Delocalization of Weakly Interacting Bosons in a 1D Quasiperiodic Potential

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DOI
10.1103/PhysRevLett.113.045304
Publication date
2014
Document Version
Other version
Published in
Physical Review Letters

Supplementary Material for: Delocalization of Weakly Interacting Bosons in a 1D Quasiperiodic Potential

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Here we present details of the derivations of some of our results: the exponential energy dependence of the first-order band (FOB) widths, the evaluation of the overlap sums in the interaction matrix elements, and the calculation of the critical interaction for the finite-temperature fluid-insulator transition.

First-order band widths. The s-th FOB represents the s-th level ($s = 0, \dots, n_1 - 1$) in a single potential well of the size n_1. The transmission (tunneling) coefficient to the neighbouring well reads [1]:

$$J_s = \frac{\omega}{2\pi} \exp\Big(- \int_{-x_*}^{x_*} dx|p| \Big), \tag{S1}$$

where ω is the spacing between FOBs (frequency of the classical periodic motion), and for $\varepsilon_s < -V + 2J$ one has:

$$x_* = \arccos[(\varepsilon_s + 2J)/V]/2\pi\kappa, \tag{S2}$$

$$|p| = \operatorname{arccosh}[(V\cos(2\pi\kappa x) - \varepsilon_s)/2J]. \tag{S3}$$

In the limit of $V - 2J \ll V$, the FOB width is equal to $8J_s$ [1] and we arrive at Eqs. (4) and (5) of the main text. In Fig. S1 we compare the predictions of Eq.(5) with the FOB width following from the spectrum obtained by exact diagonalization.

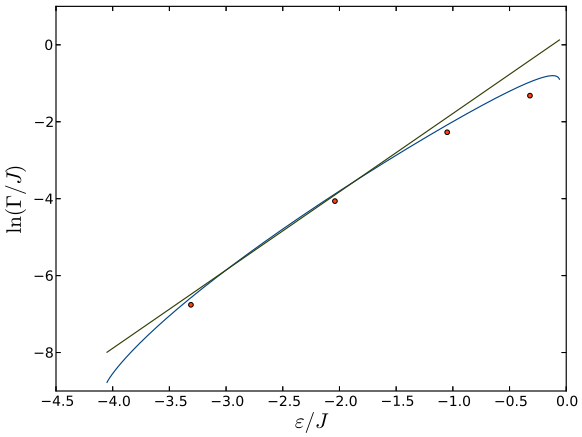

FIG. S1. The FOB width Γ_s as a function of energy ε_s at which the FOB is centered. The parameters are $V/J = 2.05$, $\kappa = 43/350$ ($n_1 = 8$, $n_2 = 7$), and $L = 350$. The blue curve corresponds to Eq.(4), the green line follows from Eq.(5), and the orange circles are the results of exact diagonalization.

Interaction matrix elements. For the one-particle AAH states α and γ (as well as β and δ) which are neighbors in energy the interaction matrix element $M^{\gamma\delta}_{\alpha\beta}$ can be expressed through the overlap sum $I^{\gamma\delta}_{\alpha\beta}$:

$$M^{\gamma\delta}_{\alpha\beta} \approx U N_\beta I^{\gamma\delta}_{\alpha\beta}, \tag{S4}$$

$$I^{\gamma\delta}_{\alpha\beta} = \sum_j \psi^\alpha_j \psi^\beta_j \psi^\gamma_j \psi^\delta_j, \tag{S5}$$

where ψ^α_j are real normalized localized eigenfunctions of the one-body Hamiltonian. Approximating the wavefunction ψ^α_j centered at j_α as

$$\begin{aligned} &\psi^\alpha_j \approx \zeta^{-1/2}; \quad |j - j_\alpha| < \zeta/2, \\ &\psi^\alpha_j \approx 0; \qquad |j - j_\alpha| > \zeta/2, \end{aligned} \tag{S6}$$

one finds that $I^{\gamma\delta}_{\alpha\beta} \neq 0$ only provided that

$$|j_\alpha - j_\gamma| < \zeta; \quad |j_\beta - j_\delta| < \zeta; \quad |j_\alpha - j_\beta| < \zeta. \tag{S7}$$

The number of sites with a non-zero product of the four wavefunctions is of the order of ζ. Using Eq.(S7) we obtain an estimate for the overlap sum:

$$I^{\gamma\delta}_{\alpha\beta} \approx 1/\zeta, \tag{S8}$$

and combining Eqs.(S4) and (S8) we find:

$$M^{\gamma\delta}_{\alpha\beta} \approx U N_\beta/\zeta. \tag{S9}$$

To check the accuracy of the estimate (S8) we computed numerically the quantity

$$W_{\alpha\beta} = \zeta \max_{\gamma\delta}(I^{\gamma\delta}_{\alpha\beta}). \tag{S10}$$

Note that here we take the maxima of matrix elements over the states $\gamma, \delta \neq \alpha, \beta$ instead of choosing nearest neighbors of α, β: $\gamma, \delta = \alpha \pm 1, \beta \pm 1$. The two choices however should be equivalent. Consider the parameters $n_1 \approx 1/\kappa \gg 1$ and $4n_1 < \zeta \leq n_1 n_2$. As the FOB width depends exponentially on energy (or on the FOB index s), only the states of the lowest energy FOB ($s = 0$) are relevant for the MBLDT. Table I presents the results of

the statistical analysis of $W_{\alpha\beta}$ for the overlapping states in the lowest FOB.

The statistics is performed as follows: For $\kappa \ll 1$ there are $\sim \kappa L$ states α belonging to the lowest FOB. If κ is not too small, $\kappa > 1/\zeta$, then for a given α there are $\sim \kappa\zeta$ lowest FOB states β that overlap with the state α. One thus obtains a set of $\sim \kappa^2\zeta L/2$ values of $W_{\alpha\beta}$ with $\alpha < \beta < \kappa L$. In agreement with (S8) we find that $\overline{W}$, the average value of $W_{\alpha\beta}$, is close to unity and depends only weakly on κ (see numerical values in Table I).

κ	$\overline{W}$	$\sqrt{\overline{(W-\overline{W})^2}}/\overline{W}$
$26/265 \approx 0.10$	1.27	0.27
$43/350 \approx 0.12$	1.27	0.21
$57/350 \approx 0.16$	1.09	0.23
$49/200 \approx 0.25$	1.12	0.26

TABLE I. Average value $\overline{W}$ and standard deviation $\sqrt{\overline{(W-\overline{W})^2}}/\overline{W}$ of $W_{\alpha\beta}$ (S10) computed numerically for $V/J = 2.05$ and various values of κ (the system size is taken as the denominator of the fractional expression for κ).

Temperature dependence of the critical interaction. The critical interaction strength U_c required for the insulator-fluid transition depends on temperature through the occupation numbers of single particle states. In order to evaluate these occupation numbers we first write an expression for the energy corresponding to the occupation number configuration $\{n_\alpha\}$ ($\alpha = 1, \ldots, L$, and n_α is a non-negative integer):

$$E(\{n_\alpha\}) = \sum_\alpha [\varepsilon_\alpha n_\alpha + U n_\alpha(n_\alpha - 1)/2\zeta]. \quad \text{(S11)}$$

The grand canonical partition function is

$$Z = \sum_{\{n_\alpha\}} \exp(-[E(\{n_\alpha\}) - \mu \sum_\alpha n_\alpha]/T). \quad \text{(S12)}$$

It factorizes as $Z = \prod_\alpha Z_\alpha$ with

$$Z_\alpha = \sum_{n=0}^{\infty} \exp\{-[(\varepsilon_\alpha - \mu)n + Un(n-1)/2\zeta]/T\}. \quad \text{(S13)}$$

If the average occupation number N_α is large we can linearize the exponent in (S13) around N_α:

$$(\varepsilon_\alpha - \mu)n + \frac{U}{2\zeta} n(n-1) \approx \Big(\varepsilon_\alpha - \mu + \frac{UN_\alpha}{\zeta}\Big)n + \text{const}, \quad \text{(S14)}$$

and the partition function becomes (up to an irrelevant constant factor):

$$Z_\alpha \approx 1/\{1 - \exp[-(\varepsilon_\alpha - \mu + UN_\alpha/\zeta)/T]\}. \quad \text{(S15)}$$

The total number of particles is $\nu L = \sum_\alpha N_\alpha$, where L is the number of sites in the system, and

$$N_\alpha = T\frac{\partial \ln Z_\alpha}{\partial \mu} \approx \Big[e^{(\varepsilon_\alpha - \mu + UN_\alpha/\zeta)/T} - 1\Big]^{-1}. \quad \text{(S16)}$$

Since $N_\alpha \gg 1$, one can further expand the exponent in Eq.(S16) and obtain a quadratic equation for N_α. The physically meaningful solution is

$$N_\alpha = \frac{\zeta}{2U}\Big\{\mu - \varepsilon_\alpha + \sqrt{(\mu - \varepsilon_\alpha)^2 + 4TU/\zeta}\Big\}. \quad \text{(S17)}$$

In the limit of $T \to 0$ equation (S17) leads to

$$N_\alpha = \begin{cases} \zeta(\mu - \varepsilon_\alpha)/U & \varepsilon_\alpha < \mu, \\ 0 & \varepsilon_\alpha > \mu. \end{cases} \quad \text{(S18)}$$

For small N_α one can neglect the interaction term in the exponent of Z_α (S13). Then for $N_\alpha \ll 1$ we obtain the Boltzmann distribution $N_\alpha \approx \exp[-(\varepsilon_\alpha - \mu)/T]$.

If $T \gg \omega$ then $(\varepsilon_0 - \mu) \gg \sqrt{TU_c/\zeta}$ which leads to

$$N_\alpha \approx \begin{cases} T/(\varepsilon_\alpha - \mu) & \varepsilon_\alpha - \mu < T, \\ 0 & \varepsilon_\alpha - \mu > T. \end{cases} \quad \text{(S19)}$$

Using Eq.(S19) one can write the number equation as

$$\nu L \approx \sum_\alpha T/(\varepsilon_\alpha - \mu), \quad \text{(S20)}$$

where the summation is over the states with energies $\varepsilon_\alpha < \min(4J, \mu + T)$. As the bandwidths are exponentially small the occupation numbers of the levels within a given FOB can be considered as energy independent. The energy dependence of ω is weak, and it can be approximated as $\omega \approx 8\kappa J$. Performing the summation over $\approx \kappa L$ levels in each FOB of energy $\varepsilon_s \approx \varepsilon_0 + s\omega$ we obtain for $\mu + T < 4J$:

$$\begin{aligned} \nu &\approx \sum_{s=0}^{(T+\mu-\varepsilon_0)/\omega} \kappa T/(s\omega + \varepsilon_0 - \mu) \\ &= \frac{\kappa T}{\omega}\Big[\psi\Big(1 + \frac{T}{\omega}\Big) - \psi\Big(\frac{\varepsilon_0 - \mu}{\omega}\Big)\Big], \end{aligned} \quad \text{(S21)}$$

where

$$\psi(x) = -\gamma + \sum_{n=0}^{\infty}[1/(n+1) - 1/(n+x)] \quad \text{(S22)}$$

is the digamma function [2], and $\gamma \approx 0.577$ is the Euler constant. Asymptotic expressions for $\psi(x)$ are known to be [2]

$$\psi(x) \approx \begin{cases} -1/x & 0 < x \ll 1, \\ \ln(x) & x \gg 1. \end{cases} \quad \text{(S23)}$$

If κ is not too small, then $(\varepsilon_0 - \mu) \ll \omega$. Assuming that $\omega \ll T \ll 8J, 8\nu J$ and using equations (S19) and

(S21) we recover the chemical potential of Eq.(22) of the main text. The particle occupation of the lowest energy FOB ($s = 0$), according to Eqs. (S15) and (S17), is

$$N_0 \approx \nu/\kappa - (T/\omega)\ln(T/\omega). \tag{S24}$$

A direct substitution of Eq.(S24) into Eq.(19) of the main text yields Eq.(23) for the critical coupling $U_c(T)$.

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