Mapping between Hamiltonians with attractive and repulsive potentials on a lattice

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Through a simple and exact analytical derivation, we show that for a particle on a lattice there is a one-to-one correspondence between the spectrum in the presence of an attractive potential $\hat{V}$ and its repulsive counterpart $-\hat{V}$. For a Hermitian potential, this result implies that the number of localized states is the same in both attractive and repulsive cases although these states occur above (below) the band continuum for the repulsive (attractive) case. For a $\mathcal{PT}$-symmetric potential that is odd under parity, our result implies that, in the $\mathcal{PT}$-unbroken phase, the energy eigenvalues are symmetric around zero and that the corresponding eigenfunctions are closely related to each other.

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The energy spectrum of a quantum particle in an attractive potential $V(\mathbf{r})$ in general consists of discrete eigenvalues for which the eigenfunctions are localized in real space, and continuum eigenvalues with non-square-integrable eigenfunctions. The energy spectrum for the corresponding repulsive potential $-V(\mathbf{r})$ has only continuum eigenvalues [1,2]. This situation changes dramatically when the particle is confined to a lattice or, equivalently, is exposed to a periodic potential. Indeed, repulsively bound two-atom states have been explored in detail since their experimental discovery in optical lattices [3,4] and continue to be a source of ongoing work [5] in the context of the Bose-Hubbard model [6,7]. We note that in the Bose-Hubbard model the interaction between the two atoms is short ranged and is tuned via the Feshbach resonance [3]. However, to our knowledge, the properties of single-particle states localized in the vicinity of a generic repulsive potential (defined below) have not been studied. In another area, localized states in parity + time-reversal ($\mathcal{PT}$)-symmetric one-dimensional lattice models, too, have been explored in recent years. These explorations have focused on the $\mathcal{PT}$ symmetry breaking in the presence of attractive (real) on-site potentials with random $\mathcal{PT}$-symmetric complex parts [8].

In this Brief Report, through a simple but exact derivation, we show that for a single particle on a lattice there is a one-to-one correspondence between its energy spectrum in the presence of an attractive potential and the repulsive counterpart, and that the corresponding eigenfunctions have identical probability distributions. For $\mathcal{PT}$-symmetric potentials that are odd under parity (and, hence, time reversal), we show that if the $\mathcal{PT}$ symmetry is unbroken, the energy spectrum must be symmetric around zero.

For the one-dimensional model, let us start with the Hamiltonian for a particle on a one-dimensional lattice with only nearest-neighbor hopping energy $J > 0$,

$$\hat{H}_0 = -J \sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i), \tag{1}$$

where $c_i^\dagger$ and c_i are creation and annihilation operators, respectively, at site i. The external potential is given by $\hat{V} = \sum_j V_j c_j^\dagger c_j$. We define the potential to be attractive provided $\sum_j V_j < 0$ and repulsive if is positive. Let $|\psi_\alpha\rangle = \sum_j f_{\alpha,j}|j\rangle$ be an eigenstate of the Hamiltonian $\hat{H}_+ = \hat{H}_0 + \hat{V}$ with energy E_α where $|j\rangle$ denotes a single-particle state localized at site j. The coefficients $f_{\alpha,j}$ obey the recursion relation

$$-J[f_{\alpha,j+1} + f_{\alpha,j-1}] + V_j f_{\alpha,j} = E_\alpha f_{\alpha,j}. \tag{2}$$

We now consider the staggered wave function $|\phi_\alpha\rangle = \sum_j f_{\alpha,j}(-1)^j|j\rangle$. Using Eq. (2), it is straightforward to show that the staggered wave function satisfies the following equation:

$$\hat{H}_0|\phi_\alpha\rangle = (-E_\alpha + \hat{V})|\phi_\alpha\rangle. \tag{3}$$

Thus, it is an eigenfunction of the conjugate Hamiltonian $\hat{H}_- = \hat{H}_0 - \hat{V}$ with eigenvalue $-E_\alpha$. When $\hat{V} = 0$, the energy spectrum is given by $\epsilon_k = -2J\cos(ka)$ and represents the well-known continuum band from $-2J$ to $2J$ where a is the lattice spacing. In this trivial case, indeed the eigenfunction $|\psi_k\rangle = \sum_j \sin(kj)|j\rangle$ and its staggered counterpart $|\phi_k\rangle = \sum_j \sin[(\pi - k)j]|j\rangle$ have energies $\pm\epsilon_k$, respectively.

Our result shows that if an attractive external potential $\hat{V}$ has n bound states below its continuum with energies E_m ($m = 1, \ldots, n$), then the corresponding repulsive potential $-\hat{V}$ must have an equal number of bound states above its continuum with energies $-E_m$. Since the staggered wave function $|\phi_\alpha\rangle$ varies over the lattice length scale a, it is energetically expensive and ill defined in the continuum limit $a \to 0$. Physically, in the continuum limit, the absence of lattice-site scattering centers makes it impossible for a particle to localize near the repulsive potential. However, on a lattice, the probability distributions for the two states—a localized bound state $|\psi_\alpha\rangle$ with energy $E_\alpha \leqslant -2J$ in an attractive potential and the localized bound state $|\phi_\alpha\rangle$ with energy $-E_\alpha \geqslant +2J$ in the repulsive potential—are identical. As a concrete example, we numerically obtain the spectrum for a lattice with $N = 29$ sites and a quadratic potential that vanishes at the ends, $V_m = \Lambda(m-1)(N-m)/N_0^2$, where $m = 1, \ldots, N$, $N_0 = (N+1)/2$ is the center of the lattice and $V_{N_0} = \Lambda$. Figure 1 shows the ground-state wave function $\psi_{G,m}$ for the attractive case, $\Lambda/J = -0.5$ [Fig. 1(a)], along with the highest-energy-state wave function ϕ_m for the repulsive case, $\Lambda/J = +0.5$ [Fig. 1(b)]. It is clear that the two wave functions are related by $\phi_m = (-1)^{m+1}\psi_{G,m}$.

For the two-particle case, we can generalize this result in a straightforward manner to treat interparticle interaction $\hat{U} = \sum_{ij} U_{i-j}\hat{n}_i\hat{n}_j$ where the on-site number operator is given by

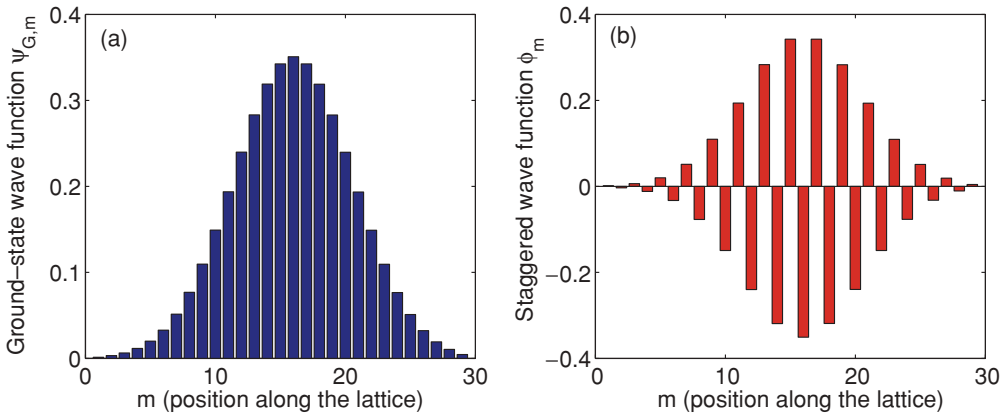

FIG. 1. (Color online) (a) Dimensionless ground-state wave function $\psi_{G,m}$ for an *attractive quadratic potential* $V_m = \Lambda(m-1)(N-m)/N_0^2$, where $N = 29 = (2N_0+1)$ is the lattice size and $\Lambda/J = -0.5$. As expected for a quadratic potential ground state, $\psi_{G,m}$ is a Gaussian with width $x_0 = a(N_0^2 t/|\Lambda|)^{1/4} \sim 4.61$. (b) Dimensionless highest-energy-state wave function ϕ_m for its *repulsive counterpart* with $\Lambda/J = +0.5$. We see that the ϕ_m is indeed the staggered version of the ground-state wave function $\phi_{G,m}$.

$\hat{n}_i = c_i^\dagger c_i$. In the two-particle sector, the recursion relation satisfied by the relative-coordinate wave function is given by [6,7]

$$-J_K\left(\psi^K_{\alpha,m+1} + \psi^K_{\alpha,m-1}\right) + U(r_m)\psi^K_{\alpha,m} = E^K_\alpha \psi^K_{\alpha,m}. \qquad (4)$$

Here $-\pi/a \leqslant K \leqslant \pi/a$ is the lattice momentum associated with the center of mass of the two particles, $J_K = J\cos(Ka)$ is the effective hopping energy, $r_m = am = a(i-j)$ is the distance between the two particles on the lattice located at sites i and j, and $U(r_m)$ is the real-space interaction between the two particles. Note that for a nonlocal interparticle interaction $U(r_m)$, multiple bound-state ψ^K_α solutions are generic, although, in the context of the Bose-Hubbard model, only one [3] or two [6] have been discussed. If ψ^K_α is an eigenfunction of the Hamiltonian $\hat{H}_0 + \hat{U}$ with energy E^K_α, Eq. (4) implies that the staggered wave function ϕ^K_α defined by $\phi^K_\alpha(r_m) = (-1)^m \psi^K_\alpha(r_m)$ is an eigenfunction of the conjugate Hamiltonian $\hat{H}_0 - \hat{U}$ with energy $-E^K_\alpha$.

Two-particle bound states in the presence of on-site and nearest-neighbor repulsive density-density interactions on a lattice have been extensively investigated [3,5,6]. Our derivation shows that they are a generic feature of any density-density interaction on a lattice, and this result is true for square lattices in higher dimensions. Note that the quantum statistics of the particles only constrains the relative wave function $\psi^K_\alpha(r_m)$ to be odd (spinless fermions) or even (bosons or spin-singlet fermions) under parity; however, it does not affect the one-to-one correspondence between the spectra for the two Hamiltonians $\hat{H}_0 \pm \hat{U}$. Thus, two-atom bound states with attractive and repulsive interactions in optical lattices (bosons) [3], the donor and acceptor impurity levels in semiconductors (fermions) [9], as well as the localized phonon modes (collective bosonic excitation) [10,11] around a soft or stiff impurity can all be thought of as manifestations of the correspondence between spectra for $\hat{H}_+$ and H_-.

The mapping between the two Hamiltonians $\hat{H}_+$ and $\hat{H}_-$ is valid independent of the properties of the potential $\hat{V}$ including its Hermiticity; the on-site potential elements V_j may be complex. However, for a $\mathcal{PT}$-symmetric potential that is odd under parity (and, hence, time reversal), $V_j^* = -V_j = V_{-j}$, it follows that $\hat{H}_+^* = \hat{H}_-$, where the asterisk denotes complex conjugation. Therefore, it follows from $\hat{H}_+|\psi_\alpha\rangle = E_\alpha|\psi_\alpha\rangle$ that the wave function $|\psi^*_\alpha\rangle = \sum_j f^*_{\alpha,j}|j\rangle$ is an eigenstate of the conjugate Hamiltonian $\hat{H}_-$ with eigenvalue $+E^*_\alpha$. In the continuum limit, it has been shown that a wide class of such potentials, including $V(x) = ix^3$ and $V(x) = i\sin^{2n+1}(x)$, have purely real energy spectra [12,13]. If the $\mathcal{PT}$ symmetry is unbroken, $E^*_\alpha = E_\alpha$, then it follows that $\hat{H}_-|\phi_\alpha\rangle = -E_\alpha|\phi_\alpha\rangle$ and $\hat{H}_-|\psi^*_\alpha\rangle = +E_\alpha|\psi^*_\alpha\rangle$.

This explicit construction of wave functions with equal and opposite energies implies that for any arbitrary $\mathcal{PT}$-symmetric potential that is odd under parity, if the $\mathcal{PT}$ symmetry is not broken, the energy spectrum must be symmetric around zero. It also shows that the corresponding wave functions in the two cases have components that are simply related: $[+E_\alpha, f^*_{\alpha,j}] \leftrightarrow [-E_\alpha, f_{\alpha,j}(-1)^j]$. As an example, we consider the simplest "finite lattice" with two points. (Our result is equally applicable to a finite lattice.) The Hamiltonian in this case is given by $\hat{H}_- = -J\hat{\sigma}_x + i\gamma\hat{\sigma}_z$, where (σ_x,σ_z) are the Pauli matrices in the site-index space [14] and a real γ ensures that the potential is odd under parity as well as time reversal. The eigenvalues in this case are given by $E_\pm = \pm\sqrt{J^2-\gamma^2}$. Thus, the $\mathcal{PT}$ symmetry in this case is not broken as long as $\gamma \leqslant J$. The corresponding (unnormalized) eigenfunctions[1] are given by [14]

$$|\pm\rangle = \begin{pmatrix} 1 \\ \pm e^{\mp i\theta} \end{pmatrix}, \qquad (5)$$

where $\theta = \arctan(\gamma/\sqrt{J^2-\gamma^2})$ is real when $\gamma \leqslant J$. Therefore, in the $\mathcal{PT}$-unbroken phase, the eigenvectors for positive and negative energies indeed are related by $f_{-,j} = (-1)^j f^*_{+,j}$, where $j = 0,1$.

[1]We consider unnormalized eigenvectors to avoid the subtleties associated with the $\mathcal{CPT}$ inner product [14] that are irrelevant for our result.

Our result, through a one-to-one mapping between attractive and repulsive potentials on a lattice, shows that localized states in repulsive potentials are ubiquitous. These states can be explored via local measurements. In contrast to the bound states with energies below the continuum band, these localized states with energies above the continuum band will decay into the continnum states. They may thus provide a useful spectroscopic tool in optical lattices as well as engineered electronic materials with a small bandwidth.

Note added in proof. Recently, we became aware of a related paper [15].

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