Mapping between Hamiltonians with attractive and repulsive potentials on a lattice

Yogesh N. Joglekar

Department of Physics, Indiana University Purdue University Indianapolis (IUPUI), Indianapolis, Indiana 46202, USA

(Dated: September 8, 2010)

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 $V(\mathbf{r})$, 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 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 ($\mathcal{PT}$) 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 [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 $\mathcal{PT}$-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.

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

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

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_α where $|j\rangle$ denotes a single-particle state localized at site j. The coefficients $f_{\alpha,j}$ obey the recursion relation

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

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

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

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 $|\phi_k\rangle = \sum_j \sin\left[(\pi - k)j\right]|j\rangle$ 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, $V_m = \Lambda(m-1)(N-m)/N_0^2$, 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 wavefunction ψ_{Gm} for the attractive case, $\Lambda/J = -0.5$, (left panel) along with the highest-energy state wavefunction ϕ_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]

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

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

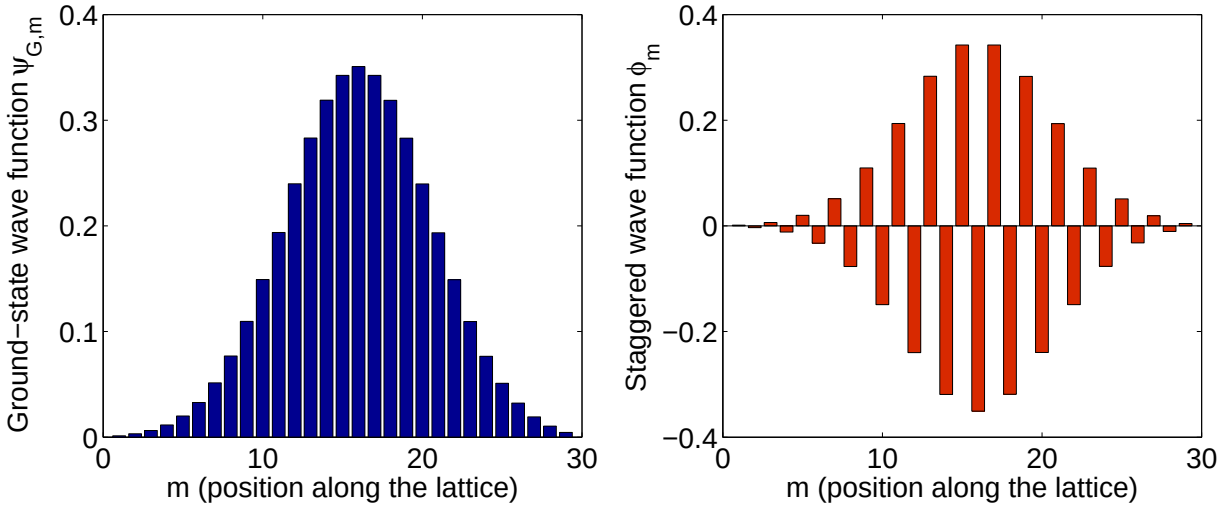

FIG. 1. (color online) (a) The left panel shows the dimensionless ground-state wavefunction $\psi_{G,m}$ for an *attractive quadratic potential* $V_m = \Lambda(m-1)(N-m)/N_0^2$ where $N = 29 = (2N_0+1)$ is the lattice size and $\Lambda/J = -0.5$. As expected for a quadratic potential ground-state, $\psi_{G,m}$ is a Gaussian with width $x_0 = a(N_0^2 t/|\Lambda|)^{1/4} \sim 4.61$. (b) The right panel shows the dimensionless highest-energy state wavefunction 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 wavefunction $\phi_{G,m}$.

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 non-local interparticle interaction $U(r_m)$, multiple bound-state ψ_α^K solutions are generic, although, in the context of the Bose-Hubbard model, only one [3] or two [6] have been discussed. If ψ_α^K is an eigenfunction of the Hamiltonian $\hat{H}_0 + \hat{U}$ with energy E_α^K, Eq. 4 implies that the staggered wavefunction ϕ_α^K defined by $\phi_\alpha^K(r_m) = (-1)^m \psi_\alpha^K(r_m)$ is an eigenfunction of the conjugate Hamiltonian $\hat{H}_0 - \hat{U}$ with energy $-E_\alpha^K$.

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 $\psi_\alpha^K(r_m)$ 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) [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 $\hat{H}_+$ and H_-.

$\mathcal{PT}$ Symmetric Potential: 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 * 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 (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 $\gamma \leq J$. The corresponding (unnormalized) eigenfunctions [15] are given by [14]

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

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 $j = 0, 1$.

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

---

[1] L.D. Landau and E.M. Lifschitz, *Quantum Mechanics* (Butterworth-Heinemann, San Francisco, 2005).

[2] Here we only consider a non-relativistic system and thus ignore the question of bound states in the Dirac equation with a repulsive potential: H. Brysk and P.F. Zweifel, Phys. Rev. C **23**, 968 (1981); H. Tezuka, Japan J. Indust. App. Math, **14**, 39 (1997).

[3] K. Winker, G. Thalhammer, F. Lang, R. Grimm, J. Hecker Denschlag, A.J. Daley, A. Kantian, H.P. Buchler, and P. Zoller, Nature (London) **441**, 853 (2006).

[4] L. Fallani and M. Inguscio, Nature (London) **441**, 820 (2006).

[5] S.M. Mahajan and A. Thyagaraja, J. Phys. A **39**, L667 (2006).

[6] M. Valiente and D. Petrosyan, J. Phys. B **41**, 161002 (2008); M. Valiente and D. Petrosyan, J. Phys. B **42**, 121001 (2009).

[7] Y.-M. Wang and J.-Q. Liang, Phys. Rev. A **81**, 045601 (2010).

[8] P.Y. Yu and M. Cardona, *Fundamentals of Semiconductors* (Springer, New York, 1996).

[9] K-Q. Chen, X-H. Wang, and B-Y. Gu, Phys. Rev. B **62**, 9919 (2000).

[10] S. Mizuno, Phys. Rev. B **65**, 193302 (2002).

[11] O. Bendix, R. Fleishmann, T. Kottos, and B. Shapiro, Phys. Rev. Lett. **103**, 030402 (2009).

[12] C.M. Bender and S. Boettcher, Phys. Rev. Lett. **80**, 5243 (1998).

[13] C.M. Bender, G.V. Dunne, and P.N. Meisinger, Phys. Phys. Lett. A **252**, 272 (1999).

[14] C.M. Bender, D.C. Brody, and H.F. Jones, Phys. Rev. Lett. **89**, 270401 (2002).

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