Universal witnesses of vanishing energy gap

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Abstract – Energy gap, the difference between the energy of the ground-state of a given Hamiltonian and the energy of its first excited state, is a parameter of a critical importance in analysis of phase transitions and adiabatic quantum computation. We present a concrete technique to determine an upper bound for the energy gap of a Hamiltonian \(H_0\) based on properties of the set of expectation values of \(H_0\) and an additional auxiliary Hamiltonian \(V\). This formalism can be applied to obtain an effective criterion of gaplessness, which we illustrate with a concrete example of the XY model—a physical system with vanishing energy gap.

Introduction. – The connection between geometry and quantum phase transitions has been studied extensively with various approaches, which include geometric phase formalism \([1]\) and studies of properties of the entropy of low-energy states \([2]\). One of the geometry-related methods is based on the notion of numerical range —the set of joint expectation values of several observables among the same quantum state. It has been applied in the analysis of uncertainty relations \([3–5]\), detection of quantum entanglement \([6,7]\), and generalized Wigner functions \([8]\).

The link between the numerical range and quantum phase transition is of special interest, as it connects the static properties of the set of quantum states (being an image of a linear map) and the dynamical properties of a Hamiltonian family depending on a single parameter, \(H_\lambda = H_0 + \lambda V\). One of the properties with important implications in quantum computing \([9]\), state distinguishing, quantum speed limits \([10]\), and properties of ground states \([11–13]\) is the value of the energy gap: the energy difference between the ground state and the first excited state. There are various ways of estimating the energy gap for various kinds of systems: finite-size criteria \([14–17]\) take into account scaling of the energy gap with dimension of the system at finite size to estimate its asymptotic value. Martingale methods \([18]\) use other properties of Hamiltonians of a finite size. Using imaginary time propagation \([19]\) and methods based on density matrix renormalization group \([20]\) the gap can be estimated numerically. There exist also techniques to determine bounds for the energy gap applicable for a certain classes of Hamiltonians \([21–25]\). Macroscopic separation of the ground-state parts \([26]\) provide an upper bound for the energy gap, another such result is based on the fluctuations of the local observables \([27]\).

In this work, we explore the connection \([28]\) between phase transitions in systems described by a parameterized Hamiltonian \(H_\lambda\) and numerical ranges further and provide a new link between the two: the vanishing energy gap is related to the geometrical features of the numerical range of operators \(H_0\) and \(V\). Hence the geometrical properties of the analyzed sets on the plane is sufficient to determine the gaplessness for certain classes of Hamiltonians. We illustrate this connection studying a well-known gapless system: a chain of interacting spins forming the XY model \([24,29]\). Our result requires determination of only a single observable to estimate the energy gap, which may be advantageous in some contexts.

Main result: gaplessness witnesses. – The main result of this work consists in Proposition 1 providing upper bounds for the energy gap in terms of discontinuous behavior of expectation values. Here, the energy gap \(\Delta H\) is the asymptotic difference between the energy \(E_0\) of the ground state and the energy \(E_1\) of the first excited state, excluding the potential degeneracy of the former. For a sequence of Hamiltonians \(H_n\), describing systems of increasing size, the system is said to be \textit{gapped} if the value

\[
\Delta H = \limsup_{n \to \infty} \left[ E_1(H_n) - E_0(H_n) \right]
\]

is nonzero. This expression determines the optimal rate of computation in adiabatic quantum computers \([30]\). If the gap vanishes, \(\Delta(H) = 0\), the Hamiltonian \(H\) is said to be \textit{gapless}.
be gapless. This nontrivial property [31] is a signature of a quantum phase transition taking place [32].

We provide here an efficient method to determine whether an arbitrary Hamiltonian $H$ is gapless with the help of an auxiliary Hermitian operator $V$, which we call a gaplessness witness of $H$.

**Proposition 1.** If for a Hamiltonian $H$ there exists a Hermitian operator $V$ and $t_+ > 0$ such that

1) the ground state $|g(t)\rangle$ of $H + tV$ is constant in $t \in [0, t_+)$ (i.e., in this region $d|g(t)\rangle/dt = 0$),

2) at the point of the phase transition, $t = t_*$, the expectation value $\langle H \rangle_{|g(t)\rangle}$ has a jump discontinuity of size

$$\varepsilon = \lim_{t \to t_*^-} \langle H \rangle_{|g(t)\rangle} - \lim_{t \to t_*^+} \langle H \rangle_{|g(t)\rangle},$$

then the Hamiltonian $H$ has its energy gap $\Delta H$ bounded from above by $\varepsilon$:

$$0 \leq \Delta(H) \leq \varepsilon. \quad (3)$$

If $\langle H \rangle_{|g(t)\rangle}$ is continuous at $t = t_*$ for any Hermitian operator $V$ meeting the assumptions (equivalent to $\varepsilon = 0$), the Hamiltonian $H$ is gapless.

By contraposition, if a Hamiltonian $H$ is gapped, $\Delta H > 0$, then the function $\langle H \rangle_{|g(t)\rangle}$ is not continuous at $t = t_*$. The mathematical background of this result is presented in the following sections.

**Preliminaries: joint numerical range.** – The methods presented here rely on the properties of low-dimensional projections (up to affine transformations) of the set of density matrices of fixed dimension $d$. Let us recall the definition of the (joint) numerical range of $k$ Hermitian operators $A_1, \ldots, A_k$ of order $d$: the numerical range $W(A_1, \ldots, A_k)$ is the set of simultaneously allowed expectation values taken over all mixed states [33–35],

$$W(A_1, \ldots, A_k) = \{(\text{Tr} \rho A_1, \ldots, \text{Tr} \rho A_k) : \rho \in \mathcal{M}_d\}, \quad (4)$$

where $\mathcal{M}_d$ denotes the set of density operators of size $d$.

The object $W$ defined above is a convex subset of $\mathbb{R}^k$, the boundary of which is formed by the images of ground states of combinations of $A_1, \ldots, A_k$ —for an example with $k = 2$ see fig. 1. The latter property is useful in the analysis of quantum phase transitions happening at zero temperature [28,36,37].

In the context of this article, the joint numerical range of two Hermitian operators, $W(X,Y)$ is the most important case. Many of the following statements do generalize to the joint numerical ranges of arbitrary number of operators $k$ —we still restrict ourselves to $k = 2$ in the interest of simplicity, it is also enough for our purposes.

**Boundary of the numerical range and quantum phase transitions.** – Boundary $\partial W$ of the numerical range $W$ contains information related to the ground states of Hamiltonians built as combinations of the input operators. This is a direct consequence of the fact that points on the boundary of a convex set are maximizers of linear functionals, formally described in the following statement.

**Proposition 2.** Let us denote the boundary of the numerical range of two Hermitian operators $W(X,Y)$ by $\partial W$. The point $\vec{p} = (x, y)$ in $\partial W$ with the inward-pointing normal vector $\vec{n} = (n_x, \ldots, n_y)$, is an image of the ground state of the Hamiltonian $n_x X + n_y Y$.

**Proof.** A point $\vec{p}$ having an (inward-pointing) normal vector $\vec{n}$ on the boundary $\partial W$ of a convex set indicates that it minimizes the functional $\vec{n} \cdot \vec{q}$ among points $\vec{q} \in W$. Since $\vec{q}$ is a vector of expectation values, this is equivalent to the minimization of $n_x \langle X \rangle + n_y \langle Y \rangle$, an expression equal to $\langle n_x X + n_y Y \rangle$. Expectation value is minimized on the ground state of $n_x X + n_y Y$, which proves the proposition.

Some properties of the ground states of Hamiltonians composed of $k$ terms, $H = \sum_{i=1}^k n_i H_i$, are visible in the boundary of the numerical range $W(H_1, \ldots, H_k)$. Flat parts of the boundary $\partial W$ indicate the degeneracy of the ground state of the Hamiltonian corresponding to the appropriate normal vectors. Cusps, having multiple normal vectors, indicate that the ground state stays constant over a range of parameters [28].

For the sake of clarity, let us state here a simplified version of this result restricted to $k = 2$ terms. In such a case, the joint numerical range of two Hermitian observables is equivalent to the numerical range of a single non-Hermitian operator, $W(A,B) = W(A + iB)$.

**Proposition 3.** Consider a numerical range $W(H,V)$ with a cusp, the preimage of which is denoted by $|g\rangle$. Then,

a) the state $|g\rangle$ is a simultaneous eigenvector of $H$ and $V$,

b) let us split $H$ and $V$ into simple sums of two operators: one restricted to the space spanned by $|g\rangle$, the
second to its orthogonal complement: \( H = H^g \oplus H^\perp \), \( V = V^g \oplus V^\perp \). The numerical range \( W(H,V) \) is then a convex hull of the set union of \( W(H^g,X^g) \) and \( W(H^\perp,V^\perp) \).

**Proof.** a) If a point \((\langle H \rangle_g, \langle V \rangle_g) \in \partial W(H,V)\) forms a cusp of \( W \), it corresponds to multiple different support lines with different (normalized) normal vectors. Let us denote two of them by \( \vec{n} \) and \( \vec{m} \). Then by Proposition 2, the state \(|g\rangle\) is the ground state of \( \vec{n} \cdot (H, V) \) and of \( \vec{m} \cdot (H, V) \),

\[
\begin{align*}
n_0 H |g\rangle + n_1 V |g\rangle &= E_\vec{n} |g\rangle, \\
m_0 H |g\rangle + m_1 V |g\rangle &= E_\vec{m} |g\rangle.
\end{align*}
\]

Since the matrix \( \begin{pmatrix} n_0 & n_1 \\ m_0 & m_1 \end{pmatrix} \) is nonsingular if \( \vec{n} \neq \vec{m} \), this system of equations can be diagonalized to form

\[
\begin{align*}
H |g\rangle &= \lambda_H |g\rangle, \\
V |g\rangle &= \lambda_V |g\rangle,
\end{align*}
\]

which shows that \(|g\rangle\) is a common eigenvector of both \( H \) and \( V \).

b) Every state vector can be written as \(|\psi\rangle = \sqrt{p} \exp(i \phi) |g\rangle + \sqrt{1-p} |\psi^\perp\rangle\), where \(|\psi^\perp\rangle\) is orthogonal to \(|g\rangle\). Since the image of \(|\psi\rangle\) is at the apex of a cusp, the vector is a simultaneous eigenstate of \( H \) and \( V \). This fact implies that the image of \(|\psi\rangle\) in the numerical range lies at

\[
\begin{align*}
\langle (H)|\psi\rangle, \langle V|\psi\rangle &= p \langle (H)|g\rangle, \langle V|g\rangle \\
&\quad + (1-p) \langle (H)|\psi^\perp\rangle, \langle V|\psi^\perp\rangle.
\end{align*}
\]

The numerical range is thus a convex hull of the point corresponding to the state \(|g\rangle\) and the numerical range \( W(H^\perp,V^\perp) \) of operators restricted to the orthogonal subspace:

\[
W(H,V) = \text{conv} \left( W(H^g,X^g), W(H^\perp,V^\perp) \right). \tag{8}
\]

\( \square \)

In the case of a 2-D numerical range \( W(A,B) \), there exists a relation [38] linking the curvature of the boundary \( \partial W \) with the spectral properties of the non-Hermitian operator \( A + iB \).

The properties of the numerical range are not only of mathematical interest: convexity implies bounds for the properties of the ground-state space of mixed Hamiltonians, which serves as a basis for semidefinite programming (which uses spectrahedra, objects dual to joint numerical ranges [39]), widely used in quantum information theory [3,4]. Sampling of the boundary of the numerical range \( W \) has been realized experimentally for three-level quantum systems [40], confirming the classification established in [41].
Fig. 3: XY model. Top: expectation value of $H_{\gamma}(\gamma)$ (minus its ground-state energy) taken in the ground-state of $H_{\gamma}(\gamma) + t V_0$ (operators defined in appendix C by eq. (C.1)) as a function of the perturbation strength $t$. Bounds for the gap value for $H_{(100)}(\gamma)$ follow from Proposition 1 and the behavior of the expectation value. Continuous (within numerical ranges of finite-dimensional systems are always of a discontinuity, the size of which approaches 0 as $N$ is increased — see fig. 3. This numerical observation is confirmed by the asymptotic analytical treatment presented in appendix B. Since the size of the gap approaches 0 as $N \to \infty$, the Hamiltonian $H$ is asymptotically gapless for $\gamma = 0$.

For $\gamma \neq 0$, the Hamiltonian $H(\gamma)$ has an energy gap equal to $\gamma$. It is reflected by the growing discontinuity in the expectation value of $H(\gamma)$ with respect to the ground state of $H(\gamma) + t V$.

**Concluding remarks.** — Estimation of the value of the energy gap is important in various applications, such as many-body physics, condensed-matter physics, theory of quantum information, and adiabatic quantum computing. In this paper, we provide a method for estimation of the value of the energy gap, which may see practical applications. The technique developed combines geometrical and algebraic properties of the numerical range — the set of simultaneously attainable expectation values. It allows us to obtain an upper bound for the value of the energy gap with knowledge of the properties of the ground states only.

Note that the technique proposed here is universal, as it can be applied in a very general setting. While gaplessness witnesses — operators used to detect gaplessness in a geometric way — exist for every gapless Hamiltonian, generically “trivial” witnesses can be difficult to implement physically as they might be nonlocal. Numerical analysis provides evidence that for a given Hamiltonian $H$ with ground-state energy $E_0 = 0$, the gaplessness of $H$ is routinely detected by a random observable of the form $V = H Z H$, where $Z$ is a random Hermitian matrix drawn from the Gaussian Orthogonal Ensemble.

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Data availability statement: The data that support the findings of this study are available upon reasonable request from the author.

**Appendix A: existence of witnesses and trivial gaplessness.** — If a Hamiltonian $H$ is gapless, there always exists at least a single witness. If the ground state energy $E_0$ of $H$ is zero, the operator $V = H^2 - H$ is capable to show that the gap $\Delta(H)$ vanishes. Furthermore, as stated in the concluding section, random observables also yield effective witnesses of vanishing energy gap.
The case associated with the gaplessness of $H$ by Proposition 1 often appears in various contexts: in the one-dimensional Bose-Hubbard model with $N$ sites, the average occupation $(n_i)/N$ is constant in the Mott insulator phase and it varies continuously as the hopping rate increases. Similar behavior is observed with the average spin $(S_z)/N$ in the XY model interacting with an external field. In these cases, the apparent gaplessness is trivial, as it pertains to operatorsaveraged over the entire system. While the total spin operator $S_z = \sum_{i=1}^{N} s_i^z$ is not gapless, the average spin $S_z/N = \sum_{i=1}^{N} s_i^z/N$ is: it has homogeneously distributed eigenvalues ranging from $-1/2$ to $1/2$ with a spacing of $1/N$.

**Appendix B: analytical treatment of the witness for the XY model.** – We wish to determine the ground-state energy and excitation spectrum of the Hamiltonian $G(N)$ acting on a finite chain of $N$ sites, parameterized by $t$ and $\gamma$:

$$H_{(N)}(\gamma) = \frac{1}{2} \sum_{i=1}^{N-1} \left( \frac{1 + \gamma}{2} \sigma_x^{(i)} \sigma_x^{(i+1)} + \frac{1 - \gamma}{2} \sigma_y^{(i)} \sigma_y^{(i+1)} \right) + t \sum_{i=2}^{N-2} \sigma_x^{(i-1)} \sigma_x^{(i)} \sigma_y^{(i+1)} - \sigma_y^{(i-1)} \sigma_y^{(i)} \sigma_x^{(i+1)} + V_{(N)}$$

(B.1)

The free fermion method [43] works remarkably well in this case. To proceed, let us express the spin operators in the following way:

$$\sigma_x^{(n)} = (c_n + c_n^\dagger) \prod_{m<n} (1 - 2c_m^\dagger c_m), \quad \sigma_y^{(n)} = i(c_n^\dagger - c_n) \prod_{m<n} (1 - 2c_m^\dagger c_m), \quad \sigma_z^{(n)} = (1 - 2c_n^\dagger c_n),$$

(B.2) (B.3) (B.4)

where $c, c^\dagger$ obey the fermionic anticommutation relations:

$$\{c_i, c_j^\dagger\} = \delta_{ij}, \quad \{c_i, c_j\} = 0, \quad \{c_i^\dagger, c_j^\dagger\} = 0.$$  (B.5)

This set allows us to write the term representing the XY part of the Hamiltonian as

$$H_{(N)} = -\sum_{i=1}^{N-1} \left( \frac{1 + \gamma}{2} \sigma_x^{(i)} \sigma_x^{(i+1)} + \frac{1 - \gamma}{2} \sigma_y^{(i)} \sigma_y^{(i+1)} \right)$$

$$= -\sum_{i=1}^{N-1} (c_i c_{i+1} + c_i^\dagger c_{i+1}^\dagger) + \gamma (c_i c_{i+1} + c_i^\dagger c_{i+1}^\dagger)$$

+ b.t.  (B.6)

The boundary term (b.t.), appearing here due to the broken translational symmetry of a finite chain has the form of a long chain of fermion operators. Its contribution to the behavior of the complete Hamiltonian is, however, relatively constant (of order $O(1)$ in all expectation values, while the rest of $H_{(N)}$ grows as $O(N)$) and independent of $N$. Since we are interested in the asymptotic behavior as $N \to \infty$, we can omit the boundary term in later calculations. The same substitution also simplifies the form of the witness part of the Hamiltonian:

$$V_{(N)} = \sum_{i=2}^{N-2} \sigma_x^{(i-1)} \sigma_x^{(i)} \sigma_y^{(i+1)} - \sigma_y^{(i-1)} \sigma_y^{(i)} \sigma_x^{(i+1)}$$

$$= -2i \sum_{i=2}^{N-2} c_i^\dagger c_{i+1}^\dagger + c_i c_{i+1}.$$  (B.7)

The total Hamiltonian, $G(\gamma, t)$ has thus the form of nearest- and next-nearest-neighbor hopping and creation/annihilation of free fermions. In general, such Hamiltonians are diagonalized by expressing the creation and annihilation operators as a sum of creation and annihilation of plane waves, followed by Bogoliubov transformation [44]:

$$c_n^\dagger = \frac{1}{\sqrt{N}} \sum_k \exp(ink) d_k^\dagger, \quad c_n = \frac{1}{\sqrt{N}} \sum_k \exp(-ink) d_k.$$  (B.8)

The resulting Hamiltonian expressed in the terms of $d$ and $d^\dagger$ operators reads

$$G_{(N)}(\gamma, t) = \sum_k \cos(k) d_k^\dagger d_k$$

$$+ \gamma (\exp(-ik) d_{-k}^\dagger d_k + \exp(ik) d_k d_{-k})$$

$$+ t \sin(2k) d_k^\dagger d_k,$$  (B.9)

where the momentum index $k$ spans $\pm \frac{\pi}{N}, \pm \frac{2\pi}{N}, \ldots, \pm \frac{(N-1)\pi}{N}$. This form is finally diagonalized by a standard Bogoliubov transformation to

$$G(\gamma, t) = \sum_k d_k^\dagger d_k \left( \sqrt{(\cos k + t \sin 2k)^2 + \gamma^2 \sin^2 k} - \frac{1}{2} \right).$$  (B.10)

The energies $E_k$ pertain to excitations, while the negative sum of them gives the ground-state energy:

$$E_0(\gamma, t) = -\sum_k E_k.$$  (B.11)

This result can be applied in the calculation of the joint numerical range, since the knowledge of the ground-state energy as a function of parameters is sufficient to determine the boundary points using the Hellmann-Feynmann theorem. If $E_0(\gamma, t)$ is known, then

$$\langle V_{(N)}(\gamma, t) \rangle = \frac{\partial E_0}{\partial t}, \quad \langle H_{(N)}(\gamma, t) \rangle = E_0(\gamma, t) - \frac{\partial E_0}{\partial t}.$$  (B.12)
Calculations done this way are necessarily approximate, since in eq. (B.6) the boundary terms were omitted. The error of approximation is of order $O(1)$ (since the boundary term consists of a fixed number of operators with bounded norm), while the expectation values grow as $O(n)$.

Calculations obtained in this way agree well with numerical investigations performed using the density matrix renormalization group for large $N$ [45]. This method can be thus used to explore the joint numerical range associated with the XY model (fig. 3) and its properties, including the geometric determination of the energy gap value (Proposition 1).

Appendix C: tapered Hamiltonians. – The Hamiltonian presented in eq. (B.1) needs a slight modification for calculations presented in fig. 3. The original form is susceptible to the finite size effects centered at the ends of spin chain. One of the methods to deal with this is to consider cyclic Hamiltonians, in which $\sigma^\alpha_{(N+k)} = \sigma^\alpha_{(k)}$ —this brings back translational invariance of eigenstates, but results in suboptimal plots (which are nevertheless technically correct and consistent with Proposition 1). We have opted for an alternative: tapering the weights of interactions toward the ends of spin chain.

The tapered Hamiltonians have very similar form to the original ones,

\begin{equation}
H'_{(N,m)}(\gamma) = -\sum_{i=1}^{N+2m-1} \left( \frac{1 + \gamma}{2} s_x^{(i)} s_x^{(i+1)} + \frac{1 - \gamma}{2} s_y^{(i)} s_y^{(i+1)} \right),
\end{equation}

\begin{equation}
V'_{(N,m)} = \sum_{i=1}^{N+2m-2} S_x^{(i-1)} S_x^{(i)} S_y^{(i)} S_y^{(i+1)} - S_y^{(i-1)} S_y^{(i)} S_x^{(i)} S_x^{(i+1)}.
\end{equation}

The spin operators $\sigma^{(i)}_{\mu}$ have been substituted with $s^{(i)}_{\mu}$ and $S^{(i)}_{\mu}$. These operators are defined as

\begin{equation}
s^{(i)}_{\mu} = w_{\mu}^{1/2} \sigma^{(i)}_{\mu},
S^{(i)}_{\mu} = w_{\mu}^{1/3} \sigma^{(i)}_{\mu},
\end{equation}

where $w_{\mu}$ is the tapering weight, equal to 1 in the bulk and approaching 0 near the spin chain boundary. It appears in different powers in $s^{(i)}_{\mu}$ and $S^{(i)}_{\mu}$ to match the spin powers in $H'$ and $V'$ —resulting two- and three-site Hamiltonian terms are weighted approximately according to $w_{\mu}$.

The weight $w_{\mu}$ used in calculations is a sigmoid one, symmetric on both ends (see fig. 4):

\begin{equation}
w_{\mu} = \begin{cases} \frac{1}{2} \left( 1 - \cos \frac{\pi (i-1)}{m} \right), & i \leq m, \\
1, & m < i \leq N - m, \\
\frac{1}{2} \left( 1 - \cos \frac{\pi (N + 2m - i)}{m} \right), & i > N - m.
\end{cases}
\end{equation}

For plots presented in fig. 3, tapering distance $m = 50$ was chosen. Hence, in addition to $N = 100$ spin sites with full weight $w_\mu = 1$ the system was surrounded with $m = 50$ sites with decreasing weight on both sides.

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