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Delocalization of Weakly Interacting Bosons in a 1D Quasiperiodic Potential

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We consider weakly interacting bosons in a 1D quasiperiodic potential (Aubry-Azbel-Harper model) in the regime where all single-particle states are localized. We show that the interparticle interaction may lead to the many-body delocalization and we obtain the finite-temperature phase diagram. Counterintuitively, in a wide range of parameters the delocalization requires stronger coupling as the temperature increases. This means that the system of bosons can undergo a transition from a fluid to insulator (glass) state under heating.

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Quantum mechanics of a single particle in a quasiperiodic potential is a standard although quite nontrivial theoretical problem [1–6] intensively studied for several decades. It turned out that for one-dimensional (1D) quasiperiodic potentials (superposition of two incommensurate periodic potentials) the eigenfunctions can be either extended or localized, depending on the parameters of the potential. The phenomenon of quantum localization was observed for 1D quantum gases in both random [7] and quasiperiodic potentials [8]. The experiments conducted in the regime of negligible interaction between the atoms of expanding Bose gas demonstrated good qualitative agreement with the single-particle theories of localization [3,9]. The same applies to spreading of wave packets of light in a quasiperiodic photonic lattice [10]. Recently [11,12], a Feshbach resonance was used to study bosons with sizable and fine-tunable interaction in the quasiperiodic potential.

Theoretical description of many-body effects in disordered fermionic [13,14] and bosonic [15] systems is based on the idea of the localization of many-body wave functions in the Hilbert space—many-body localization. The quasiperiodic potential represents an intermediate case between periodic and disordered systems. Zero temperature phase diagram for 1D bosons in the quasiperiodic potential has been previously discussed and calculated numerically [16–18], and the case of an infinite temperature for (nearest-neighbor) interacting spinless fermions has been studied in Ref. [19]. The problem of localized and extended states of two interacting particles in the 1D quasiperiodic potential has been discussed in Refs. [20,21].

In this Letter we study finite-temperature transport properties of interacting bosons in the 1D quasiperiodic potential and predict the physical behavior which differs drastically from the many-body localization of bosons caused by random potentials. We show that, counterintuitively, in a

broad temperature range an increase in temperature induces a transition from fluid to glass.

The standard model of a 1D quasiperiodic potential is the Aubry-Azbel-Harper (AAH) model [1–3]—a tight-binding Hamiltonian with hopping amplitude J and periodically modulated on-site energies, at a period incommensurate with respect to the primary lattice. The eigenstate ψ_j^α at energy ε_α is determined by the equation

$$J(\psi_{j+1}^\alpha + \psi_{j-1}^\alpha) + V \cos(2\pi\kappa j)\psi_j^\alpha = \varepsilon_\alpha \psi_j^\alpha. \quad (1)$$

Here V is the modulation amplitude, and κ is an irrational number. In 1D random potentials all single-particle states are localized [22,23]. On the contrary, in the AAH model all states are extended unless the amplitude of the modulation exceeds a critical value $2J$. Then all states are localized, and the localization length in units of the lattice constant is given by [3]

$$\zeta = \frac{1}{\ln(V/2J)} \Rightarrow \zeta \approx \frac{V}{V-2J} \gg 1 \quad \text{for } V-2J \ll V. \quad (2)$$

Below we assume $\zeta \gg 1$. Our analytical consideration based on the semiclassical approach [2,5,24,25] to the single-particle problem, is valid when the period of the modulation is much larger than the period of the lattice, $\kappa \ll 1$. We supplement this analysis by numerical calculations for $\kappa \sim 1$, in particular for κ equal to the golden ratio $(\sqrt{5}-1)/2$.

The semiclassical one-particle spectrum is organized according to the continued fraction decomposition [2,5] of the irrational parameter $\kappa = 1/[n_1 + 1/(n_2 + \dots)]$. For $n_1, n_2, \dots \gg 1$ the spectrum has a hierarchical structure: it consists of n_1 narrow first-order bands (FOBs)—clusters of L/n_1 energy levels (L is the size of the system). Each FOB contains n_2 second-order bands, so that there are $\sim n_1 n_2$ second-order bands in total, etc. All eigenstates are located

in the energy interval $-V - 2J < \varepsilon < V + 2J$. The spacing ω between FOBs is the frequency of the classical periodic motion [26] in a single potential well of the size $1/\kappa \approx n_1$ [27], which includes n_1 levels,

$$\omega = \frac{2\pi}{\oint dx/v} \approx \frac{2\pi^2\kappa V}{\ln(64V^2/|\varepsilon^2 - V^2/\zeta^2|)}, \quad (3)$$

where $v = \sqrt{4J^2 - [\varepsilon - V \cos(2\pi\kappa x)]^2}$ is the classical velocity of a particle. The widths of FOBs are determined by the tunneling between neighboring wells [5],

$$\Gamma_s = \frac{4\omega}{\pi} \exp\left(-\int dx|p|\right). \quad (4)$$

The integral is taken over the classically forbidden region, and $|p| = \text{arccosh}[(V \cos(2\pi\kappa x) - \varepsilon_s)/2J]$. The index s labels FOBs centered at the energies ε_s . The action can be approximated as $\int dx|p| \approx |\varepsilon_s|/4\kappa J$, which yields an exponential dependence of the bandwidth on energy

$$\Gamma_s \approx \frac{32\kappa J}{\pi} \exp(-|\varepsilon_s|/4\kappa J). \quad (5)$$

Can the localization of the bosons be destroyed by the interaction? It is known that the interaction can delocalize fermions [14] and 1D bosons [15] in the case of a random potential. Experiments with interacting bosons in 1D quasiperiodic potentials [11,12] indicated an interaction-induced localization-delocalization transition. It is also worth noting that experiments in quasiperiodic photonic lattices [10] have found that nonlinearity (interactions) increases the width of localized wave packets of light. Here we consider the AAH model with a weak on-site interaction,

$$H_{int} = \frac{U}{2} \sum_j a_j^\dagger a_j^\dagger a_j a_j; \quad U \ll J, \quad (6)$$

with a_j being the bosonic field operators. In order to estimate the critical coupling constant U_c corresponding to the many-body localization-delocalization transition (MBLDT), we use the method developed in [14,15], which is similar to the original estimation for the single-particle Anderson localization [9]. One has to consider the localized one-particle states $|\alpha\rangle$ and analyze how different two-particle states $|\alpha, \beta\rangle$ hybridize due to the interaction. The criterion of MBLDT is

$$P_\alpha \sim 1, \quad (7)$$

where P_α is the probability that for a given one-particle state $|\alpha\rangle$ there exist three other states $|\beta\rangle, |\gamma\rangle, |\delta\rangle$, such that the two-particle states $|\alpha, \beta\rangle$ and $|\gamma, \delta\rangle$ are in resonance; i.e., the matrix element $\langle \gamma, \delta | H_{int} | \alpha, \beta \rangle \equiv M_{\alpha\beta}^{\gamma\delta}$ exceeds the

energy mismatch $\Delta_{\alpha\beta}^{\gamma\delta} \equiv |\varepsilon_\alpha + \varepsilon_\beta - \varepsilon_\gamma - \varepsilon_\delta|$ where $\varepsilon_\alpha, \varepsilon_\beta, \varepsilon_\gamma$ and ε_δ are one-particle energies.

For large occupation numbers N_β, N_γ , and N_δ of the states $|\beta\rangle, |\gamma\rangle$ and $|\delta\rangle$ the fluctuations are small. Selecting a given single-particle state α and taking into account both direct and inverse processes we find [28]

$$M_{\alpha\beta}^{\gamma\delta} = \sqrt{|N_\beta(1+N_\gamma)(1+N_\delta) - N_\gamma N_\delta(1+N_\beta)|} U_{\alpha\beta}^{\gamma\delta}, \quad (8)$$

with

$$U_{\alpha\beta}^{\gamma\delta} = U \sum_j \psi_j^{\delta*} \psi_j^{\gamma*} \psi_j^\beta \psi_j^\alpha. \quad (9)$$

As discussed in Refs. [14,15], the matrix elements of the interaction are small unless the energies $\varepsilon_\alpha, \varepsilon_\beta, \varepsilon_\gamma, \varepsilon_\delta$ are almost equal pairwise, e.g., $\varepsilon_\alpha \approx \varepsilon_\gamma$ and $\varepsilon_\beta \approx \varepsilon_\delta$, while ε_α and ε_β can differ substantially. Accordingly, $M_{\alpha\beta}^{\gamma\delta} \approx N_\beta U_{\alpha\beta}^{\gamma\delta}$. The approximation (8) for the matrix elements remains valid for small occupation numbers.

If α and γ (as well as β and δ) are nearest neighbors in energy the energy mismatch is

$$\Delta_{\alpha\beta}^{\gamma\delta} = \delta_\alpha + \delta_\beta, \quad (10)$$

where $\delta_\alpha = |\varepsilon_\alpha - \varepsilon_\gamma|$ is a typical spacing between the states on the length scale ζ at energy close to ε_α . We estimate the matrix element [29]:

$$M_{\alpha\beta}^{\gamma\delta} \approx UN_\beta/\zeta. \quad (11)$$

According to Eqs. (10) and (11) the probability $P_{\alpha\beta}^{\gamma\delta}$ of having $M_{\alpha\beta}^{\gamma\delta} \gtrsim \Delta_{\alpha\beta}^{\gamma\delta}$ is

$$P_{\alpha\beta}^{\gamma\delta} \approx UN_\beta/\zeta(\delta_\alpha + \delta_\beta). \quad (12)$$

The probability P_α which enters the criterion (7) of MBLDT is the sum of $P_{\alpha\beta}^{\gamma\delta}$ over all single-particle states $|\beta\rangle, |\gamma\rangle, |\delta\rangle$. Since for given α and β the number of relevant pairs of states $|\gamma\rangle, |\delta\rangle$ is of order unity, only the summation over β is important,

$$P_\alpha = \sum_{\beta, \gamma, \delta} P_{\alpha\beta}^{\gamma\delta} \approx \sum'_\beta UN_\beta/\zeta(\delta_\alpha + \delta_\beta), \quad (13)$$

where \sum' means that the summation is over the eigenstates on the length scale of ζ . Substitution of Eq. (13) into Eq. (7) leads to the criterion of MBLDT:

$$\sum'_\beta U_c N_\beta / \zeta(\delta_\alpha + \delta_\beta) = 1. \quad (14)$$

The critical coupling strength U_c in Eq. (14) depends on the choice of the state α through the quantity δ_α . One has to

choose α which minimizes U_c . Besides, Eq. (14) expresses the critical coupling U_c in terms of the occupation numbers N_β which are determined by the chemical potential. In order to formulate the MBLDT criterion in terms of the experimentally controllable filling factor ν one has to complement Eq. (14) with the number equation, which relates ν to the occupation numbers:

$$\nu = \sum_{\alpha} N_{\alpha}/L. \quad (15)$$

We are now ready to apply the MBLDT criterion to interacting bosons in the AAH model. On the insulator side, the occupation numbers are given by

$$N_{\alpha} = \{\exp[(\varepsilon_{\alpha} - \mu + UN_{\alpha}/\zeta)/T] - 1\}^{-1}, \quad (16)$$

where μ is the chemical potential shifted by the interaction energy of a particle in the state $|\alpha\rangle$ with particles in all other states. Equations (14), (15), and (16) yield the critical coupling U_c as a function of temperature.

On the length scale ζ there are $\sim\zeta$ states with a significant amplitude of the wave function. Thus, there are at most ζ states contributing to the sum in Eq. (14). The calculation simplifies in the limit $n_1 \ll \zeta \ll n_1 n_2$ where each FOB contains $\sim\zeta/n_1 \approx \kappa\zeta$ overlapping states. The related example is shown in Fig. 1: κ is close to $1/8$, the localization length is $\zeta \approx 40$, and $n_2 = 7$.

At temperatures much smaller than the spacing between the FOBs, i.e., $T \ll \omega$, only single-particle states from the lowest energy FOB participate in MBLDT. We assume that the spacing between the states in this band is approximately constant and thus equal to $\delta_{\beta} \approx \Gamma_0/\kappa\zeta$. Using the fact that

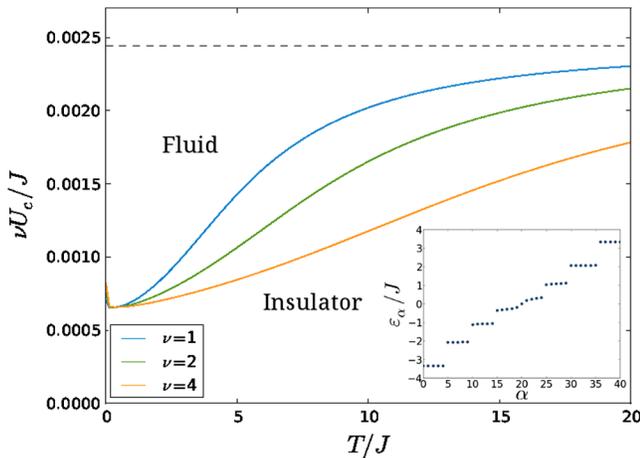


FIG. 1 (color online). The critical coupling strength U_c versus temperature obtained by directly using Eqs. (14)–(16) and the one-particle spectrum computed by exact diagonalization, for κ close to $1/8$, $V = 2.05J$, and the filling factor $\nu = 1, 2, 4$. At $T = 0$ we recover universality in νU_{c0} . The dashed line is the $T \rightarrow \infty$ asymptotics. The inset shows the spectrum on the length scale of ζ (the number of states is $\zeta \approx 40$).

the sum $\sum_{\beta} N_{\beta}/\zeta$ over the states on the length scale ζ in Eq. (14) is equal to the sum $\sum_{\alpha} N_{\alpha}/L$ in Eq. (15) over all states we obtain [30]:

$$\nu U_c \approx 2\Gamma_0/\kappa\zeta; \quad T \ll \omega. \quad (17)$$

At temperatures $T \gg \omega$ many FOBs are occupied and particles in these bands participate in MBLDT. The bands are so narrow that all levels in the s th FOB have the same occupation, so that the corresponding level spacing is $\delta_{\beta} \approx \Gamma_s/\kappa\zeta$. Then, summing over β within each FOB one can rewrite Eq. (14) as

$$\sum_{s=0}^{n_1-1} \zeta U_c N_s \kappa^2 / (\Gamma_0 + \Gamma_s) \approx 1 \quad (18)$$

(we selected the state $|\alpha\rangle$ to be in the lowest energy band, $s = 0$). According to Eq. (5) the width Γ_s exponentially increases with ε_s (i.e., s) in the interval $0 > \varepsilon_s > \varepsilon_0 \approx -V - 2J$, since $|\varepsilon_s|$ decreases. Hence, at $T \ll 8J$ the sum over s in Eq. (18) is dominated by $s = 0$, which leads to

$$U_c \approx 2\Gamma_0/N_0\kappa^2\zeta. \quad (19)$$

For $\varepsilon_s - \mu < T$ we may use the occupation number expression [29]

$$N_s \approx T/(\varepsilon_s - \mu), \quad (20)$$

and put $N_s \approx 0$ for larger ε_s . In particular $N_0 \approx T/(\varepsilon_0 - \mu)$. With the use of Eq. (20), one can rewrite Eq. (15) as

$$\nu \approx \sum_{s=0}^{(T+\mu-\varepsilon_0)/\omega} \kappa T / (s\omega + \varepsilon_0 - \mu). \quad (21)$$

In the temperature range $\omega \ll T \ll 8J$ we then find the chemical potential dependence on temperature [29]

$$\mu \approx \varepsilon_0 - \frac{\kappa T}{\nu} \left[1 + \frac{T}{8\nu J} \ln\left(\frac{T}{\omega}\right) \right], \quad (22)$$

and using equation (19) we obtain the critical coupling:

$$\nu U_c \approx \frac{2\Gamma_0}{\kappa\zeta} \left[1 + \frac{T}{8\nu J} \ln\left(\frac{T}{\omega}\right) \right]. \quad (23)$$

Since $T \ll 8J$, the second term in square brackets is a small correction. Nevertheless, it is important. According to Eq. (23) the temperature dependence of the critical coupling is anomalous: U_c increases with T ; i.e., an increase in temperature favors the insulator state.

This behavior originates from the cluster structure of the spectrum, with exponentially increasing cluster width when going from the lowest (highest) cluster energy to the middle of the spectrum. Therefore, at $T \ll 8J$ (and $\zeta \gg n_1 \approx \kappa^{-1}$)

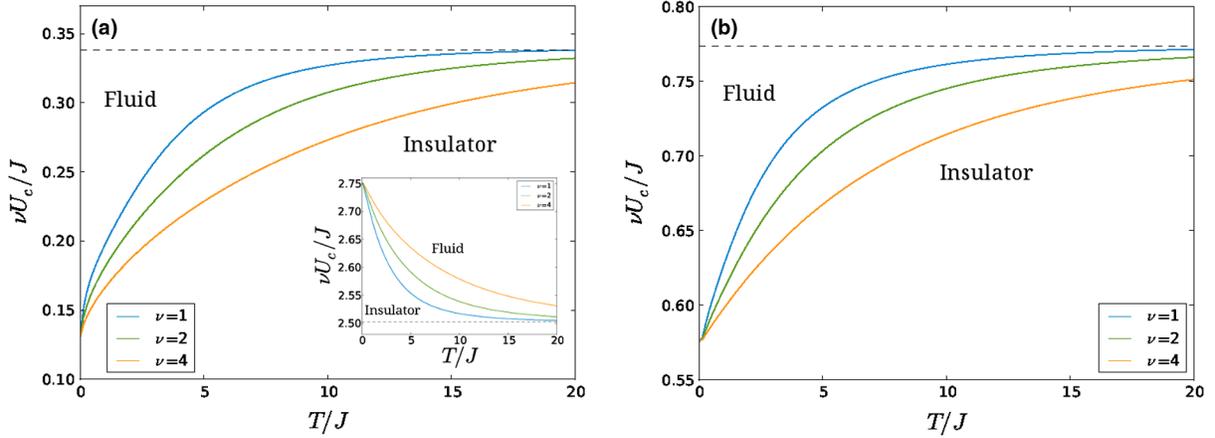


FIG. 2 (color online). The same as in Fig. 1 for $V = 2.3J$ ($\zeta \approx 7$). In (a) $\kappa \approx 0.24$, and in (b) κ is equal to the golden ratio. The inset in (a) shows $\nu U_c(T)$ for $\kappa \approx 1/8$ and $V = 2.25J$ ($\zeta \approx 8$).

the localization-delocalization transition is provided only by the particle states in the lowest energy cluster. The fraction of these particles decreases with increasing temperature, thus ensuring an increase in the critical coupling strength U_c .

For temperatures $T \rightarrow \infty$ ($T \gg 8J, 8\nu J$) all eigenstates are equally populated and $N_s = \nu$. Then the main contribution to the sum in Eq. (18) comes from $s = 0$ and $s = n_1 - 1$ as $\Gamma_{n_1-1} \approx \Gamma_0 \approx (32\kappa J/\pi) \exp(-1/\kappa)$. Having in mind Eq. (17) we thus obtain

$$\nu U_{c\infty} \approx \Gamma_0/\kappa^2 \zeta \approx \nu U_{c0}/2\kappa \gg \nu U_{c0}, \quad (24)$$

where U_{c0} is the zero temperature critical coupling at $\zeta \gg n_1 \approx \kappa^{-1}$. Therefore, under this condition we always expect the anomalous "freezing with heating" behavior at high enough temperatures.

Our analytical results are confirmed by numerics using the single-particle spectrum obtained by exact diagonalization. The results for $\kappa \approx 1/8$ and $\zeta = 40$ are shown in Fig. 1. The critical coupling turns out to be very small since it is proportional to the width Γ_0 , which is several orders of magnitude smaller than J . This justifies the validity of our perturbative approach with respect to the interparticle interaction.

In the opposite limit $1 \ll \zeta \lesssim \kappa^{-1}$, the situation changes. Indeed in this case single-particle states participating in MBLDT belong to different FOBs (not more than one state from a given cluster). The characteristic spacing between these states is $\sim 8J/\zeta$ and the cluster structure of the spectrum is not important. The resulting critical coupling νU_c is $\sim J$. For $\kappa \ll 1$ one can use the quasiclassical approach with the density of states $\kappa/\omega(\epsilon)$ and $\omega(\epsilon)$ given by Eq. (3). The results are consistent with our calculations based on exact diagonalization for the one-particle spectrum and Eqs. (14), (15), and (16). They suggest a slow decrease of U_c with increasing temperature and are

displayed in the inset of Fig. 2(a) for ζ and κ^{-1} both close to 8. However, since our approach is based on the perturbative treatment of the interactions, its predictions at $\nu U_c \gtrsim J$ at least require a large filling factor ν . A detailed analysis of this question will be given elsewhere.

For $\kappa \sim 1$ the quasiclassical approach is no longer valid and one has to rely only on the numerics based on exact diagonalization for the one-particle problem and Eqs. (14), (15), and (16). The results for $\kappa = 1/(1 + 1/(1 + \dots)) = (\sqrt{5} - 1)/2$ (golden ratio) and for κ close to 0.24 at $\zeta \approx 7$ are shown in Fig. 2. For the latter case our results at $T = 0$ and $\nu = 1$ are consistent with the DMRG calculations of Refs. [16] and [17] (using $\kappa = 0.77$ which is equivalent to $\kappa = 0.23$) extrapolated to $V = 2.3J$.

Reference [19] presented results of the numerical simulation for spinless fermions with nearest neighbor interaction subject to a quasiperiodic potential at $T = \infty$. This problem (different from bosons with the onsite interaction), can also be attacked with our approach at any temperature. The results will be published elsewhere, but already now we can say that at $T \rightarrow \infty$, they agree fairly well with Ref. [19].

Our results at finite temperatures indicate an anomalous $U_c(T)$ dependence. The experiment [11] has been performed for $\kappa \approx 1.24$, which according to Eq. (1) is equivalent to $\kappa = 0.24$. The extrapolation of experimental results to $V \approx 2.3J$ gives $\nu U_c/J \sim 0.3$, which is consistent with our calculations.

In conclusion, we have developed the many-body localization theory of weakly interacting bosons in a 1D quasiperiodic potential and obtained the phase diagram in terms of temperature and interaction. The most unexpected prediction based on our calculations is the transition from fluid to insulator (glass) with heating.

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- [27] Hereinafter considering the limit $\kappa \ll 1$, we put everywhere $n_j = \kappa^{-1}$.
- [28] The matrix element $\langle \gamma, \delta | H_{int} | \alpha, \beta \rangle$ by itself is proportional to $\sqrt{N_\alpha}$. However, the related probability (proportional to N_α) determines the time derivative of N_α , so that N_α drops from the expression for the probability of hybridization of a given state of the N_α manifold. This is equivalent to considering a single particle state $|\alpha\rangle$ with $N_\alpha = 1$.
- [29] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevLett.113.045304> for details on the approximate exponential energy dependence of the FOB widths, evaluation of the overlap sums, and calculation of the critical interaction temperature dependence.
- [30] In fact, the level spacing δ_β is minimal in the center of the FOB and somewhat increases closer to the band edges. This slightly increases the critical coupling compared to the result of Eq. (17). However, the quantity $\nu U_c \kappa \zeta / 2\Gamma_0$ remains equal to unity within a factor of 2 up to $\kappa \approx 0.25$, where the cluster structure of the spectrum is still pronounced but the quasiclassical approach is strictly speaking not valid. A decrease in the level spacing with increasing energy in the low-energy part of the FOB can also influence the temperature dependence of U_c at $T < \omega$. Indeed, as shown in Fig. 1, the curve $U_c(T)$ has a dip at very low temperatures. If $T < \omega$ and the occupation of the lowest energy FOB is large, the critical coupling U_c first decreases with increasing temperature (this is analogous to the behavior of $U_c(T)$ displayed in the inset of Fig. 2, where not more than one state of a given FOB participates in MBLDT). Once the temperature exceeds the spacing between the FOBs the exponential dependence of the FOB widths dominates and the temperature dependence of U_c becomes anomalous.