To date, the rigorous results are available for the case of non-interacting particles only, while the complexity of the many-body localization problem leaves it essentially open, despite some recent advances [11–13].

In this light, much attention is devoted to the computationally accessible case of a few interacting quantum particles. The earlier studies of the two interacting particles (2IP) in random lattices concluded that interaction inflates the single particle localization length ξ_1 up to another finite localization length ξ_2 [14–20]. For quasi-periodic potentials the predictions differed from incremental increase of localization length to decrease of localization length in the insulating regime [21–23].

The recent results reveal much more dramatic and unexpected effects of interactions. First, it was shown that some of the 2IP states in quasi-periodic lattices can become completely delocalized under the non-perturbatively strong interaction, giving rise to an unconstrained wave packet propagation [24, 25]. Second, in disordered lattices, it was found that 2IP produce self-sustained subdiffusive propagation beyond the single particle

localization length, provided that the disorder is weak and $\xi_2 \gg \xi_1$ [26]. This regime was associated with the quantum chaos and high effective connectivity of states due to interaction [26, 27].

These findings intriguingly correlate with the results obtained in the mean field approximations, which lead to the Gross–Pitaevsky type nonlinear wave equations [28,29]. There nonlinearity breaks localization and leads to subdiffusive wave packet propagation, underpinned by nonintegrability and dynamical chaos [30–37]. The particular footprints of the chaotic nature of subdiffusion are seen in the asymptotically self-similar expansion of the wave packet [38–40] and the nonlinearity-dependent subdiffusion exponent [39, 41].

In this paper we demonstrate that a few interacting particles can propagate beyond the single-particle localization length in two main regimes, determined by the presence or absence of quantum chaos [42, 43]. Quantum chaos develops in random lattices and shapes the self-similar wave packet profiles, which tails are localized exponentially, with the corresponding length diverging in time. The pure three particle interaction does exhibit subdiffusion but with a weaker exponent, completing the similarity to the classical nonlinear chaotic spreading. In contrast, 2IP on quasi-periodic lattices do not develop a pronounced quantum chaos, according to level statistics, and delocalize in a regular regime, as ballistically propagating plane waves. Its analogy for the nonlinear classical lattices is currently not known. In case of mixed potentials, the regular propagation is broken already by weak disorder.

1. Model and Numerics

We study the few particle dynamics in the framework of the Hubbard model with the Hamiltonian

$$\hat{\mathcal{H}} = \sum_j \left[\hat{b}^+_{j+1}\hat{b}_j + \hat{b}^+_j\hat{b}_{j+1} + \varepsilon_j \hat{b}^+_j\hat{b}_j + \frac{U_k}{k}\left(\hat{b}^+_j\right)^k \left(\hat{b}_j\right)^k \right] \tag{1}$$

where $\hat{b}^+_j$ and $\hat{b}_j$ are creation and annihilation operators of indistinguishable bosons at lattice site j. U_k measures the k-particle on-site interaction strength. The on-site energies are either random uncorrelated numbers with a uniform probability density function on the interval $\varepsilon_j \in [-W/2, W/2]$ as in the original Anderson problem, or quasi-periodically modulated $\varepsilon_j = W\cos(2\pi\alpha j + \theta)$, as in the Aubry–Andre case.

For the 2IP case we make use of the vacuum state $|0\rangle$ and the basis $|j,k\rangle \equiv \hat{b}^+_j b^+_k|0\rangle$ and write the 2IP wave function as $\Psi = \sum\limits_{j,k} \varphi_{j,k}|j,k\rangle$:

$$i\dot{\varphi}_{j,k} = \varepsilon_{j,k}\varphi_{j,k} + \sum_{\pm}(\varphi_{j\pm1,k} + \varphi_{j,k\pm1}), \tag{2}$$

where $\varepsilon_{j,k} = \varepsilon_j + \varepsilon_k + U_2\delta_{j,k}$ and $\delta_{j,k}$ is the Kronecker symbol.

For three interacting particles (3IP), when pairwise interactions are absent, $U_2 = 0$, the corresponding equations read:

$$i\dot{\varphi}_{j,k,m} = \varepsilon_{j,k,m}\varphi_{j,k,m} + \sum_{\pm}(\varphi_{j\pm1,k,m} + \varphi_{j,k\pm1,m} + \varphi_{j,k,m\pm1}), \tag{3}$$

where $\varepsilon_{j,k,m} = \varepsilon_j + \varepsilon_k + \varepsilon_m + U_3\delta_{j,k,m}$. A mixture of two and three particle interactions can also be considered, $\varepsilon_{j,k,m} = \varepsilon_j + \varepsilon_k + \varepsilon_m + U_3\delta_{j,k,m} + U_2\left(\delta_{j,k} + \delta_{k,m} + \delta_{j,m}\right)$. However, we did not find qualitative differences with the 2IP case.

In the absence of interactions, $U_k = 0$, solutions to (2) break into a product of single particle (SP) solutions that follow

$$i\dot{\varphi}_m = \varepsilon_m \varphi_m + \varphi_{m+1} + \varphi_{m-1}. \tag{4}$$

In the disordered case all eigenstates $\{A_m^{(r)}\}_{r=1,\ldots N}$ of (4) are exponentially localized with the maximal localization length $\xi \approx 96/W^2$ for $W < 4$ [3]. In the quasi-periodic case all eigenstates are delocalized below the mobility edge, $W = 2$, and localized above, sharing the same localization length $\xi = [\ln(W/2)]^{-1}$ [2].

Numerical integration of (2) and (4) is performed on finite lattices $N \times N$ and $N \times N \times N$ with the PQ-method [34], the particle identity appropriately made use of. The initial conditions correspond to the particles placed at the adjacent sites. To characterize the wave packet dynamics we calculate the one-dimensional probability distribution function (PDF) of the particle density as $\mathrm{PDF}_j = \sum\limits_k |\varphi_{j,k}|^2$ for 2IP and $\mathrm{PDF}_j = \sum\limits_{k,m} |\varphi_{j,k,m}|^2$ for 3IP. We monitor the wave packet expansion computing its mass center $m_1 = \sum_j j\mathrm{PDF}_j$ and the second moment $m_2 = \sum_j (j - m_1)^2 \mathrm{PDF}_j$. The system size is varied within $N = 5000...15000$ (2IP) and $N = 1000$ (3IP).

2. Results

It has been previously found that in both types of localizing lattices, Anderson and Aubry–Andre, interactions can induce propagation of two quantum particles much beyond the SP localization length ξ_1 [24–27]. Fig. 1 presents the global picture of the regimes, the brighter color corresponding to greater values of the wave packet second moment m_2, as measured after $t = 10^5$ time of evolution from localized initial conditions. In the disordered case the phase diagram is smooth and shows gradual delocalization, while in the quasi-periodics case it consists of several sharp tongues. The details of 2IP expansion also differ. In the Anderson model the wave packets propagate ballistically up to the SP localization length, ξ_1, and then make a crossover towards the subdiffusive spreading up to the 2IP localization length $\xi_2 \gg \xi_1$ (also believed to be finite), $m_2(t) \propto t^\alpha$,

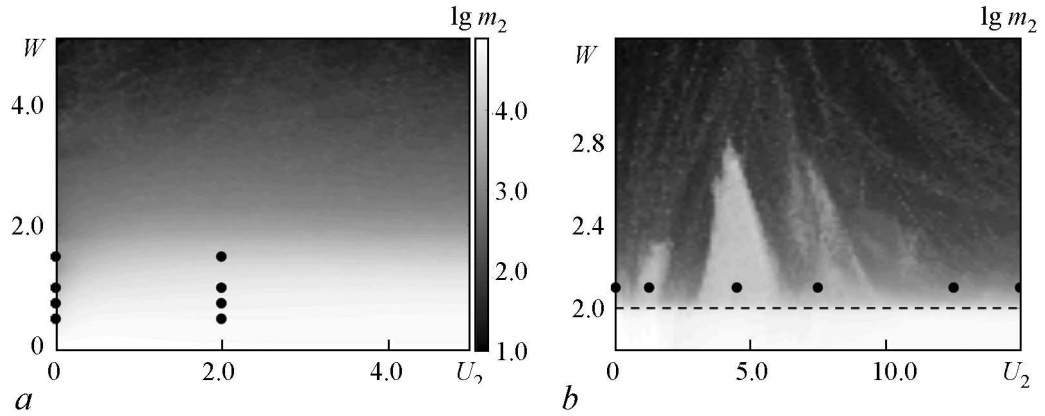

Fig. 1. Phase diagrams of the 2IP localization for the (*a*) random and (*b*) quasi-periodic lattices as suggested by the wave packet second moment m_2 (color coded) after its long-term evolution ($N = 1000$, $t = 10^5$). Dashed horizontal line in (*b*) indicates a SP metal–insulator transition. Black dots mark the points, for which $m_2(t)$ is shown in Fig. 3, *a*, 5,*a*

$\alpha \approx 1/2$ [26,27]. These stages can be clearly seen in the respective PDF, cf. Fig. 2, *a*, and the scaling of the wave packet second moment for the parameters marked in Fig. 1, *a*, cf. Fig. 3, *a*. In contrast, 2IP in quasi-periodic lattices can become completely delocalized, as demonstrated by the wave packet divergence and the formation of the system-wide two-particle states [24,25]. The visual wave packet expansion does not present a slowdown on the observable spatiotemporal scale, cf. Fig. 2, *b*.

We start the detailed analysis of the particle spreading with the Anderson model. There two main observations lead to the conjecture of the quantum chaotic nature of 2IP subdiffusion: the high connectivity of the SP states due to interactions and the Wigner–Dyson type level statistics [26].

Let us first explore the effect of the order of interaction on the spreading exponent that is a trait of chaotic spreading in classical nonlinear lattices [39,41].

Consider diffusion of the norm between few-particle states composed of SP ones, $\mathbf{r} \equiv (r_1, \ldots, r_k)$, $\mathbf{s} \equiv (s_1, \ldots, s_k)$. The diffusion rate D should be proportional to the coupling between them, $\Gamma_{\mathbf{r},\mathbf{s}}$, which can be written as [44]:

$$\Gamma_{\mathbf{r},\mathbf{s}} = 2\pi \frac{|\langle \mathbf{r}|\mathcal{H}_{int}|\mathbf{s}\rangle|^2}{|\omega_{\mathbf{r}} - \omega_{\mathbf{s}}|},$$
$$\mathcal{H}_{int} = \sum_j \frac{U_k}{k} \left(\hat{b}_j^+\right)^k \left(\hat{b}_j\right)^k, \tag{5}$$

where $\omega_{\mathbf{r},\mathbf{s}}$ are respective eigenfrequencies. It follows that $D \sim U_k^2 \mathbf{n}^{2(k-1)}$, where $\mathbf{n}$ is the local norm density, PDF. For a one-dimensional expansion, the wave packet second moment and norm density relate as $m_2 \sim 1/\mathbf{n^2}$. Substituting it into $m_2 = D\,t$ we finally obtain

$$m_2 \propto t^{\alpha}, \alpha = 1/k. \tag{6}$$

The results of numerical experiments for the 3IP case (the numerics for 3IP in case $U_2 \neq 0$ reveals qualitatively the same results as for 2IP, and is not presented here) clearly confirm the predicted decrease of the subdiffusion exponent for higher order of interactions, $\alpha \approx 0.25$ for a set of disorder strengths and $U_3 = 2.0$ ($U_2 = 0$) as it is

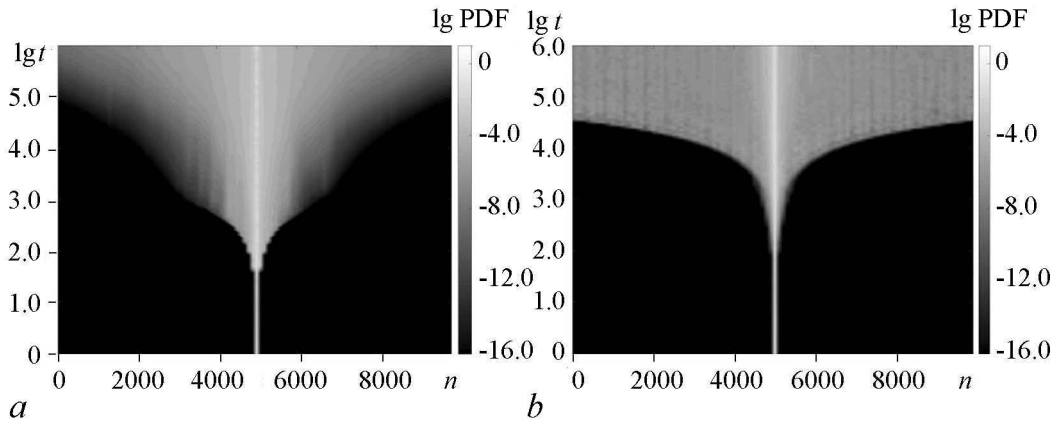

Fig. 2. Characteristic PDF evolution of expanding 2IP wave packets on (*a*) a disordered lattice, $W = 1.0$, $U_2 = 2.0$, $N = 10000$, and (*b*) a quasi-periodic lattice, $W = 2.02$, $U_2 = 7.5$, $N = 10000$. Note the crossover from ballistic to subdiffusive expansion in (*a*) at about $t = 10^3$, once the wave packet goes beyond ξ_1, and the persistently uniform expansion in (*b*)

read from Fig.3, *b*, similar to the existing effect for the nonlinear classical lattices. At the same time, the quantitative validation of the exponent in (6) remains unattainable given the limited spatiotemporal scales of numerical observation, attainable in the 3IP case.

The other key trait of the nonlinear chaotic wave packet spreading is the approximate self-similarity of solutions, in analogy to the nonlinear diffusion equation [38–40]. Remarkably, self-similarity is also discovered in the quantum disordered case. However, at variance to the nonlinear case, the wave packet is well approximated by a decaying exponent with the time-dependent localization length:

$$|\psi_l| \sim \exp[-|l - l_0|/\xi(t)]. \tag{7}$$

Fig. 4, *a* illustrates self-similar expansion of the wave packet from a localized initial state on a disordered lattice through snapshots at different times. It demonstrates that the wave packet profile is well-described by the exponential decay at any time moment; its slope is monotonously decreasing in time. It allows to introduce the dynamical

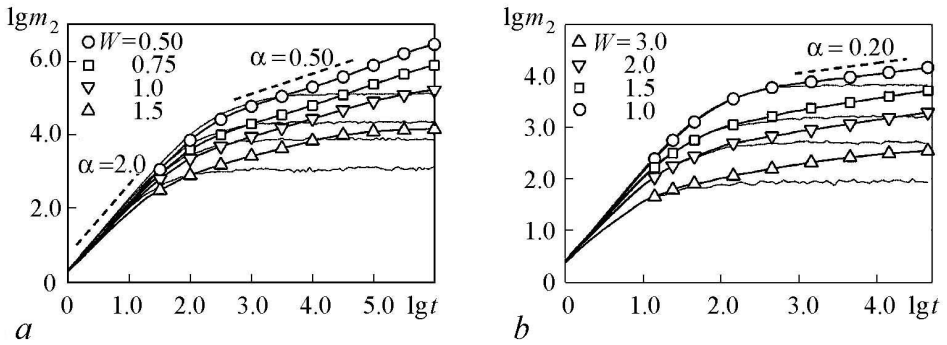

Fig. 3. Dynamics of the wave packet second moment, $m_2(t)$ from a localized initial state on a random lattice. *a* – The curves for 2IP (from top to bottom) correspond to disorder $W = 0.5$ (circles), 0.75 (squares), 1.0 (down-triangles), 1.5 (up-triangles), and interaction $U_2 = 2.0$ and $U_2 = 0$ (dash-dotted lines), cf. Fig. 1, *a*. Dashed lines exemplify $m_2 \sim t^\alpha$, $\alpha = 2.0$ and $\alpha = 0.5$. *b* – The curves for 3IP (from top to bottom) correspond to disorder $W = 1.0$ (circles), 1.5 (squares), 2.0 (down-triangles), 3.0 (up-triagles), and interaction $U_3 = 2.0$ (solid lines) and $U_3 = 0$ (dash-dotted lines). Dashed lines exemplify $m_2 \sim t^\alpha$, $\alpha = 0.2$

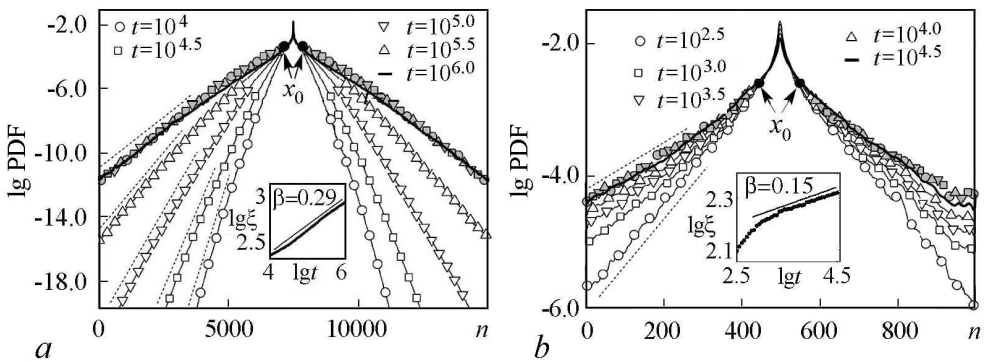

Fig. 4. Self-similar expansion of the wave packet from a localized initial state on a disordered lattice with exponentially falling out tails: $|\psi_l| \sim \exp[-|l - l_0|/\xi(t)]$. *a* – 2IP, $W = 1.0$, $U_2 = 2.0$, grey symbols demonstrate rescaling of PDF profiles at $t = 10^4$ (circles), $t = 10^{4.5}$ (squares), $t = 10^5$ (down-triangles), and $t = 10^{5.5}$ (up-triangles) to the final time $t = 10^6$ according to (8); *b* – 3IP, $W = 1.0$, $U_3 = 2.0$ ($U_2 = 0$), grey symbols demonstrate rescaling of PDF profiles at $t = 10^{2.5}$ (circles), $t = 10^3$ (squares), $t = 10^{3.5}$ (down-triangles), and $t = 10^4$ (up-triangles) to the final time $t = 10^{4.5}$ according to (8). The dashed lines guide an eye. Insets: the dynamical localization length scales as $\xi(t) \sim t^\beta$, $\beta \approx 0.29$ (*a*) and $\beta \approx 0.15$ (*b*)

localization length and study its evolution (Fig. 4, *a*, inset). The self-similarity of solutions is established by scaling between the two moments of time, $t_1 < t_2$, defined as follows:

$$\mathrm{PDF}\left(|x - x_0|, t_2\right) = \mathrm{PDF}\left((t_1/t_2)^{\beta}|x - x_0|, t_1\right), \tag{8}$$

where x_0 mark the distance from the central peak, at which self-similarity of tails begins. In particular, for $W = 1, U_2 = 2$ we find $\xi(t) \sim t^{\beta}, \beta \approx 0.29$ (cf. Fig. 4, *a*, inset), which corroborates well the theoretical expectation $\beta = \alpha/2$. The 3IP model also displays this kind of self-similarity (cf. Fig. 4, *b*). Let us now turn to the quasi-periodic case. Analysing the wave packet expansion we find an almost ballistic growth of its second moment, $\alpha \approx 1.5 \ldots 1.7$ for the parameters in the delocalization regime (Fig. 5, *a*), cf. marks in Fig. 1, *b*. The diffusion exponent decreases only on the border of the spreading regime. The wave packet profiles exhibit the wave fronts typical of the plain wave propagation in the disorder-free lattice (Fig. 5, *b*).

To shed light on the nature of the difference to the disordered case, we study the level spacing statistic for the systems of the size $N \sim \xi_1$, for which full diagonalization is numerically accessible (in particular, $N = 100, 200, 300$ were tested). There one recovers the transition to the Wigner–Dyson type distribution $P(s) = \pi s/2 \exp\left(-\pi s^2/4\right)$ from the Poisson-type distribution $P(s) = \exp\left(-s\right)$ as interaction prompted subdiffusive propagation, Fig. 6, *a*. In contrast, the level spacing statistics for quasi-periodic systems develops an even a sharper peak about $s = 0$, manifesting regular quantum dynamics in different delocalization tongues, consistently. There is indication that it drops to $P(0) = 0$ equally sharp, pointing out the possibility of a mixture with weak chaos. Further numerical studies, more massive then we could currently attain, are needed to validate the hypothesis.

Finally, we address the transition between the regular and chaotic few quantum particle propagation. For that we introduce a mixed potential $\varepsilon_j = (1-q)W_Q \times \times \cos(2\pi\alpha j + \theta) + qW_D\zeta_j$, $\zeta_j \in [-W/2, W/2]$ where q parametrizes the weights of the pure quasi-periodic (W_Q) and disordered (W_D) potentials. We choose $U_2 = 4.5$, $W_Q = 2.1$ and $W_D = 1.0$ such that in the limiting cases one has regular and chaotic quantum wave packet spreading, respectively. Changing $q \in [0, 1]$ we start from localized initial conditions and obtain the second moment at $t = 10^5$ as a function of q, cf. in

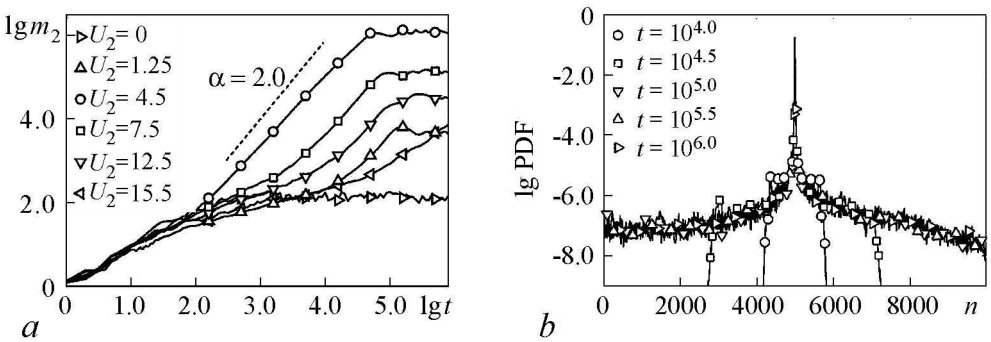

Fig. 5. Quasi-periodic lattice: *a* – Dynamics of the wave packet second moment, $m_2(t)$ from a localized initial state, $W = 2.1$, U_2 varied, $N = 10000$. The almost ballistic propagation persists in delocalization region throughout free expansion, $\alpha \approx 1.5...1.7$, $U_2 = 1.25$, 4.5, 7.5. The exponent decreases on the border of the region ($U_2 = 12.5$, 15.0); *b* – Plane wave type expansion of the wave packet, $W = 2.4$, $U_2 = 4.5$, $t = 10^4$, $10^{4.5}$, 10^5, $10^{5.5}$, 10^6

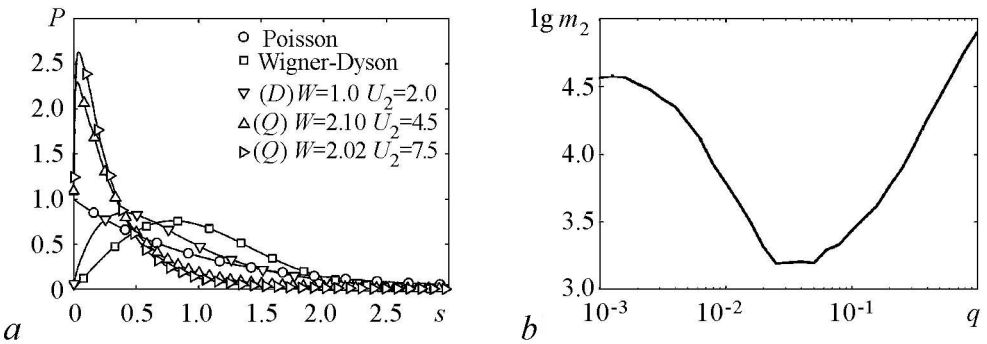

Fig. 6. *a* – Normalized 2IP level spacing distribution ($\langle P(s)\rangle = 1$) for disordered and quasi-periodic lattices, $N = 100$. In all cases wave packet spreading beyond ξ_1 is observed. Distinctly non-Poissonian in the disordered case indicate quantum chaos, and the Poisson-type in the quasi-periodic one manifest regular dynamics. Testbed Poisson $P(s) = \exp(-s)$ (circles) and Wigner–Dyson $P(s) = \pi s/2 \exp(-\pi s^2/4)$ (squares) distributions are also shown. *b* – The wave packet expansion at $t = 10^5$ depending on the balance between the quasi-periodic ($q = 0$) and random ($q = 1$) potentials

Fig. 6, *b*. The results demonstrate that even a weak mixture of disorder destroys regular propagation: the almost ballistic expansion at $q = 0$ is taken over by a quickly saturating growth of $m_2(t)$ already for $q \sim 10^-2$. The minimum of m_2 at $t = 10^5$ is reached for $q \approx 0.05$. Interestingly, going back from the purely disordered case, $q = 1$, one also observes decay of the final m_2, suggesting that mixing potentials hampers either types of pure spreading.

Conclusion

We establish the two fundamental regimes of 2IP spreading, determined by the presence or absence of quantum chaos. Disordered potentials produce chaotic quantum dynamics, that leads to subdiffusion, $m_2 \sim t^\alpha, \alpha = 1/k$ for the $k-$particle interaction, and self-similarity of the expanding wave-packets, $|\psi_l| \sim \exp[-|l - l_0|/\xi(t)]$, $\xi(t) \sim t^\beta$, $\beta \approx \alpha/2$. It is worth drawing attention to the imprecise agreement between the theoretical and numerically estimated subdiffusion exponent for the 3IP case, which reasons are currently unclear.

Delocalization in quasi-periodic potentials is attributed to regular quantum spreading, as it follows by the level spacing statistics and the almost ballistic expansion of plane waves. Remarkably, even a weak mixture of disorder in quasi-periodic potentials destroys this regime. Unexpectedly, already two interacting quantum particles are able to reproduce all basic features of nonlinear wave packet subdiffusion in classical lattices, which are, strictly speaking, are obtained only in the mean field approximation for the many-body quantum dynamics. Even more puzzling is the second, regular spreading regime in the few particle quantum problem for quasi-periodic potentials that does not seemingly possesses an nonlinear classical counterpart. Beside open theoretical challenges we also forsee a keen interest from the experimental physics of ultracold atomic condensates in modulated potentials to our findings.

The Authors acknowledge RFBR No.15-42-02670, T.V.L. also acknowledges Dynasty Foundation.

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Поступила в редакцию *22.11.2016*
После доработки *16.01.2017*

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