Mapping between Hamiltonians with attractive and repulsive potentials on a lattice

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Abstract

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 spectra 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-continnum 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.
**Introduction:** The energy spectrum of a quantum particle in an attractive potential \( V(r) \), 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 \(-V(r)\) 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 Feschback 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 (\(PT\)) symmetric one-dimensional lattice models, too, have been explored in recent years. These explorations have focused on the \(PT\)-symmetry breaking in the presence of attractive (real) on-site potentials with random \(PT\)-symmetric complex parts [11].

In this note, 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 \(PT\)-symmetric potentials that are odd under parity (and hence time-reversal), we show that if the \(PT\)-symmetry is unbroken, the energy spectrum must be symmetric around zero.

**One-dimensional Model:** Let us start with the Hamiltonian for a particle on a one-dimensional lattice with only nearest-neighbor hopping energy \( J > 0 \),

\[
\hat{H}_0 = -J \sum_i \left( c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right)
\]  

where \(c_i^\dagger\) and \(c_i\) are creation and annihilation operators at site \(i\) respectively. 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 \(E_\alpha\) where \(|j\rangle\) denotes a single-particle state localized at site \(j\). The coefficients \(f_{\alpha,j}\) obey the recursion relation

\[
-J [f_{\alpha,j+1} + f_{\alpha,j-1}] + V_j f_{\alpha,j} = E_\alpha f_{\alpha,j}.
\]
We now consider the staggered wavefunction $|\phi_\alpha\rangle = \sum_j f_{\alpha,j} (-1)^j |j\rangle$. Using Eq.(2) it is straightforward to show that the staggered wavefunction satisfies the following equation

$$\hat{H}_0 |\phi_\alpha\rangle = (-E_\alpha + \hat{V}) |\phi_\alpha\rangle.$$  \hspace{1cm} (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 wavefunction $|\phi_\alpha\rangle$ 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 $E_\alpha \leq -2J$ in an attractive potential and the localized bound state $|\phi_\alpha\rangle$ with energy $-E_\alpha \geq +2J$ 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, $V_m = \Lambda(m - 1)(N - m)/N^2$, 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 wavefunction $\psi_{G,m}$ for the attractive case, $\Lambda/J = -0.5$, (left panel) along with the highest-energy state wavefunction $\phi_m$ for the repulsive case, $\Lambda/J = +0.5$ (right panel). It is clear that the two wavefunctions are related by $\phi_m = (-1)^{m+1} \psi_{G,m}$.

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

$$-J_K \left[ \psi_{\alpha,m+1}^{K} + \psi_{\alpha,m-1}^{K} \right] + U(r_m) \psi_{\alpha,m}^{K} = E_\alpha^K \psi_{\alpha,m}^{K}. \hspace{1cm} (4)$$

Here $-\pi/a \leq K \leq \pi/a$ 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
FIG. 1. (color online) (a) The left panel shows the dimensionless ground-state wavefunction \( \psi_{G,m} \) 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 \( x_0 = a(N_0^2t/|\Lambda|)^{1/4} \sim 4.61 \). (b) The right panel shows the dimensionless highest-energy state wavefunction \( \phi_m \) for its repulsive counterpart with \( \Lambda/J = +0.5 \). We see that the \( \phi_m \) is indeed the staggered version of the ground-state wavefunction \( \phi_{G,m} \).

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 wavefunction \( \psi^K_{\alpha}(r_m) \) to be odd (spin-less 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) [8], as well as the localized phonon modes (collective bosonic excitation) [9, 10] around a soft or stiff impurity can all be thought of as manifestations of the correspondence between spectra for $\hat{H}_+\pm\hat{H}_-$. 

**$\mathcal{PT}$ Symmetric Potential:** The mapping between the two Hamiltonians $\hat{H}_+\pm\hat{H}_-$ 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 $^*$ denotes complex conjugation. Therefore, it follows from $\hat{H}_+|\psi_\alpha\rangle = E_\alpha|\psi_\alpha\rangle$ that the wavefunction $|\psi_\alpha^*\rangle = \sum_j f_{\alpha,j}^*|j\rangle$ 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 wavefunctions 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 wavefunctions 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 2 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 $\hat{\sigma}_x, \hat{\sigma}_z$ are the Pauli matrices in the site-index space [14] and a real $\gamma$ 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 $\gamma \leq J$. The corresponding (unnormalized) eigenfunctions [15] are given by [14]

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

where $\theta = \arctan(\gamma / \sqrt{J^2 - \gamma^2})$ is real when $\gamma \leq J$. 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 $j = 0, 1$. 

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Conclusion: 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 continuum states. They may thus provide a useful spectroscopic tool in optical lattices as well as engineered electronic materials with a small bandwidth.

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