Energy as Rate of Computing

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Abstract

We offer well-motivated and basis-independent definitions for the total *amount of change* occurring along any continuous trajectory of a quantum state vector, as well as the *amount of computational effort* required for a given unitary transformation in an abstract setting, given a set of possible "input" quantum states, and a set of available Hamiltonians. Our definitions are based on the action of the Hamiltonian, which we show is equal to (2×) the area swept out in the complex plane by the vector coefficients (in any basis). Using our definitions, we show that the rate of change of any state is exactly given by its average energy (relative to a given ground state), while the *rate of computing* in the abstract situation could be considered to be the energy of the highest-energy state in the input set. The minimum amount of computational work required to carry out various types of quantum and classical logic operations is explored.

1. Introduction

The average energy E of any quantum system relative to its ground state was shown by Margolus and Levitin [1] to directly limit the rate at which the system can undergo transitions between distinguishable (orthogonal) states, such as individual steps within a digital computation. The maximum (and achievable) rate is $R_\perp(N) = 2EN/[h(N-1)]$ for a dynamical orbit which cycles through a sequence of $N \geq 2$ mutually orthogonal states, with the extreme cases being $R_\perp(2) = 4E/h$ and $R_\perp(\infty) = 2E/h$. Related results concerning the minimum time required to perform unitary transforms of specific types have also been explored in other papers, such as [2].

Results such as these suggest that energy might fruitfully be *exactly* identified with the rate of raw, low-level quantum-physical "computing" that is taking place within a given physical system, if only the quantity "amount of computing" could be appropriately defined. We would like to understand better what this means, and show that some well-defined and well-justified measure of the rate at which "computational work" is being carried out within any quantum system is indeed *exactly* equal to the energy of that system.

In this paper, we address this goal by proposing a well-defined, real-valued measure of the total *amount of change* undergone over the course of *any* continuous trajectory of a state vector along the unit sphere in Hilbert space. This measure is simply given by the line integral of the magnitude of the *imaginary* component of the inner product between infinitesimally-adjacent state vectors along the given path. This quantity is invariant under any time-independent change of basis, since the inner product itself is. (And for closed paths, it even turns out to be invariant not only under rotations but also under *translations* of the complex plane.) Our quantity is also equal to twice the

complex-plane area (relative to the origin) that is circumscribed or "swept out" by the coefficients of the basis vector components (in any basis). We show that the instantaneous rate at which change (under our definition) occurs for any state (under any time-dependent Hamiltonian) is exactly given by the instantaneous (Hamiltonian) energy of the state. Our quantity is thus also equal to the action of the Hamiltonian over the system's trajectory.

Finally, we propose that (and motivate why) the *amount of computational work* performed by a given *transformation trajectory* (that is, a unitary transform described as $U=e^{iA}$, where A is the time-integral of a given time-dependent Hamiltonian) might best be defined as the *maximum* amount of change (under our definition) over the set of all initial states of the system that are under consideration in a given situation. (Similarly to how the *information capacity* or maximum entropy of a system also depends on what set of states is considered to be "available.") For time-independent Hamiltonians, an abstract system's *rate of computing* is then given exactly by the energy of its highest-energy state under consideration. And for any system of given energy, its rate of computing is exactly given by its energy. For a "bare" unitary transform (that is, one that is not associated with any specific Hamiltonian), the *computational effort* required to perform it in a given situation can be defined by minimizing the amount of computational work over all available transformation trajectories that result in that unitary.

The Margolus-Levitin theorem can then be reinterpreted (sightly) as showing us that the minimum Hamiltonian action or computational effort required to flip a bit in isolation is $h/4$, while the total action required to complete a cycle through N distinct neighboring states is $(N-1)h/2$. The other previous results concerning minimum times to perform other quantum operations can also be subsumed under our new framework.

2. Basic framework

Let $\mathcal{H}$ be any Hilbert space, and let $H(t)$ be any continuous mapping from a real-valued parameter t ("time") to Hermitian operators on $\mathcal{H}$, in other words, H can be considered to be a (most generally) time-dependent Hamiltonian, given appropriate energy units. For any times $t_1,t_2 \in \mathbb{R}$, define the *action operator of H from t_1 to t_2* to be:

$$A_H(t_1,t_2) = \int_{t=t_1}^{t_2} H(t)\,\mathrm{d}t \qquad (1).$$

Of course, in the special case where we have a time-independent $H(t) = H$ (const.), we can simplify the action operator to just $A_H(t_1,t_2) = A_H(\Delta t) = H\Delta t$ where $\Delta t = t_2 - t_1$.

Note that, although the action quantity that is most frequently used in physics (*e.g.* in Hamilton's principle) is the action of the *Lagrangian* $L = pv - H$, it is also perfectly valid and reasonable for us to define a more general notion of the action "of" any quantity that has units of energy, by integrating that energy quantity over time. In this case, we are referring to the action of the *Hamiltonian*, rather than the action of the Lagrangian.

Also define the *unitary transform from t_1 to t_2 under H* to be:

$$U_H(t_1,t_2) = \exp[iA_H(t_1,t_2)]. \qquad (2)$$

(In this document, we will use roman font for the constant imaginary unit i where $\mathrm{i}^2 = -1$, to distinguish it from italic variables *i* used as indices. Likewise for e, the constant base of the natural logarithms.) This is just the usual quantum time-evolution operator which transforms state vectors from time t_1 to t_2 under a given time-dependent Hamiltonian $H(t)$. (Sometimes, by convention a minus sign is inserted inside the exponential, but this is a purely arbitrary choice.) Henceforth, we will almost always omit the H subscript from U and A, although they should still be understood, in the context of the present discussion, to be always still implicitly dependent on H.

Taylor-expanding the expression for U, we note that (suppressing the t_1,t_2 parameters for clarity):

$$\begin{aligned} U &= \exp[\mathrm{i}A] \\ &= \sum_{n=0}^{\infty} \frac{(\mathrm{i}A)^n}{n!} \\ &= 1 + \mathrm{i}A - \frac{A^2}{2} - \frac{\mathrm{i}A^3}{6} + \ldots \\ &= 1 + \mathrm{i}A + \mathrm{O}(A^2) \end{aligned} \tag{3}$$

where the $\mathrm{O}(A^2)$ notation here is expressing the fact that if we were to scale to ever *smaller A*, *e.g.* by considering what happens to $A(k) = A_{\mathrm{H}}(t_1, t_1 + (t_2 - t_1)/k)$ as $k \to \infty$, the sum of the A^2, A^3, *etc.* terms would become asymptotically bounded in magnitude by a term that goes as A^2, and that thus would be negligible in comparison with A. In other words, as $k \to \infty$,

$$U(k) \to 1 + \mathrm{i}A(k). \tag{4}$$

Assuming that $H(t)$ is a continuous function, then for any infinitesimal time interval of magnitude $\Delta t = \mathrm{d}t$, $H(t)$ can be considered effectively time-independent over the "entire" infinitesimal interval between t_1 and $t_2 = t_1 + \mathrm{d}t$, and so we can say that at any time t, the "infinitesimal" (here meaning, close to 1) unitary transform applying "at" that time t can be expressed as

$$\begin{aligned} U(t, t+\mathrm{d}t) &= 1 + \mathrm{i}A(t, t+\mathrm{d}t) \\ &= 1 + \mathrm{i}A_{H(t)}(\mathrm{d}t) \\ &= 1 + \mathrm{i}H(t)\mathrm{d}t \end{aligned} \tag{5}$$

with the equality here being both rigorous and exact.

This simple (and well-known) relationship between U and H over infinitesimal time intervals could be seen as suggesting that important characteristics of U over arbitrarily large intervals can usefully be found by integrating properties of the infinitesimal unitary $U(t, t+\mathrm{d}t)$ over time between t_1 and t_2, or in other words by integrating properties of the instantaneous $H(t)$. Indeed, we will see that this is the case. Also, we will see that the imaginary unit i in (5) ends up playing an important role, and leads us to consider the imaginary part of the inner product in our definition of total action.

Now, to simplify further notation, let us henceforth write $U'(t)$ to mean $U(t, t+\mathrm{d}t)$. We will refer to the entire function $U'(t)$ over values of t between any t_1 and t_2 as the *transformation trajectory* between those times. Note that the overall transformation $U(t_1,t_2)$ is the product of all the infinitesimal $U'(t)$ over all times t in the range from t_1 to t_2. That is, we can write:

$$U(t_1,t_2) = \prod_{t=t_1}^{t_2} U'(t)\,. \tag{6}$$

Although the product operator $\prod$ is more traditionally applied only over discrete sets of terms, there is no reason it can't also be applied to a set of values that are each infinitesimally close to 1, analogously to how an integral $\int$ can be viewed as simply a generalization of the sum operator $\sum$ to a continuous set of infinitesimal terms.

Note that although $U'(t)$ completely determines $U(t_1,t_2)$, knowing the total transformation $U(t_1,t_2)$ for a particular pair of times t_1,t_2 is not sufficient to determine the specific complete transformation trajectory $U'(t)$, even for values of t falling in the range $[t_1, t_2]$.

3. Defining the amount of change

Now, let us proceed to define our concept of the *amount of change* performed by a transformation trajectory $U'(t)$ between two times, and by the resulting over unitary transform U. We will find it easiest to analyze this by first considering U's behavior when operating on its eigenvectors.

Let us first pause and look back at equation (3), the Taylor-expansion of the definition of U as $\exp[\mathrm{i}A]$, and reflect on it a moment. This equation immediately implies that all eigenvectors of A are eigenvectors of U as well. Why? Let $Av = av$ (with v a vector, a a scalar), then, spelling out the steps explicitly,

$$Uv = \left[\sum_{n=0}^{\infty} \frac{(\mathrm{i}A)^n}{n!}\right] v = \sum_{n=0}^{\infty} \frac{\mathrm{i}^n A^n v}{n!} = \sum_{n=0}^{\infty} \frac{\mathrm{i}^n a^n v}{n!} = \left(\sum_{n=0}^{\infty} \frac{\mathrm{i}^n a^n}{n!}\right) v = uv \tag{7}$$

where u is the scalar value $u = \sum_{n=0}^{\infty} (\mathrm{i}a)^n / n! = \mathrm{e}^{\mathrm{i}a}$. Since Uv is equal to a scalar (namely u) times v, we have that v is an eigenvector of U. Now, since U and A are of equal dimensionality, and all eigenvectors of A are eigenvectors of U, the converse also holds, and the two operators have identical sets of eigenvectors. Since U is unitary, it preserves vector length, and so its eigenvectors v remain unchanged under U except for a phase rotation, namely a multiplication by $u = \mathrm{e}^{\mathrm{i}a}$, where a is the eigenvalue of A corresponding to v. Note that A must have real eigenvalues, since it is an integral of H (which has real eigenvalues since it is Hermitian) and anyway, since we know $|u| = 1$, and $u = \mathrm{e}^{\mathrm{i}a}$, a must be real. In other words, the action operator is giving us the total angle of phase-rotation undergone by those vectors that end up unchanged by $U(t_1, t_2)$ aside from a phase-rotation.

Of course, we would also like to understand and quantify what happens to other vectors as well. We will see how to do this shortly. First, we will begin by analyzing in more detail what happens to a given eigenvector v over time as it is transformed by U.

Given any an initial vector v (at time t_1 which without loss of generality we set equal to 0), we can let $v(t) = U(t_1, t)v$. In other words, $v(t)$ traces out a continuous path on an origin-centered sphere in Hilbert space having radius $|v|$, which WLOG we can consider to be 1.

For simplicity, first suppose that H is time-independent (later, we will see how to remove this restriction). Then $A(\Delta t) = H\Delta t$ and $U(\Delta t) = \exp[iH\Delta t]$, so that for times $t = t_1+\Delta t = \Delta t$, we have $v(t) = U(\Delta t)v = \exp[iH\Delta t]v$. If v is an eigenvector of U (thus of A, and of H) let its eigenvalue under H be ω. Then $v(t) = \exp[i\omega t]v$. In other words, $v(t)$ simply phase-rotates continuously in the complex plane at angular velocity ω. Note that the inner product between the initial v and $v(t)$, which we can write $\langle v|v(t)\rangle$, has the value $\exp[i\omega t] = \cos(\omega t) + i \sin(\omega t)$. The imaginary part of the inner product is $\sin(\omega t)$. Note now that for an infinitesimal $t = dt$, we have that $\sin(\omega dt) = \omega dt = dA$, *i.e.*, the infinitesimal increment in angle (or action) accumulated over the time dt. In other words, over infinitesimal time intervals, the imaginary part of the inner product between the "before" vector $v(t_1)$ and the "after" vector $v(t_1+dt)$ gives exactly the amount of action (or phase angle accumulation) over that time. At least, we have shown this in the case of a time-independent Hamiltonian H, and an initial vector v which is an eigenvector of that Hamiltonian. Let us now see how to generalize this to other cases.

First, suppose the initial vector v is not an eigenvector of H. However, let $\{v_i\}$ be a maximal set of unit-length mutually orthogonal vectors which are all eigenvectors of H, in other words, H's orthonormal eigenbasis. Then, any arbitrary v can be expressed in terms of components in the v_i basis, that is $v = \sum_i c_i v_i$ where the c_i are complex coefficients.

Of course, since U is a linear operator, we can express Uv in terms of v's components in that basis, *i.e.*,

$$\begin{aligned} v(t) = U(t)v &= U(t)\left(\sum_i c_i v_i\right) \\ &= \sum_i c_i U(t) v_i \\ &= \sum_i c_i \exp[i\omega_i t] v_i \end{aligned} \tag{8}$$

where ω_i is just the eigenvalue of H that is associated with eigenvector v_i. Now, note that the exponential terms can be absorbed into the coefficients. That is, we can look at the coefficients as being time-dependent quantities, $c_i(t) = c_i \exp[i\omega_i t]$, and say that always $v(t) = \sum_i c_i(t) v_i$. Note that each coefficient, whatever its magnitude, still just phase-rotates in the complex plane with an angular velocity ω_i that is given by the corresponding eigenvalue of H.

At this point, let us pause to preview the next steps. We are going to study several quantities, and show the close identities between them:

1. The average rate of phase angle accumulation of the coefficients $c_i(t)$, weighted by their squared modulus (magnitude).
2. The *energy* of the given vector v considered as a quantum state.
3. The rate at which the coefficients $c_i(t)$ sweep out area in the complex plane.

4. The imaginary component of the inner product between infinitesimally-adjacent state vectors.
5. The rate at which the coefficients $c_j(t)$ in *any* orthonormal basis v_j sweep out area in the complex plane.

First, let us describe each coefficient c_i in phase-magnitude representation as $c_i = m_i \exp[\mathrm{i}\theta_i]$, where $m_i = |c_i|$ is the modulus (absolute value, magnitude, norm, length) of the complex number c_i, and $\theta_i = \arg(c_i)$ is its argument (phase angle). Another notation for this relation is $c_i = m_i \angle \theta_i$. Perhaps the most popular notation in use today is $c_i = m_i \mathrm{e}^{\mathrm{i}\theta_i}$, although the notation e^x may be confused with the ordinary complex exponentiation operation, which is, strictly speaking, multi-valued in the case of non-integer exponents. (*E.g.*, $1^{1/3}$ technically has 3 distinct complex values, namely 1, $\exp[2\pi\mathrm{i}/3]$, and $\exp[4\pi\mathrm{i}/3]$.) To avoid confusion, we use the $\exp[\cdot]$ notation here.

Let us now consider the following quantity:

$$\overline{\omega} = \sum_i m_i^2 \omega_i \tag{9}$$

Recall that ω_i is the eigenvalue of H corresponding to eigenvector v_i, and is the rate of phase rotation (or angular velocity) of the coefficient c_i in the complex plane. So, $\overline{\omega}$ is simply the average angular velocity of the coefficients, weighted by their squared modulus. Weighting by the squared modulus of the amplitudes (complex coefficients) of the basis states is the normal way of taking the average or mean value of an observable quantity in quantum mechanics, for a pure state that is a complex superposition of the eigenstates of the given observable. Thus, we can say $\overline{\omega}$ is simply the average complex-plane angular velocity for the quantum state v.

We pause to note that aside from a conversion of units, $\overline{\omega}$ is also the *energy* of the quantum state v. For example, if $\overline{\omega}$ has been implicitly quantified in terms of radians per second, then we can write $\overline{e} = \overline{\omega}\hbar$, using some standard physical unit for $\hbar$ such as Joule-seconds, to obtain the average energy $\overline{e}$ in a more traditional energy unit such as Joules. (The constant $\hbar$ can be considered to represent the angle "1 radian," and thus serves to make this implicit angle-unit explicit.) However, I emphasize that this is merely a matter of unit-conversion, and we can equally well say that $\overline{\omega}$ *is* the energy of the state.

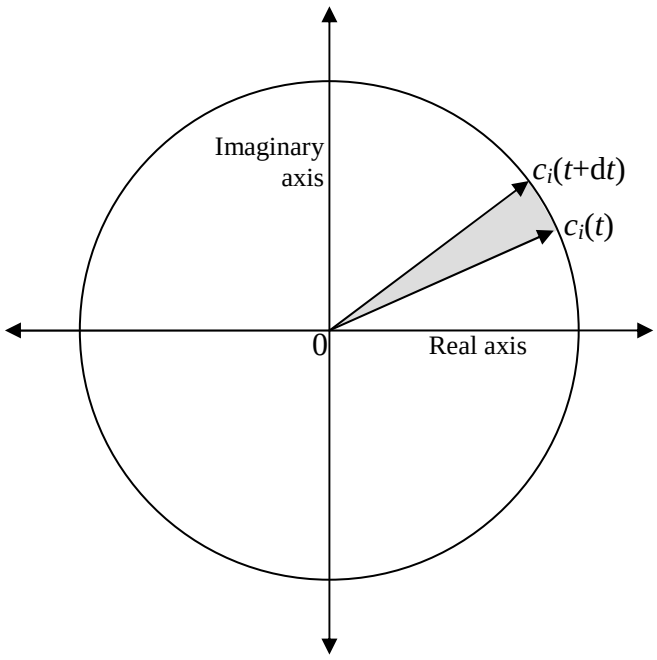

Figure 1. A complex coefficient c_i sweeps out a small wedge-shaped area (shown exaggerated) in the complex plane over an infinitesimal time interval dt.

Let us now consider the rate at which the complex coefficients sweep out area in the complex plane. To illustrate what we mean by this, refer to figure 1, which illustrates a region of the complex plane centered on the origin. Consider first just one of the coefficients c_i. At time t, it has value $c_i(t)$, shown as an arrow on the diagram. A short time dt later, the arrow has rotated to $c_i(t+\mathrm{d}t)$, and we say that the arrow has "swept out" the region shown in gray. Between these times, the arrow has rotated by an angle $\mathrm{d}\theta_i = \omega_i \mathrm{d}t$. What is the area of the wedge-shaped region of the disc? This is easy to calculate, if we recall that, were we to let the arrow sweep out a full circle, it would rotate by a total angle of $\theta_i = 2\pi$ radians, while sweeping out an area of $a_i = \pi m_i^2$, since m_i (the magnitude of c_i) is the radius of the circle shown. Thus, for the full circle, $a_i = \theta_i m_i^2/2$. By symmetry, this relation between a and θ also holds for each part of the circle, so we have $\mathrm{d}a_i = \mathrm{d}\theta_i m_i^2/2 = \omega_i m_i^2 \mathrm{d}t/2$.

To find the total area da swept out by *all* coefficients c_i over time dt, we merely do the same for each of them, and sum them all up:

$$\begin{aligned} \mathrm{d}a &= \frac{1}{2}\sum_i \omega_i m_i^2 \mathrm{d}t \\ &= \frac{1}{2}\overline{\omega}\,\mathrm{d}t \end{aligned} \tag{10}$$

Thus, the total rate da/dt at which area is swept out in the complex plane by all the various coefficients taken together is exactly half of the average component phase velocity, *i.e.*, half the state's energy.

This brings us to the fourth item in the preview above, namely the inner product between infinistesimally-adjacent state vectors $v(t)$ and $v(t+\mathrm{d}t)$. For conciseness, we will let $v=v(t)$ and $v' = v(t+\mathrm{d}t)$ and likewise for the coefficients c_i and phase angles θ_i. The

inner product $v \bullet v' = \langle v|v'\rangle = v^\dagger v'$ (these are three common alternative notations for it) can be defined in terms of the coefficients c_i, c_i' by:

$$v \bullet v' = \sum_i c_i^* c_i' \tag{11}$$

where the * denotes complex conjugation of c_i'. Now, in the phase-magnitude representation, $c_i^* = (m_i \exp[\theta_i])^* = m_i \exp[-\theta_i]$. Note that $m_i'=m_i$ because the complex magnitudes are not changed by phase rotation. Thus, $c_i^* c_i' = (m_i \exp[-\theta_i])(m_i \exp[\theta_i']) = m_i^2 \exp[\theta_i'-\theta_i]$. But, note that $\theta_i' = \theta_i + \omega_i dt$, so we have

$$\begin{aligned} c_i^* c_i' &= m_i^2 \exp[\omega_i dt] \\ &= m_i^2 \left[\cos(\omega_i dt) + i \sin(\omega_i dt)\right] \\ &= m_i^2 \left[1 + i\omega_i dt\right] \end{aligned} \tag{12}$$

where in the last step we are using the identities $\cos(d\theta)=1$ and $\sin(d\theta)=d\theta$ which hold for infinitesimal angles $d\theta$, where in our case $d\theta=\omega dt$. Now, we just sum equation (12) over the values of the index i to get the overall inner product. The real part of the inner product is just $\sum m_i^2 = 1$ always, so it is not very useful, but the imaginary part of the inner product, $\mathrm{Im}[v \bullet v'] = \sum m_i^2 \omega_i dt = \overline{\omega}\, dt$, in other words, it is the average energy times the time increment dt. Recall that $\overline{\omega}$ is the average phase velocity or average Hamiltonian energy of the state v, thus $dA = \overline{\omega}\, dt$ is the average increment in phase, or the increment in action over the time dt. Note that we have $dA = 2da$, where recall da was the increment in area swept out in the complex plane.

Of course, even for a non-infinitesimal time interval Δt, we can obtain the total average accumulation of phase angle ΔA, or the total area Δa swept out, by just using the expressions $\Delta A = \overline{\omega}\, \Delta t$ and $\Delta a = \Delta A/2$.

As an interesting aside, for any closed trajectory that eventually brings all coefficients back to their initial complex-plane locations simultaneously, it does not even matter where we choose to locate the complex origin for purposes of calculating the area, relative to the geometric curves traced out in the plane by the coefficients. The total area swept out by the points as they travel around the curves remains exactly the same no matter where the "center" is chosen.

4. Generalizing to arbitrary bases

The above discussion proceeded under the context of a set of basis vectors $\{v_i\}$ which were taken to be orthonormal eigenvectors of the (temporarily presumed constant) Hamiltonian operator H. Now, we will see that this choice of basis is in fact unnecessary, and that the same statements concerning the relationship between the area swept out and the action would hold true in any (time-independent) basis.

That this is true is suggested by considering the relationship between dA (the increment of action, the energy $\overline{\omega}$ times dt) and the inner product $v \bullet v' = v(t) \bullet v(t+dt)$ between infinitesimally neighboring vectors along the trajectory. We saw that $dA = \mathrm{Im}[v \bullet v']$. However, a fundamental property of the inner product that it is itself a unitary invariant; that is, it is a product of two vectors considered as pure *geometric* objects, and

thus it is independent of the basis which we use to express those vectors in terms of components. Therefore, this basis-independence also holds for the imaginary part of the inner product. So, if we were to just define dA = Im[v•v'], this definition would rely not at all on any particular basis; we do not even have to find the eigenstates of the Hamiltonian to determine it. Yet, it is still true that dA/dt is the energy of the state v.

Now, however, we would like to see whether the other quantities we investigated that explicitly invoke a choice of basis nevertheless remain consistent under a change of basis. In particular, we saw that in the energy basis v_i, the area swept out by the coefficients c_i in the complex plane was exactly given by half of the action A, that is, a=A/2. Does this remain true in other bases? We will see that it does.

At first, it may seem non-obvious that the area swept out is still half of the action. Note that our previous arguments for this relied on the fact that in the energy basis $\{v_i\}$, the coefficients all rotated at uniform angular velocity in a circle in the complex plane, while their individual magnitudes m_i remained constant. In a different basis v_j, this is no longer true. Each basis vector v_j is in general some superposition of the v_i, like

$$v_j = \sum_i u_j^i v_i \,, \tag{13}$$

where the matrix $\mathbf{U} = [u_j^i]$ of complex coefficients (j indexing rows, i columns) is, most generally, any unitary matrix. We can also write this equation in matrix-vector form as $\vec{v}_j = \mathbf{U}\vec{v}_i$. Now, for a general vector v,

$$v = \sum_i c_i v_i = \sum_j c_j v_j = \sum_j c_j \sum_i u_j^i v_i = \sum_{ij} c_j u_j^i v_i = \sum_i \left(\sum_j c_j u_j^i \right) v_i \,, \tag{14}$$

so, equating the coefficients on the v_i components of v, we have that

$$\begin{aligned} c_i &= \sum_j u_j^i c_j \\ \vec{c}_i &= \mathbf{U}^T \vec{c}_j \,, \end{aligned} \tag{15}$$

or, solving for the c_j's,

$$\begin{aligned} \vec{c}_i &= \mathbf{U}^T \vec{c}_j \\ (\mathbf{U}^T)^{-1} \vec{c}_i &= \vec{c}_j \\ (\mathbf{U}^T)^{T*} \vec{c}_i &= \vec{c}_j \\ \mathbf{U}^* \vec{c}_i &= \vec{c}_j \\ c_j &= \sum_i (u_j^i)^* c_i . \end{aligned} \tag{16}$$

In other words, each complex coefficient in the new basis is just a particular linear combination of what the various complex coefficients were in the old basis. If the coefficients c_i in the old energy basis are describing perfect circles around the complex origin at a variety of radii and angular velocities, there is no guarantee that the

coefficients c_j in the new basis will be describing circular paths, although their paths will of course still be continuous. In general, the c_j will follow a complex looping trajectory in the complex plane, generated exactly as if by Ptolemaic planetary epicycles, *i.e.*, as a sum of circularly rotating vectors. A given c_j will in general return to its initial location in the complex plane only when its components c_i that have nonzero values of u_j^i simultaneously return to their initial locations exactly (which could take infinitely long, if the corresponding ω_i values were relatively irrational).

Anyway, the important point for our present purposes is that the c_js do not, in general, maintain a constant magnitude (distance from the origin), and so the area swept out by the c_j over a given time is no longer just a section of a circle, which was easy to analyze. Instead, while c_j's phase angle θ_j is rotating, simultaneously its magnitude m_j may also be growing or shrinking. Figure 2 illustrates the situation.

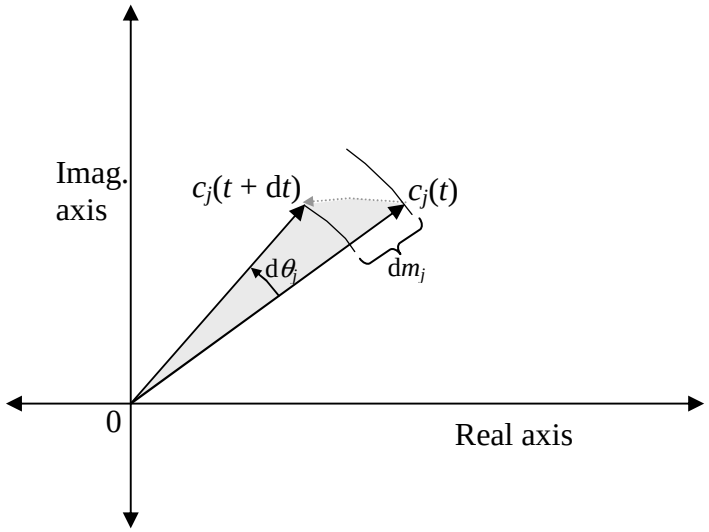

Figure 2. Area swept out (exaggerated) by a coefficient c_j (in a basis other than the energy eigenbasis) over an infinitesimal time interval dt. Note that both its phase and magnitude change in general.

What, now, is the area swept out in this more general situation? Notice that it is (in the infinitesimal limit which we are discussing) exactly half the area of the parallelogram spanned on two adjacent sides by $c_j = c_j(t)$ and $c_j' = c_j(t+dt)$, considered as vectors in the complex plane. See figure 3.

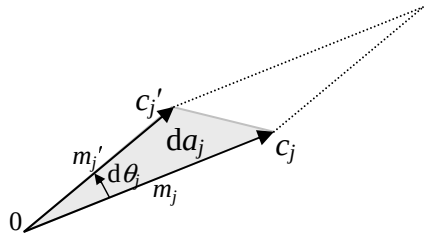

Figure 3. The infinitesimal area da_j swept out approaches one-half the parallelogram area $m_j m_j' \sin d\theta_j$.

The parallelogram area, itself, is $dA_j = m_j m_j' \sin(d\theta_j)$, where m_i and m_i' are the magnitudes of the old and new coefficients, respectively, and $d\theta_j$ is the increment in phase angle. However, note that the area dA_j of this parallelogram is also the magnitude of the "cross product" $c_j \times c_j'$ between the coefficients, considered as two-dimensional vectors. (The

traditional cross-product, defined in three dimensions, would be a vector perpendicular to the complex plane having this value dA_j as its length.) There is a beautiful identity connecting the cross product and dot product with the conjugate multiplication of complex numbers, namely:

$$a^* b = a \cdot b + i(a \times b) \tag{17}$$

where a^* means the complex conjugate of a, and $a \cdot b$ denotes the real "dot product" between a and b considered as vectors, namely $|a||b| \cos[\arg(b) - \arg(a)]$, and $a \times b$ denotes the real "cross product" previously mentioned between a and b considered as vectors, namely $|a||b| \sin[\arg(b) - \arg(a)]$. That this is true can be shown easily:

$$\begin{aligned} a^* b &= (|a| \exp[-i \arg(a)]) (|b| \exp[i \arg(b)]) \\ &= |a||b| \exp\{i[\arg(b) - \arg(a)]\} \\ &= (|a||b| \cos \theta) + i(|a||b| \sin \theta) \end{aligned} \tag{18}$$

where $\theta = \arg(b) - \arg(a)$. Applying this identity to our situation, we can see that the area swept out is exactly ½ of the *imaginary* part of the conjugate product between our two coefficients, in other words,

$$da_j = dA_j/2 = \mathrm{Im}[c_j^* c_j']/2. \tag{19}$$

Now, this is the area swept out by this single component c_j. To find the total area da swept out by all components, we merely sum over components:

$$\begin{aligned} da &= \sum_j \mathrm{Im}[c_j^* c_j'] / 2 \\ &= \frac{1}{2} \mathrm{Im}\left[\sum_j c_j^* c_j' \right] \\ &= \frac{1}{2} \mathrm{Im}[v_j \bullet v_j'] \end{aligned} \tag{20}$$

In other words, *just like in the energy basis*, in an arbitriary basis, the infinitesimal increment da in the area swept out is *still* exactly one-half of dA the imaginary component of the inner product between infinitesimally adjacent vectors along the trajectory. We saw earlier that dA was exactly the action of the Hamiltonian over the time increment dt. Integrating over time, we see now that the total area a swept out by the coefficients in any basis is exactly $A/2$, where A is indeed exactly the action of the Hamiltonian, *i.e.* the quantum average value of the observable operator $A = H\Delta t$ when applied to the initial state vector v.

5. Time-dependent Hamiltonians

In the above we have established that $2da = dA = \mathrm{Im}[v \bullet v'] = H dt$ for infinitesimal changes of the state vector $v \rightarrow v'$ along its trajectory over infinitesimal time intervals dt under a *constant* Hamiltonian. But, as long as the Hamiltonian only changes in continuous fashion, it can always be considered "constant" throughout any infinitesimal interval dt, even if it is varying over non-infinitesimal timescales. Therefore the above

identities still hold true even for a time-dependent Hamiltonian $H(t)$, as we originally started with. Thus, when we integrate over time, it remains true that:

$$2a = A = \int_{t=t_1}^{t_2} \mathrm{Im}[v(t) \bullet v(t+\mathrm{d}t)] = \int_{t=t_1}^{t_2} \overline{\omega}(t)\mathrm{d}t = \int_{t=t_1}^{t_2} H(t)\mathrm{d}t\,. \tag{21}$$

In other words, $2a$ (twice the area swept out by the complex coefficients, in any basis) is equal to A, the action of the Hamiltonian (the average eigenvalue $\langle v|A|v\rangle$ of the operator $A(t_1,t_2)$ applied to the initial state v), which is equal to the integral along the trajectory $v(t)$ of the imaginary component of the dot product between neighboring vectors, and to the integral of the average phase velocity of the coefficients in the energy eigenbasis (weighted by the instantaneous eigenstate probability $[m_i(t)]^2$), and to the integral of the instantaneous Hamiltonian energy (the average eigenvalue of the operator $H(t)$ applied to the instantaneous state $v(t)$) over time. We might even consider this quantity to be a reasonable definition of the geometric *length* of the path that the state vector describes as it drifts along the unit sphere in Hilbert space, except that it could be negative if $\langle H\rangle$ (the instantaneous average value of H) was sometimes negative.

Anyway, the fact that this measure of "amount of change" is so stable with respect to changes of basis as well as multifarious ways of defining it, and that it connects so strongly with fundamental physical concepts such as action and energy, as well as with primitive geometric concepts such as angles and areas, all feeds into our motivation for proposing it as being the most natural and genuine measure of the "amount of change" that is undergone by a physical quantum state vector v as it changes dynamically under a (possibly-varying) physical influence $H(t)$.

If we like, we can consider the dynamical trajectory of the system to comprise a *computation*, and then A (or equally well, a) becomes a natural measure of the total raw *amount of computational work that is* performed physically by the system. Note this is not to imply that all of the raw physical computation that is occurring in the given system is necessarily being harnessed and applied by humans to meet our calculational needs, only that this is the total amount of raw computational work that occurring "in nature."

The only caveat to all of this is that the quantity A is itself dependent on where we choose to draw our zero of energy. As is well-known, energies are only defined up to an additive constant, and so the total action is only defined up to this constant times the time Δt. Although it is natural to define the least eigenvalue of the Hamiltonian (the "ground state") to be the zero of energy, this is by no means mandated mathematically, and in the context of a time-dependent or infinite-dimensional Hamiltonian, there might not even be any minimum eigenvalue. One should keep these caveats in mind, although they seemingly end up not much affecting the practical applications of this concept, which we will address in a later section.

6. More abstract scenarios

Consider an abstract physical situation wherein we know that a particular time-dependent Hamiltonian $H(t)$ will be applied to a system, but we do not know the exact initial state v of the system to which it will be applied. Instead, suppose we are given only a set of possible initial states, or a probability distribution over initial states. Can we

meaningfully define the amount of computational work performed by the resulting action $A(t_1,t_2)$ between two times, in the absence of knowledge of the particular state?

In the case where we have a probability distribution over initial states, of course one natural thing to do is to quantify the weighted average action over all those states. This is then the expectance value of the action, or of the amount of computation.

If we are only given a set of states, we might construct a uniform probably distribution over that set (or if it is a continuous set, a uniform probability density function, according to some natural measure on that set), and then proceed to define the expected action according to that distribution.

However, an interesting alternative is to also consider what we would get by taking the *minimum* and *maximum* action over the set of initial states.

For large sets of possible states, the minimum action may frequently be zero, for example, it will be 0 as long the Hamiltonian is time-independent and its lowest-energy eigenstate (the ground state, defined to have energy 0) happens to be included in the set of possible initial states. So, minimizing the action over initial states may not tell us anything useful that we don't already know.

On the other hand, the *maximum* action $A(t_1,t_2)$ over the set of possible initial states is a measure of the maximum amount of "computational work" that could be performed by the given dynamics $H(t)$ operating on an element of the given input set, between two given times t_1 and t_2. This is perhaps a better measure of the computational "power" of the dynamics. It is a dynamics that *could* perform a given amount of computational work. Insofar as the actual state *might* be the one that invokes maximal work, we can say that a system with an unknown or unspecified state is, at least, performing this much "potential" computational work. At least, even if the actual state is not the maximum-action one, the system could be thought of as still "doing the work" of determining that the actual state is *not* the one that should transition through the given maximal distance.

To summarize:

$$\text{(potential computational work represented by action operator } A) = \mathrm{W}[A] = \max_{v \in V} Av$$

where V is the set of available initial state vectors, and Av denotes the action of the operator A when applied to v, that is,

$$Av = \langle v | A | v \rangle = \sum_k A_k m_k^2 \tag{22}$$

where the basis k is the orthonormal eigenbasis of the operator A. In other words, Av is just the quantity we were calling A earlier, for the particular case of initial vector v. If we can obtain the eigenvalues A_k and can determine the magnitudes m_k of the coefficients c_k of the eigenvectors v_k in this basis, then we can calculate the action by the summation shown.

7. Computational effort

Suppose now that we are given nothing except a unitary operator U on the Hilbert space $\mathcal{H}$, and we want to address the question: How much *computational effort* does it require

to *implement U*, in the sense that *U* ends up being generated by the dynamics, according to $U = e^{iA}$ for some *A*? The above discussion provides us a way to answer this question.

Among the set of *all* Hermitian operators *A*, or among at least a set of available action operators, we can choose one generating *U* that has the *smallest* value of the potential computational work $W[A] = \max_{v \in V} Av$, given a set *V* of available initial states. This *A* then can be considered the "best" action operator for generating the given unitary *U*, in the sense that the length of the longest trajectory that would be undergone by any possible state vector $v \in V$ is minimized.

Formally, given *U* we can define the *effort* to implement *U*, E[*U*], by

$$E[U] = \min_{A \in \aleph} \max_{v \in V} Av \tag{23}$$

where $\aleph$ is the set of available action operators on $\mathcal{H}$, *i.e.*, some subset of the set of all Hermitian operators on $\mathcal{H}$, determined by what constitutes an "available" dynamics. For example, $\aleph$ might reasonably be constrained to only those action operators that are obtainable by time-integrating instantaneous Hamiltonians $H(t)$ that are themselves constructed by summing over local interaction terms between neighboring subsystems, or by integrating a Hamiltonian density function that includes only local terms over some topological space, *e.g.*, to reflect the local structure of spacetime in a quantum field-theory picture. Or, we might constrain ourselves to action operators that are obtainable from time-independent Hamiltonians only.

Now, given this notion of the computational effort of a given unitary *U*, one can reinterpret previous results (such as [1,2]) regarding "quantum speed limits" or minimum times to implement various specific unitary transforms of interest (or classes of transforms), given states of specified average energy above the ground state, as follows: These analyses are specifying an $\aleph$ (usually, just all Hermitian operators) and a *V* (usually, just the entire Hilbert space), and showing that E[*U*] for the transform *U* has a specific value, assuming a time-independent Hamiltonian with a ground state energy of 0. In other words, a certain minimum "worst-case" action is required to implement *U*.

As an example, Margolus and Levitin's result [1] can be interpreted as saying that any *U* that rotates any state *v* to an orthogonal state requires an effort $E[U] \geq h/4$. Also, if there is a *v* such that $v, Uv, U^2v, \ldots, U^{N-1}v, U^Nv=v$ comprises a cycle of *N* states, with each orthogonal to the preceding and succeeding states in the cycle, then E[*U*] is *exactly* $(h/2)(N-1)/N$, so long as we are given complete freedom in constructing the Hamiltonian, aside from the requirement that it be time-independent. For $N=2$, this expression reduces to $h/4$; while for $N \to \infty$, $E[U] \to h/2$.

We note that this form of the Margolus-Levitin theorem at first only seems to concern the amount of *action A* required to implement the given *U*; however, in light of our previous discussions, this immediately also implies that an initial state of given energy *E* (above the ground state) will take time $t = A/E$ to accumulate this amount of action under a time-independent Hamiltonian, and thus it will take at least this much time to undergo the given transformation (namely, a transition between two orthogonal states, in the case of the Margolus-Levitin theorem).

It is anticipated that, armed with the new definitions proposed in this document, it would be a highly useful and worthwhile exercise to systematically go through a variety

of the quantum unitary transforms that have already been studied in the context of quantum computing as comprising useful "quantum logic gate" operations, and quantify their computational effort according to the above definition. This would directly tell us how much physical action is required for those operations (given a best-case Hamiltonian implementation, while operating on a worst-case input state). We can likewise do the same for classical reversible Boolean logic operations embedded within unitary operations, and classical irreversible Boolean operations embedded within these (with ancilla bits available as needed for carrying away unwanted information to be discarded).

This will, for the first time, give us a natural and physically well-founded measure for the computational effort or physical action needed to physically implement various logic operations. This in turn would directly translate to a minimum physical time to perform these operations within any physical system or subsystem using a set of states having a given maximum energy above the ground state, given any known or prespecified constraints on the system's initial state and its available Hamiltonian dynamics. This new quantification of computational effort may also allow us to derive lower bounds on the number of quantum gates of a given type that would be required to implement a given larger transformation, and possibly to show that certain constructions of larger gates out of smaller ones are optimal.

8. Effort to perform various operations

In this section [under construction], we explore the amount of computational effort (according to our previous definitions) that is required to implement a variety of important quantum and classical logic operations.

References

[1] Norman H. Margolus and Lev B. Levitin, "The maximum speed of dynamical evolution," *Physica D*120 (1998) 188-195, http://arXiv.org/abs/quant-ph/9710043.

[2] Lev B. Levitin, Tommaso Toffoli, and Zachary Walton, "Operation time of quantum gates," http://arXiv.org/abs/quant-ph/0210076, October 25, 2002.