Many-particle localization by constructed disorder: enabling quantum computing with perpetually coupled qubits

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We demonstrate that, in a many-particle system, particles can be strongly confined to their sites. The localization is obtained by constructing a sequence of on-site energies that efficiently suppresses resonant hopping. The time during which a many-particle state remains strongly localized in an infinite chain can exceed the reciprocal hopping frequency by $\gtrsim 10^5$ already for a moderate energy bandwidth. The results show viability of quantum computers with time-independent qubit coupling.

Disorder-induced localization has been one of the central problems of condensed-matter physics\textsuperscript{[1]}. The problem is particularly challenging for many-body systems, where only a limited number of results has been obtained\textsuperscript{[2]}. Recently it has also attracted much interest in the context of quantum computing. In many proposed physical implementations of a quantum computer (QC) the qubit-qubit interaction is not turned off\textsuperscript{[3, 4, 5, 6, 7, 8]}. Generally, the interaction leads to hopping of excitations between the qubits. Preventing hopping is a prerequisite for quantum computation. To control a QC and measure its state excitations must remain localized between operations. Several approaches to quantum computation with interacting qubits were proposed recently\textsuperscript{[9, 10, 11, 12]}. In this paper we study strong on-site many-particle localization. It implies that each particle (or excitation) is nearly completely confined to one site. This is a stronger condition than just exponential decay of the wave function, and it is this condition that must be met in a QC.

Strong on-site localization does not arise in a disordered many-particle system with bounded random on-site energies\textsuperscript{[12]}. Indeed, consider a state where particles occupy $N$ sites. For short-range hopping it is directly coupled to $\sim N$ other $N$-particle states. With probability $\propto N$ one of them will be in resonance with the initial state, provided the on-site energies are uniformly distributed over a finite-width band. For large $N$ this leads to state hybridization over time $\sim J^{-1}$, where $J$ is the intersite hopping integral (we set $\hbar = 1$).

Here we show that many-particle localization can be obtained in an infinite chain by constructing a sequence of on-site energies. For the proposed narrow-band sequence, all many-particle states remain confined for a time that largely exceeds $J^{-1}$. We find that stationary many-particle states in moderately long chains are also strongly localized.

A QC allows both studying and using strong localization. Here, on-site excitation energies are interlevel distances of the qubits. They can often be individually controlled, which makes it possible to construct an arbitrary energy sequence. However, since the qubit tuning range is limited, so should be the energy bandwidth. A smaller bandwidth is also desirable for a higher speed of quantum gate operations.

To localize one particle, the difference between excitation energies on neighboring sites should be much larger than $J$. In addition, even for nearest neighbor coupling, the energies of remote sites should also differ to prevent virtual transitions via intermediate sites. However, the further away the sites are, the smaller their energy difference can be. We use this to obtain strong on-site single-particle confinement for a bounded energy bandwidth.

For many-particle localization one has to suppress not only single-particle, but also combined resonances, where several interacting excitations make a transition simultaneously. There is no known way to eliminate all such resonances. However, the problem can be approached from a different point of view by looking at a lifetime of a localized state. The effective many-particle hopping integral quickly falls off with the increasing number of involved excitations and intermediate nonresonant sites, which gives the effective “order” of a transition. To obtain a desired lifetime it is sufficient to eliminate resonances up to a certain order. As we show, this can be done for an infinite system.

We will consider a one-dimensional chain of $S = 1/2$ spins in a magnetic field. This model also describes an array of qubits. The excitation energy of a qubit is the Zeeman energy of a spin. The qubit-qubit interaction is the exchange spin coupling. For many proposed realizations of QC’s\textsuperscript{[3, 4, 5, 6, 7, 8]} it has a form $\frac{1}{2} \sum_{nm} J_{nm} S_n^\mu S_m^\mu$, where $n, m$ are spin sites, $\mu = x, y, z$ are spin projections, and $J_{nm} = J_{nm}^{\mu \mu}$ for the effective magnetic field in the $z$-direction. The 1D spin system can be mapped, via Jordan-Wigner transformation, onto a system of fermions. For nearest neighbor coupling, the
fermion Hamiltonian is
\[ H = \sum_n \varepsilon_n a_n^\dagger a_n + \frac{1}{2} J \sum_n (a_n^\dagger a_{n+1} + a_{n+1}^\dagger a_n) + J\Delta \sum_n a_n^\dagger a_n^\dagger a_{n+1} a_{n+1}. \] (1)

Here, \( a_n^\dagger, a_n \) are the fermion creation and annihilation operators. Presence of a fermion on site \( n \) corresponds to the \( n \)th spin (qubit) being in the excited state. The on-site energies \( \varepsilon_n \) in Eq. (1) are the Zeeman energies counted off from the characteristic central energy, \( J \equiv J_{n+n+1}^z \) is the hopping integral, and \( J\Delta \equiv J_{n+n+1}^\text{eff} \) is the fermion interaction energy; we set \( J, \Delta > 0 \).

Localization of stationary states can be conveniently characterized by the inverse participation ratio (IPR), which shows over how many sites the wave function spreads. For an \( N \)-particle eigenstate \( |\psi_{N\lambda}\rangle \) (\( \lambda \) enumerates the eigenstates) it is given by
\[ I_{N\lambda} = \left( \sum_{n_1 < \ldots < n_N} |\langle \Phi_{n_1^{\ldots n_N}} | \psi_{N\lambda} \rangle|^4 \right)^{-1}, \] (2)
where \( |\Phi_{n_1^{\ldots n_N}}\rangle = a_{n_1}^\dagger \ldots a_{n_N}^\dagger |0\rangle \) is an on-site \( N \)-particle wave function (quantum register).

For fully localized stationary states \( I_{N\lambda} = 1 \). For delocalized states \( I_{N\lambda} \gg 1 \) [for an \( L \)-site chain \( I_{N\lambda} \approx L^2! / N! (L-N)! \)]. Strong localization corresponds to \( I_{N\lambda} \) being close to 1 for all states.

Localization requires that the on-site energies \( \varepsilon_n \) be tuned away from each other. For nearest neighbor coupling a natural first step is to separate \( \varepsilon_n \)'s into two subbands, for even and odd \( n \), with the inter-subband distance \( h \) that significantly exceeds \( J \). Then we further split each subband into two subbands to detune next nearest neighbors. Here the splitting can be smaller, because next-nearest-neighbor hopping occurs via a nonresonant site, and the effective hopping integral is \( \sim J^2/h \).

The procedure of band splitting is continued, with higher-order splitting being smaller and smaller.

A simple sequence of \( \varepsilon_n \) that implements the above idea has the form
\[ \varepsilon_n = \frac{1}{2} h \left[ (-1)^n - \sum_{k=2}^{n+1} (-1)^{\lfloor n/k \rfloor} \alpha^{k-1} \right], \quad n \geq 1 \] (3)
(\( \lfloor \cdot \rfloor \) is the integer part). The energies (3) are illustrated in Fig. 1(a). Besides the scaling factor \( h \), they are characterized by one dimensionless parameter \( \alpha < 1 \). For small \( \alpha \), the two major subbands have width \( \approx \alpha h \) and are separated by a gap of width \( \approx h \). The splitting of higher-order subbands is proportional to higher powers of \( \alpha \). For \( \alpha \gtrsim 0.4 \) all subbands overlap and the subband structure disappears.

One can see from Eq. (3) and Fig. 1(a) that sites with close energies are indeed spatially separated. Analytical estimates of the energy difference can be obtained for small \( \alpha \). We have \( |\varepsilon_{n+m} - \varepsilon_n| \sim h \) for odd \( m \) and \( \sim \alpha h \) for odd \( m/2 \). In general, the larger is \( m \) the higher may be the order in \( \alpha \) of the leading term in \( |\varepsilon_{n+m} - \varepsilon_n| \).

It is important for localization that the sequence (3) has no simple symmetry. It is neither self-similar nor quasi-periodic (which is another example of “constructed” disorder [13]). For analytical estimates it is essential that the coefficients at any given power \( \alpha^q \) are repeated with period \( 2(q+1) \) [14].

A convenient characteristic of the on-site energy sequence is the amplitude of a particle transition from site \( n \) to site \( n + m \). To the lowest order in \( J \) it has the form
\[ K_n(m) = \prod_{k=1}^{m} J/\left[ 2(\varepsilon_n - \varepsilon_{n+k}) \right]. \] (4)
It can be shown using some results from number theory that \( K_n(m) \) decays with \( m \) nearly exponentially [14]. For small \( \alpha \) and large \( |m| \) we have
\[ K_n(m) \propto \alpha^{-|m|} \left( J/2h \right)^{|m|}. \] (5)
The decrement \( \nu \) depends on \( n, m \). However, it is limited to a narrow region around \( \nu = 1 \) with \( 0.89 < \nu < 1.19 \), cf. Fig. 1(b). For estimates one can use \( \nu = 1 \), i.e., set \( K_n(m) = K^m \). The inset shows the maximal IPR, \( I_{1\text{max}} = \max_{\lambda} I_{1\lambda} \), demonstrating strong localization.

Equation (6) describes the tail of the transition amplitude for \( J/2h\alpha \ll 1 \). Strong single-particle localization occurs for \( \alpha \gg \alpha_{th} \), where the threshold value of \( \alpha \) is \( \alpha_{th} \approx J/2h \). The condition \( \alpha_{th} \ll \alpha < 0.4 \) can be satisfied for a moderately large ratio of the energy bandwidth \( h \) to the hopping integral \( J \).
Strong single-particle localization for $\hbar/J = 20$, as evidenced by $I_{1\alpha}$ being very close to 1, is seen from Fig. 1(c). The data are obtained by diagonalizing the Hamiltonian (1) for open chains with different numbers of sites $L$.

In the limit $\alpha \to 0$ the stationary single-particle states are sinusoidal, which gives $\langle I_1 \rangle \approx L/3$, cf. Fig. 1(c) (⟨⟩ means averaging over the eigenstates). As $\alpha$ increases, the bands are split into more and more subbands, and $\langle I_1 \rangle$ decreases. It sharply drops to $\approx 1$ in a narrow region, which can be conditionally associated with a smeared transition to strong localization. The center of the transition region gives $\alpha_{\text{th}}$. It appears to be independent of the chain length $L$. The estimate $\alpha_{\text{th}} = J/2\hbar$ is in good agreement with the numerical data for different $h/J$.

When $\alpha \gg \alpha_{\text{th}}$, all states are localized. The wave function tails are small and limited mostly to nearest neighbors. At its minimum over $\alpha$ for given $h/J$, for all states $I_{1\alpha} - 1 \approx J^2/\hbar^2$, see inset in Fig. 1(c). The agreement with the above estimate becomes better with increasing $h/J$. For $\alpha \gtrsim 0.4$, when the bands of $\varepsilon_n$ start overlapping, the IPR increases with $\alpha$.

The difference in the localization problems for many-particle and single-particle systems stems from the interaction term $\propto J\Delta$ in the Hamiltonian (1). If $\Delta = 0$ (the interaction between the underlying spins or qubits is of the $XY$-type), the above single-particle results apply to the many-particle system. For nonzero $\Delta$, on the other hand, (i) the energy levels are shifted depending on the occupation of neighboring sites, potentially leading to many-particle resonances, and (ii) there occur interaction-induced many-particle transitions.

To analyze many-particle effects, it is convenient to change from $a_n^\dagger, a_n$ to new creation and annihilation operators $b_n^\dagger, b_n$ that diagonalize the single-particle part of the Hamiltonian (1), $a_n = \sum_k U_{nk} b_k$. The interaction part of the Hamiltonian becomes

$$H_i = J\Delta \sum_k V_{k1,k2,k3,k4} b_{k1}^\dagger b_{k2}^\dagger b_{k3} b_{k4},$$

where the sum runs over $k_{1,2,3,4}$, and $V_{k1,k2,k3,k4} = \sum_p U_{pk1}^* U_{p+1,k2}^* U_{p+1,k3} U_{pk4}$. If all single-particle stationary states are strongly localized, the off-diagonal matrix elements $U_{nk}$ are small. They are determined by the decay of the wave functions and fall off exponentially. $U_{nk} \sim K^{k-n}$ for $|k-n| \gg 1$. At the same time, the diagonal matrix element is $U_{nn} \approx 1$. Therefore the major terms in the matrix $V_{k1,k2,k3,k4}$ are those with $\varkappa = 0$, where

$$\varkappa = \min_p (|k_1 - p| + |k_2 - p - 1| + |k_3 - p - 1| + |k_4 - p|).$$

They lead to an energy shift $\propto J\Delta$ for the many-particle states with occupied neighboring sites.

The terms $V_{k1,k2,k3,k4}$ with $\varkappa > 0$ lead to two-particle intersite transitions $(k_3,k_4) \rightarrow (k_1,k_2)$, and $V J \Delta$ plays the role of a two-particle hopping integral. The parameter $\varkappa$ gives the number of intermediate steps involved in a transition. The steps are counted off from the configuration where the particles occupy neighboring sites $\Phi_n$. For large $\varkappa$ and $\alpha \gg \alpha_{\text{th}}$ we have $V \propto (J/2\hbar)^{\varkappa} \ll 1$, i.e., many-particle hopping integrals are small and rapidly decrease with the number of involved steps.

Numerical results on the many-particle IPR are shown in Fig. 2. We have studied chains of length $L = 10, 12, \text{and} 14$ with $L/2$ excitations, which have the largest number of states for given $L$ ($\propto 2^L$ for large $L$). The results were similar, and we present the data for $L = 12$, in which case the total number of states is 924.

For small $\alpha$, the IPR is independent of $\alpha$ and is large because of the large number of resonating on-site states $|\Phi_{n_1,\ldots,n_6}\rangle$. It is reduced by the interaction $\propto J\Delta$ that splits the energy spectrum into subbands depending on the number of occupied neighboring sites. On the whole, the IPR decreases with increasing $\alpha$ as long as $\alpha \lesssim 0.4$. In the region $0.2 \lesssim \alpha \lesssim 0.4$ we have $\langle I_0 \rangle \approx 1.01$ except for narrow peaks. This indicates that away from the peaks all stationary states are strongly localized, as confirmed by the data on $I_{6\text{max}} = \max_\lambda I_{6\lambda}$.

A distinctive feature of the many-particle IPR as function of $\alpha$ are multiple resonant peaks, a part of which is resolved in Fig. 2. They occur when two on-site states resonate, which gives $I_{6\text{max}} \lesssim 2$. The strongest peaks come from two-particle resonances. They happen when the two-particle energy difference

$$\delta \varepsilon = |\varepsilon_{k_1} + \varepsilon_{k_2} - \varepsilon_{k_3} - \varepsilon_{k_4}|$$

is close to $MJ\Delta$ with $M = 0, 1, 2$.

As we increase $\alpha$ starting from $\alpha = 0$, pronounced peaks of $\langle I_0 \rangle$ appear first for $\delta \varepsilon \approx soh \approx J\Delta$ with $s = 1, 2$. They are due to hybridization of pairs on sites $(n,n+1)$ and $(n,n+3)$ for $s = 1$, and $(n,n+1)$ and $(n-1,n+2)$ for $s = 2$, for example ($\varkappa = 2$-transitions).
For larger $\alpha$, resonances occur when $\omega_n h \approx MJ\Delta$ with $n \geq 2$. Such resonances require more intermediate steps, with $\omega \geq 4$. The widths of the IPR peaks are small and are in good agreement with simple estimates based on Eq. (9). In between the peaks $I_{6\text{max}} = 1.02$ for $0.2 \lesssim \alpha \lesssim 0.4$ and $h/J = 20$.

A special role is played by two-particle resonances where $\delta\varepsilon \ll J$ for all $\alpha < 0.4$. They emerge already for $\omega = 2$-transitions $(n, n + 1) \leftrightarrow (n - 1, n + 2)$. Here, if $n$ and $n + 2$ are prime numbers, $\delta\varepsilon \sim \alpha^{n-1}h$ is extremely small for large $n$. Strong resonance occurs for all $n = 6k - 1$, in which case $\delta\varepsilon/h \propto \alpha^2$ with $\xi \geq 4$. Such $\delta\varepsilon$ is unusually small for $\omega = 2$. More many-particle resonances happen for higher $\omega$. For different sections of the chain (3) we found that they could increase $I_{\text{max}}$ up to $1.15$ between the peaks, for $h/J = 20, 0.2 < \alpha < 0.4$, and $\Delta = 1$. These resonances can be eliminated by modifying the sequence $\varepsilon_n \rightarrow \varepsilon_n + \alpha'h/2$ for $n = 6k$. For appropriate $\alpha' \sim 0.1$, this modification brings $(I_6)$ and $I_{6\text{max}}$ back to $\approx 1.01$ and $\approx 1.02$, respectively (10, 12).

We now outline an alternative approach to the problem of strong localization, which is particularly relevant for quantum computing. Qubit states have finite coherence time, estimated as $\lesssim 10^5 - 10^6 J^{-1}$ for most models. It is sufficient to show that the states remain localized for a time that exceeds the coherence time. This will enable both gate operations, that take time $\sim J^{-1}$, and measurement, that often requires more time.

Delocalization occurs through a transition to a resonating on-site state. All resonant two-particle transitions up to a given number of steps $\omega_0$ will be eliminated if, for $\omega < \omega_0$, the on-site energy difference $\delta\varepsilon$ exceeds the maximum change of the interaction energy $\propto J\Delta$. For $\omega_0 = 4$ this requires $\Delta/h < \alpha^2, \alpha'/2, |\alpha - \alpha'/2|$. From Eq. (6), if the time needed for a transition with $\omega_0$ steps is $\gtrsim K^{-\omega_0}/J\Delta$, it scales as $h^{\omega_0}$. Then if $\omega_0 = 4$, the lifetime of all on-site states exceeds $J^{-1}$ by a factor $10^5$ for $h = 30, \alpha = 0.3, \alpha' \approx 0.2$, and $\Delta \lesssim 1$.

The transition time is further dramatically increased if $\omega = 4$ resonances are eliminated. The low-energy gap in $\delta\varepsilon$ for the corresponding transitions is $\sim \alpha^3h$ when $\alpha' \sim \alpha^3$. For example, for $\alpha = 0.25$ and $\alpha' = 0.22$ this gap is $\delta\varepsilon/h > 0.01$ for all sites $n > 4$, cf. Fig. 3. This means that all states will remain localized on their sites for a time $\gtrsim K^6(J\Delta)^{-1}$, if $2J\Delta/h < 0.01$.

In terms of the operation of a quantum computer, the on-site energy sequence (3) is advantageous, since one radiation frequency can be used to resonantly excite different qubits. Selective tuning to this frequency can be done without bringing neighboring qubits in resonance with each other. In our approach, localization does not require refocusing (3), which is not always easy to implement. We avoid delocalization due to indirect resonant $n \rightarrow n + 2$ transitions, which undermines the approach (10). Compared to Ref. (3), in our approach the interaction does not have to be ever turned off, and no multiqubit encoding is necessary. In addition, our results are not limited to systems with nearest neighbor coupling.

In conclusion, we have proposed a sequence of on-site energies that leads to strong localization of single- and many-particle stationary states of interacting spins or qubits. For an infinite chain, we eliminate resonances between on-site states with the effective interstate hopping integral up to $(J/h)^5$. This leads to a long lifetime of localized many-particle states already for a comparatively narrow energy bandwidth. The results show viability of scalable quantum computers where the interrogating interaction is not turned off.

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The obtained $\langle I_6 \rangle - 1$ were much smaller than for a chain with random $\varepsilon_n$ uniformly distributed over a band of the same width as (4). On the other hand, $\langle I_6 \rangle$ for the sequence (3) did not increase when random terms up to $\sim \hbar \alpha^4$ were added to $\varepsilon_n$, which indicates that the sequence (3) is robust with respect to errors.