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Localization by entanglement

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Abstract – We study the localization of bosonic atoms in an optical lattice, which interact in a spatially confined region. The classical theory predicts that there is no localization below a threshold value for the strength of interaction that is inversely proportional to the number of participating atoms. In a full quantum treatment, however, we find that localized states exist for arbitrarily weak attractive or repulsive interactions for any number (> 1) of atoms. We further show, using an explicit solution of the two-particle bound state and an appropriate measure of entanglement, that the entanglement tends to a finite value in the limit of weak interactions. Coupled with the non-existence of localization in an optimized quantum product state, we conclude that the localization exists by virtue of entanglement.

Spatial localization of quantum interacting particles and formation of bound states are of fundamental interest to modern physics. One intriguing aspect is the correspondence between localized states in classical and quantum-mechanical theories [1]. Usually, one expects quantum fluctuations to weaken localization, as the binding of particles with an attractive but shallow pair potential can be inhibited by quantum-mechanical zero-point motion. Then, localization can be interpreted essentially as a classical property that would emerge in a quantum system due to decoherence [2]. On the other hand, it was recently suggested that localization of quantum particles may be achieved when they are entangled through suitable measurements [3]. Here, we consider the role of entanglement in the localization of specific eigenstates of a multiple-boson system, *e.g.* the ground state. Specifically, we show that spatially confined interaction between atoms in an optical lattice induces entanglement and leads to localization, while the corresponding classical atomic field fails to localize. Remarkably, the effect that we demonstrate in this letter does not depend on whether the interaction is attractive or repulsive. Recent experiments on the formation of repulsive atomic pairs on optical lattices [4] imply the possibility of experimental observation of the effect reported here.

If a translationally invariant lattice with interactions is considered, its classical limit allows for localized solutions known as lattice solitons or discrete breathers [5]. A particular realization of such a system is a Bose-Einstein condensate (BEC) in an optical lattice [6]. Due to the band structure with Bragg reflection gaps in the optical lattice, localized soliton solutions are possible not only with attractive but also with repulsive interactions. Experimental evidence for the band gap solitons with repulsive BECs has been reported for one-dimensional lattices [7]. For two- and three-dimensional lattices the classical theory predicts non-zero energy and particle number thresholds for the existence of band gap solitons [8], as opposed to the case of dimension one. Quantum effects in this system are expected to be most dramatic for a small number of particles [9,10]. The extreme quantum limit of a three-dimensional lattice has been realized in the experiment of Winkler *et al.* [4], where bound pairs of repulsively interacting atoms have been reported using spectroscopic tools. According to quantum theory, these quantum solitons describe bound states of atoms that delocalize spatially [11–13]. It is an open question, whether these observed bound states persist below the above-mentioned classical threshold.

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In this letter we study localization of atoms in an optical lattice, where interactions between atoms are present in a spatially confined region only. This can be achieved experimentally by tuning the s-wave scattering length by the Feshbach resonance with inhomogeneous magnetic [14,15] or laser fields [16,17]. We show that localization occurs in the full quantum system when it is forbidden classically. The crucial difference between the quantum and the classical models is the presence or absence of entanglement (see [18–20]) between the constituent particles. The predicted quantum localization is due to entanglement. For the case of two particles we quantify the entanglement and show that it reaches a finite value in the limit of weak interactions. Beyond the specific model studied we also comment on the relation between entanglement in eigenstates, localization, and the existence of bound states for higher-dimensional and translationally invariant systems. It is worth mentioning here that bound states for two electrons (fermions) in the negative hydrogen ion also appear only in the presence of quantum correlations beyond the Hartree-Fock approximation [21].

The model. – We initially consider the dynamics of atoms in a one-dimensional optical lattice in which the atoms interact in a spatially confined region. The Hamiltonian is given by

$$H = -\sum_n (a_n^\dagger a_{n+1} + a_{n+1}^\dagger a_n) + \lambda a_0^\dagger a_0^\dagger a_0 a_0, \qquad (1)$$

where $a_n^\dagger$ (a_n) creates (destroys) a boson on the lattice site n and bosonic commutation relations $[a_n, a_m^\dagger] = \delta_{nm}$ hold. The Hamiltonian (1) describes bosonic atoms on a lattice that interact either repulsively ($\lambda > 0$) or attractively ($\lambda < 0$) only on the single lattice site $n = 0$. Single atoms with the Hamiltonian (1) on a lattice with M sites and periodic boundary conditions do not localize and the eigenstates are plane waves $1/\sqrt{M}\sum_n \exp(ikn)\, a_n^\dagger|\mathrm{vac}\rangle$, where $|\mathrm{vac}\rangle$ is the vacuum state (no particles). However, with more than one particle localized states may exist around the site $n = 0$. In this current model the binding of particles implies spatial localization and vice versa.

Classical treatment. – The quantum Hamiltonian (1) can also be understood as posing a *classical* Hamiltonian lattice problem if we replace the particle creation and destruction operators by complex valued functions of time. In order to enable a detailed comparison between classical and quantum predictions it is necessary to establish the precise relation between both pictures. An unambiguous route to relate the classical with the quantum problem can be found by the Hartree ansatz and variational procedure: For the many-body wave function with N particles we use the ansatz of a product state $|\Psi_{\mathrm{H}}^{(N)}\rangle = 1/\sqrt{N!}\,(b^\dagger)^N|\mathrm{vac}\rangle$, where $b^\dagger = 1/\sqrt{N}\sum_n \psi_n^* a_n^\dagger$ creates a single particle with the complex amplitude ψ_n on the lattice site n. The corresponding equation emerges from the standard Lagrangian variational procedure with $g = 2\lambda(N-1)/N$ assuming normalized solutions with $\sum_n |\psi_n|^2 = N$. This equation is the discrete non-linear Schrödinger (DNLS) model with non-linearity present only on the site $n = 0$,

$$i\frac{\partial}{\partial t}\psi_n = -(\psi_{n+1} + \psi_{n-1}) + g\delta_{0,n}|\psi_0|^2\psi_n. \qquad (2)$$

This model was originally introduced to study the transport of electrons coupled to lattice phonons [22]. The model also applies to BECs in an optical lattice and has been discussed in connection with Fano resonances in the transport of cold atoms [23]. Here, ψ_n describes the complex matter wave field at the lattice site n after the introduction of appropriately rescaled dimensionless variables. $N = \sum_n |\psi_n|^2$ is the number of atoms in the BEC.

We have now used the Hartree procedure to *derive* the set of classical equations (2) from the quantum problem (1). The same set of equations (2) would have also emerged from a more standard approach using a coherent-state ansatz for the many-body wave function. However, the Hartree procedure here serves a dual purpose in also characterizing the classical equations (2) as an *approximation* to the quantum problem that provides strict variational bounds for the latter.

The model of eq. (2) supports plane-wave solutions in the linear ($g = 0$) case,

$$\psi_n^{(\mathrm{pw})} = \psi_0 \exp(ikn)\exp(-i\omega t) \qquad (3)$$

with the dispersion relation $\omega = -2\cos k$ defining a band continuum $[-2, 2]$. In addition, for non-zero g, there are localized solutions

$$\psi_n^{(\mathrm{loc})} = Ae^{-\delta|n|}e^{-i\Omega t}e^{i\theta n}, \qquad (4)$$

with $\Omega = -Ng$, where the frequency $|\Omega| = 2\cosh\delta > 2$ lies outside the linear band. Furthermore, $\theta = 0$ for the attractive interactions $g < 0$, where the localized solution is the ground state, whereas $\theta = \pi$ for the repulsive interactions $g > 0$ introduces a staggered phase profile and $\psi_n^{(\mathrm{loc})}$ corresponds to the highest excited state. From the expression $A^2 = \sqrt{N^2 - 4/g^2}$ for the amplitude, we find that the system exhibits a threshold for the existence of localized states [22], which are only found for $N > 2/|g|$. Since g may be tuned to any small value, the threshold for the number of particles can be made arbitrarily large. Conversely, for a given number of particles, there is a threshold value of g for localization to occur. Figure 1 shows the dependence of the energy $E_{\mathrm{class}}^{(N)} = \sum_n -(\psi_{n-1}^{(\mathrm{loc})}\psi_n^{(\mathrm{loc})*} + \mathrm{c.c.}) + \frac{g}{2}|\psi_0^{(\mathrm{loc})}|^4 = \frac{2}{g} + \frac{N^2 g}{2}$ on the coupling constant in the case of $N = 2$ particles. In particular, no bound state is found classically in this system if $|g| < 1$.

Quantum case of two particles. – We study the two-particle sector, where we expect to find the most obvious deviations from the classical theory. In order to solve for the eigenstates $|\Psi^{(2)}\rangle$ of the Hamiltonian (1) for two-particles, we introduce the projected amplitudes

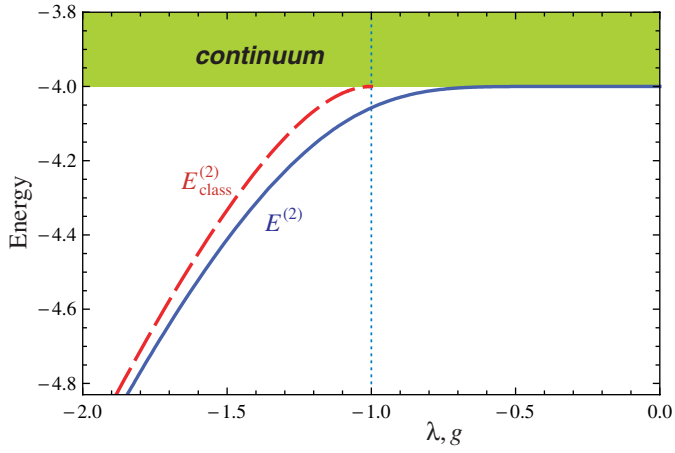

Fig. 1: Relation between energy and coupling constant for two-particle defect states. The dashed line shows the classical (Hartree) solution $E^{(2)}_{\rm class} = 2(g + \frac{1}{g})$. The shaded region at $E > -4$ indicates the edge of the continuum band of linear waves. At the classical threshold of $g = 1$ (the dotted line) the classical solution reached the continuum edge. The solid line shows the exact solution $E^{(2)}$ of the two-particle problem of eq. (8), which persists even below the classical threshold down to zero coupling.

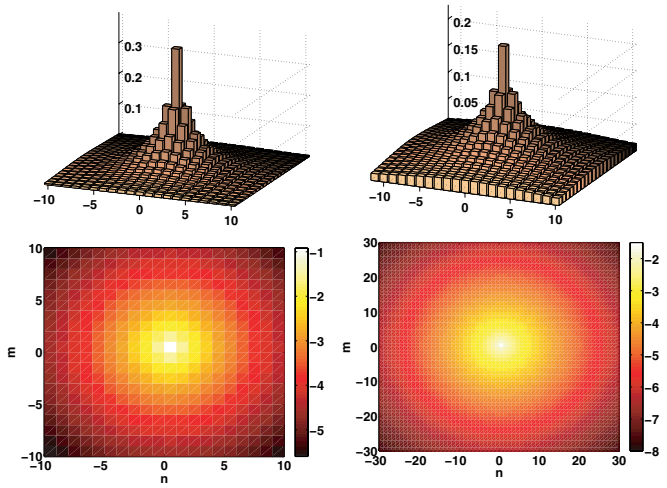

Fig. 2: Two-particle wave function (top panels: $|\varphi_{nm}|$, bottom panels: $\ln(|\varphi_{nm}|)$) for the localized state. Left panels: strong localization $\lambda = -0.978$ and $E = -4.05$. Right panels: weak localization $\lambda = -0.779$ and $E = -4.01$. The s-wave symmetry visible in the far field is a signature of entanglement, as a product wave function $\phi_n \phi_m$ would only allow fourfold symmetry. Because of the (near) cylindrical symmetry of the true wave function, the kinetic energy cost of bringing additional amplitude to the site (0, 0) is significantly reduced compared to that of the product wave function.

or two-particle wave functions $\varphi_{n,m} = \langle \mathrm{vac} | a_n a_m | \Psi^{(2)} \rangle$, which obey the equation

$$E\varphi_{n,m} = -(\varphi_{n,m+1} + \varphi_{n,m-1} + \varphi_{n+1,m} + \varphi_{n-1,m}) + 2\lambda\delta_{n,0}\delta_{m,0}\varphi_{0,0}. \quad (5)$$

This can be interpreted as the Schrödinger equation of a single particle on a two-dimensional lattice with a point defect at the lattice site (0,0). The problem is known to have a localized solution for any non-zero value of λ [24]. Introducing the Fourier transform

$$\chi_{\mathbf{k}} = \frac{1}{M} \sum_{m,n} e^{-i\frac{2\pi}{M}(k_1 n + k_2 m)} \varphi_{n,m}, \quad (6)$$

for a square lattice of $M \times M$ sites with $\mathbf{k} = (k_1, k_2)$ being the quasimomentum vector, eq. (5) becomes

$$\chi_{\mathbf{k}} = \frac{1}{E - \mathcal{E}_{\mathbf{k}}} \frac{2\lambda}{M} \sum_{\mathbf{k}'} \chi_{\mathbf{k}'}. \quad (7)$$

Looking for localized solutions with $|E| > 4$ lying outside the band of plane-wave energies $\mathcal{E}_{\mathbf{k}} = -2(\cos\frac{2\pi}{M}k_1 + \cos\frac{2\pi}{M}k_2)$, we find in the limit $M \to \infty$

$$\lambda = \frac{1}{2F(E)}, \qquad F(E) = \frac{2}{\pi E} K(16/E^2) \quad (8)$$

for the relation of the coupling parameter and the bound-state energy E (see fig. 1). Here, K is the complete elliptic integral of the first kind. It is important to emphasize that for $4 > |E| > 4.05753$ one has $|\lambda|, |g| < 1$ and thus no classical localized states persist. However, in the quantum case the asymptotic relation,

$$E(|\lambda| \to \infty) \to 2\lambda, \qquad |E(|\lambda| \to 0)| \to 4 + e^{-\frac{2\pi}{|\lambda|}}, \quad (9)$$

holds and the localized-state wave function is characterized by

$$\varphi_{n,m} = \frac{\sqrt{Z}}{M} \sum_{\mathbf{k}} \frac{1}{E - \mathcal{E}_{\mathbf{k}}} e^{i\frac{2\pi}{M}(k_1 n + k_2 m)}, \quad (10)$$

with the normalization factor $Z = -1/[M^2 F'(E)]$. The bound-state wave function $\varphi_{n,m}$ is plotted in fig. 2 for two classically forbidden cases. It is easy to see that this bound and localized state is the ground state or the highest energy state in the two-particle sector for attractive ($\lambda < 0$) or repulsive ($\lambda > 0$) interactions, respectively.

Entanglement. – A system of N particles is entangled if the multi-particle wave function $\phi_{n_1,n_2,\ldots,n_N}$ cannot be expressed as a product $\phi^1_{n_1}\phi^2_{n_2}\ldots\phi^N_{n_N}$ of single-particle wave functions. If the state of the system can be expressed by a product wave function, it is separable. The Hartree method becomes exact when no entanglement is present. Since the Hartree method is variational, it gives the *best* separable approximation in the sense that the Hartree energy will be the closest approximation to the true eigenvalue of the multi-particle Hamiltonian that can be obtained with a separable wave function.

Let us discuss the two-particle problem. If the two-particle state were separable, due to the Bose symmetry, it would be possible to write it in the form $\phi_n\phi_m$. This is inconsistent with the result that in the far field, where the underlying lattice structure becomes less important, we observe cylindrical (s-wave) symmetry as seen in fig. 2. A separable product approximation, on the contrary, is inconsistent with the s-wave symmetry and

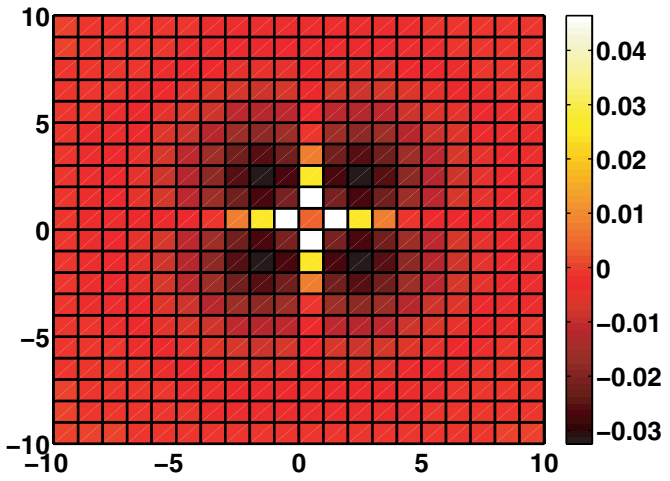

Fig. 3: Difference $\varphi_{n,m} - \psi_n^{(\mathrm{loc})}\psi_m^{(\mathrm{loc})}$ between the exact two-particle wave function and the separable (Hartree) approximation of eqs. (4) and (10), respectively, at $\lambda = -1.26$.

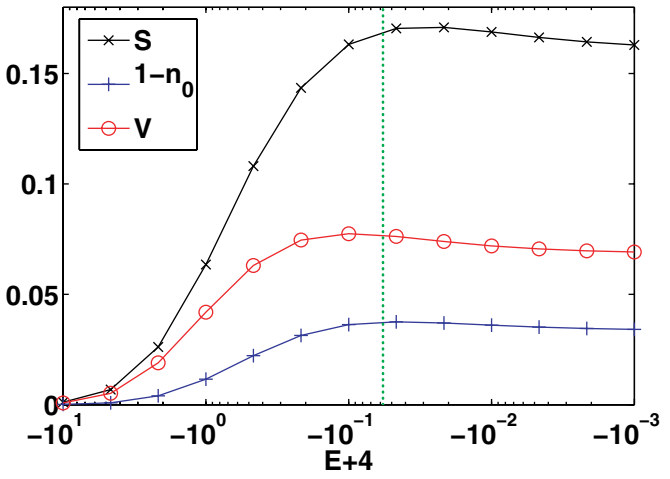

Fig. 4: Entanglement in the two-particle wave function $\varphi_{n,m}$ as a function of the energy $E^{(2)}$. Above the classical threshold $\lambda > -1$ or $E^{(2)} > -4.05753$ (shown as a dotted line) entanglement is essential for localization. Shown are the von Neumann entropy S, the condensate depletion (geometric measure) $1 - n_0$, and the entanglement measure V as defined in eq. (11).

is characterised by ridge-like structures along the $n = 0$ and $m = 0$ co-ordinate axes. These structures are clearly seen in the difference between the exact and the Hartree two-particle wave functions shown in fig. 3.

In order to quantify the entanglement of the two particles in the bound state (10) we compute various measures of entanglement, as shown in fig. 4. First we used the von Neumann entropy $S = \mathrm{Tr}(\rho \ln \rho)$ [20]. Here ρ is the single-particle density matrix (SPDM) with elements $\rho_{i,j} = F^{-1}\langle\Psi^{(2)}|a_j^\dagger a_i|\Psi^{(2)}\rangle$, normalized with $F = \sum_i \langle\Psi^{(2)}|a_i^\dagger a_i|\Psi^{(2)}\rangle$ to have $\mathrm{Tr}\rho = 1$. Another measure derived from the SPDM is the condensate depletion $1 - n_0$ (also coined geometric measure of entanglement [25]). Here, n_0 is the largest eigenvalue of ρ and measures the fraction of particles in a Bose-condensed state. Because ρ describes a pure state, $1 - n_0$ measures quantum depletion, which, as we argue here, characterizes quantum entanglement. This would not be the case in the presence of incoherent, *e.g.* thermal, excitations.

A third measure, V, that is amenable to analytic calculations is also shown in fig. 4. It uses projected orbitals defined as $g_n = G^{-1}\sum_m \varphi_{m,n}$, where $G = \sum_{m,n}\varphi_{m,n}$. Since we expect for separable states that $\varphi_{m,n}$ is equal to the product $g_n g_m$, where $g_n = \sum_m \varphi_{nm}$, the deviation

$$V = \sum_{m,n} |\varphi_{n,m} - g_n g_m|^2 \tag{11}$$

is a measure of entanglement. Calculating V from eq. (10) analytically we find

$$V \to -7 + \frac{17}{4}\pi - 8\arctan 1 \approx 0.06858 \tag{12}$$

in the limit $\lambda \to 0$, in excellent agreement with the numerical result shown in fig. 4. As this figure shows, the different entanglement measures provide a similar picture, although they are not, in general, monotonic functions of each other. In particular we note that the entanglement quickly reaches its maximum value near the classical threshold. It remains finite as the two particles become infinitely weakly bound at $\lambda \to 0$.

Three or more particles. – We now show that bound states with any number of atoms larger than two exist in the quantum model (1) for any value of the coupling constant $\lambda \neq 0$ as well. Without loss of generality we assume $\lambda < 0$. We have already found a two-body bound state. It will suffice to show that any bound p-particle ground state $|\psi\rangle$ binds another particle for any $p \geqslant 2$. For this we have to find a $(p+1)$-particle wave function $|\phi\rangle$ with $\langle\phi|H|\phi\rangle < E^{(p)} - 2$, where $E^{(p)}$ is the energy eigenvalue of $|\psi\rangle$ and the minimum energy of a free particle is -2. We use the ansatz $|\phi\rangle = \alpha\sum_n x^{-|n|}a_n^\dagger|\psi\rangle$, which is normalizable if $x > 1$. We choose $\alpha > 0$ as a normalization constant to ensure $\langle\phi|\phi\rangle = 1$. We find that $\langle\phi|H|\phi\rangle \leqslant E^{(p)} + F(x)$, where $F(x) = (1 + 2\lambda c)x^2 - 1 - x - x^{-1} + (x - x^{-1})p$ and $c = \langle\phi|a_0^\dagger a_0|\phi\rangle > 0$. Since $F(1) = -2 + 2\lambda c < -2$ it follows from continuity that there is an $x > 1$ such that $\langle\phi|H|\phi\rangle \leqslant E^{(p)} + F(x) < E^{(p)} - 2$ as required. This concludes the proof that bound states with any particle number exist in the quantum problem.

We further remark that having found an N-particle bound state that persists below the classical threshold $\lambda < \lambda_{\mathrm{thresh}} = 1/(N-1)$, we automatically know that entanglement plays an essential role in its binding. This is because the best separable wave function is in fact the Hartree approximation, which does not bind there.

Translationally invariant systems. – In interacting lattice problems with translational invariance the quantum eigenstates are delocalized due to fundamental properties of the quantum theory. However, the existence of lattice solitons in the corresponding classical theory indicates the existence of quantum states with

local second-order correlation known as quantum lattice solitons, which can be interpreted as bound states of quantum particles [9,11,12]. Both lattice solitons and quantum lattice solitons are characterised by frequencies and energies, respectively, outside of the bands of delocalized solutions in the non-interacting system. A framework for detailed comparison between the thresholds predicted by classical and quantum theory is, again, enabled by establishing the classical theory as a Hartree approximation to the quantum problem. In the classical theory, there is no threshold in a one-dimensional lattice with a cubic non-linearity (corresponding to two-particle interactions) but there are thresholds for higher dimensions [8]. The variational properties of the Hartree approximation guarantee that the existence of lattice solitons in the classical theory implies the existence of quantum lattice solitons but not vice versa. If quantum solitons exist below a classical threshold in these systems we thus know that entanglement between quantum particles plays a vital role. However, we also expect entanglement to be relevant for delocalised quantum soliton states above the thresholds (*i.e.* for stronger interactions). It is known that thresholds for quantum solitons exist in dimensions higher than one [26].

Extending the current model with spatially localized interactions into more than one dimensions, there will generally be thresholds for localization in both the quantum and the classical models [27]. However, these thresholds will generally differ. The detailed study of such systems lies beyond the scope of this letter and presents an interesting opportunity for future work.

Conclusion. – We have shown that localized states of a few atoms in an optical lattice with spatially confined s-wave interaction persist below the classical threshold. Moreover, wave function entanglement plays a crucial role in that localization. A one-dimensional optical lattice with spatially inhomogeneous interactions can be engineered with presently available techniques using magnetic or optically induced Feshbach resonances [6]. Increasing the size of the spatial interaction domain will decrease the classical threshold, but it will stay finite. Thus, quantum localization by entanglement is robust and will disappear only in the limit of an infinite interaction domain, where the classical model is known to have zero thresholds for localized states [8]. In an experiment where interactions are tuned below the classical threshold the observation of localized modes will indicate the vital role of entanglement. This entanglement between atoms is distillable [20] and could possibly be measured with entanglement witnesses or by reconstruction of the single-particle density matrix from position and momentum-space measurements. Beyond the currently studied model we expect that quantum entanglement favors localization in other quantum lattice or quantum field theories as well.

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