Quantum Diagonalization of Hermitean Matrices

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Abstract

To measure an observable of a quantum mechanical system leaves it in one of its eigenstates and the result of the measurement is one of its eigenvalues. This process is shown to be a *computational resource*. It allows one, in principle, to diagonalize hermitean $(N \times N)$ matrices by quantum mechanical measurements only. To do so, one considers the given matrix as an observable of a single spin with appropriate length s which can be measured using a generalized Stern-Gerlach apparatus. Then, each run provides one eigenvalue of the observable. As it is based on the 'collapse of the wave function' associated with a measurement, the procedure is neither a digital nor an analog calculation—it defines thus a new *quantum mechanical* method of computation.

Non-classical features of quantum mechanics such as Heisenberg's uncertainty relation and entanglement have intrigued physicists for several decades. From a classical point of view, quantum mechanics imposes constraints on the ways to talk about nature. An electron does not "have" position and momentum as does a billiard ball. Similarly, if a photon is entangled with a second one—possibly very far away—one cannot ascribe properties to it as is done for an individual classical particle. The lesson to be learned is that classical intuition about the macroscopic world simply does not extrapolate into the microscopic world.

In recent years, an entirely different attitude towards quantum theory has been put forward. The focus is no longer on attempts to come to terms with its strange features but to capitalize on its both counter-intuitive and well-established properties. In this way, surprising methods have been uncovered to solve specific problems by means which have no classical equivalent: *quantum cryptography*, for example, allows one to establish

secure keys for secret transmission of information [1]; entanglement [2] is used as a tool to set up powerful *quantum algorithms* which do factor large integers much more efficiently than any classical algorithm [3]. Throughout, these new techniques rely on the *measurement* of quantum mechanical observables as a reliable tool. This is also true for *quantum error correction* [4, 5] required to let any potential algorithm run.

Here the purpose is to point out that the bare 'projection' [2] effected by a quantum mechanical measurement does possess computational power itself. As will be shown below, it can be used to solve explicitly at least one specific computational task, namely to determine eigenstates and eigenvalues of hermitean $(N \times N)$ matrices.

The diagonalization of hermitean matrices is a recurrent problem in mathematics, physics, and related fields. Using the notation of a quantum physicist the problem reads as follows. Given a self-adjoint operator $\widehat{A}$ acting on a Hilbert space $\mathcal{H}$ of dimension N, one needs to determine its eigenstates $|A_n\rangle, n = 1, \ldots, N$, and its N real eigenvalues A_n satisfying $\widehat{A}\,|A_n\rangle = A_n|A_n\rangle, n = 1, \ldots, N$. If normalized to one, the eigenstates constitute a complete orthonormal basis of the space $\mathcal{H}$: $\sum_{n=1}^{N} |A_n\rangle\langle A_n| = 1, \langle A_n|A_{n'}\rangle = \delta_{nn'}$. The standard solution from linear algebra [6] is to write down the eigenvalue equation with respect to a given orthonormal basis $|k\rangle, k = 1, \ldots, N$, say. The N^2 matrix elements $\mathsf{A}_{kk'} = \langle k|\widehat{A}|k'\rangle$ determine the operator $\widehat{A}$ uniquely and its eigenstates are characterized by the coefficients $(\vec{A}_n)_k = A_{nk}$ in the expansion $|A_n\rangle = \sum_k A_{nk}|k\rangle$. The number λ is an eigenvalue of $\widehat{A}$ if the characteristic polynomial $P_A(\lambda)$ of the matrix A vanishes, $P_A(\lambda) = \det(\mathsf{A} - \lambda\mathsf{E}) = 0$, where E is the $(N \times N)$ unit matrix. Once the N roots A_n of the polynomial P_A are known, the non-zero solutions of the equation

$$(\mathsf{A} - A_n)\,\vec{A}_n = 0\,, \qquad n = 1, \ldots, N\,, \tag{1}$$

provide the eigenvectors $|A_n\rangle$ in the basis $|k\rangle$. Analytic expressions for the eigenvalues A_n in terms of the elements of A exist only if $N \leq 4$. In general, numerical methods are required to determine approximately the roots of $P_A(\lambda)$.

The *quantum diagonalization* of hermitean matrices is based on the assumption that the behaviour of a spin s is described correctly by non-relativistic quantum mechanics. This method will make use of the 'collapse of the wave function' as computational resource. Note that the procedure does *not* depend on a particular interpretation of quantum mechanics. Five steps are necessary to achieve the diagonalization of a given matrix A (supposed for simplicity not to have degenerate eigenvalues). The individual steps will be described first in a condensed form; subsequently, commentaries explain the technical details.

1. Standard form of A: Write the hermitean $(N \times N)$ matrix A as a combination of linearly independent hermitean *multipole* operators $\mathsf{T}_\nu, \nu = 0, \ldots, N^2 - 1$,

$$\mathsf{A} = \sum_{\nu=0}^{N^2-1} \mathbf{a}_\nu \mathsf{T}_\nu\,, \qquad \mathbf{a}_\nu = \frac{1}{N}\ \mathrm{Tr}\ [\mathsf{A}\mathsf{T}_\nu] \in \mathbf{R}\,. \tag{2}$$

2. Identification of an observable: Interpret the matrix A as an observable H_A for a single quantum spin S with quantum number $s = (N-1)/2$,

$$\mathsf{H}_A(\mathsf{S}) = \sum_{\nu=0}^{N^2-1} \mathbf{a}_\nu \mathsf{T}_\nu(\mathsf{S})\,, \tag{3}$$

using the expression of the multipoles $\mathsf{T}_\nu(\mathsf{S})$ in terms of the components of a spin.

3. Setting up a measuring device: Construct an apparatus app(H_A) suitable to measure the observable H_A.

4. Determination of the eigenvalues: Carry out measurements with the apparatus app(H_A) on a spin s prepared in a homogeneous mixture $\hat{\rho} = \mathsf{I}/(2s+1)$. The output of each measurement will be one of the eigenvalues A_n of the matrix A. After sufficiently many repetitions, all eigenvalues will be known.

5. Determination of the eigenstates: Calculate the eigenstates $|A_n\rangle$ of the matrix A on the basis of Eq. (1) and the experimentally determined eigenvalues A_n. Alternatively, determine the eigenstates $|A_n\rangle$ *experimentally* by methods of state reconstruction.

Thus, the matrix A has been diagonalized without *calculating* the zeroes of its characteristic polynomial by traditional means. The fourth step solves the hard part of the eigenvalue problem since it provides the eigenvalues A_n of the matrix A. The comments to follow provide the background necessary to perform the individual steps. Emphasis will be both on the construction of a device measuring for a given hermitean operator (Step 3) and on the working of a quantum mechanical measurement (Step 4).

Ad 1: The N^2 self-adjoint multipole operators $\mathsf{T}_\nu = \mathsf{T}_\nu^\dagger$ form a basis in the space of hermitean operators acting on an N-dimensional Hilbert space $\mathcal{H}$ [7]. Two multipoles are orthogonal with respect to a scalar product defined as the trace of their product: $(1/N)\ \mathrm{Tr}\ [\mathsf{T}_\nu \mathsf{T}_{\nu'}] = \delta_{\nu\nu'}$.

Consider now a Hilbert space $\mathcal{H}_s$ of dimension $(2s+1)$ which carries an irreducible representation of the group $SU(2)$ with the spin components $(\mathsf{S}_1, \mathsf{S}_2, \mathsf{S}_3)$ as generators. Then, the multipoles $\mathsf{T}_\nu, \nu = 1, \ldots, N^2-1$, are given by the symmetrized products $\mathsf{S}_{j_1}\mathsf{S}_{j_2}\cdots\mathsf{S}_{j_a}, j_i = 1,2,3$, and $a = 0, 1, \ldots, 2s$, after subtracting off the trace (define $\mathsf{T}_0 \equiv \mathsf{T}^{(0)} = \mathsf{E}$, the $(N \times N)$ unit matrix). The index a labels $(2s+1)$ classes with $(2a+1)$ elements transforming among themselves under rotations; for the sake of brevity, a collective index $\nu \equiv (a; j_1, \ldots, j_k)$ is used. Explicitly, the lowest multipoles read

$$\mathsf{T}_j^{(1)} = \mathsf{S}_j\,, \quad \mathsf{T}_{j_1 j_2}^{(2)} = \frac{1}{2}\left(\mathsf{S}_{j_1}\mathsf{S}_{j_2} + \mathsf{S}_{j_2}\mathsf{S}_{j_1}\right) - \frac{\delta_{i_1 j_2}}{3}\mathsf{S}_{j_1}\mathsf{S}_{j_2}\,. \tag{4}$$

The set $\{\mathsf{T}_\nu\}$ is a basis for the hermitean operators on $\mathcal{H}_s$.

Ad 2: Since the multipoles are expressed explicitly as a function of the spin components not exceeding the power $2s$, it is justified to consider them and, *a fortiori*, the quantity H_A as an *observable* for a spin s.

Ad 3: It is natural to expect that every self-adjoint operator $\widehat{B}$ comes along with an apparatus app$(\widehat{B})$ capable of measuring it [8] . For particle systems, setting up such a device remains a challenging task for an experimenter.

For spin systems, the situation is different, however. Swift and Wright [7] have shown how to devise, in principle, a *generalized Stern-Gerlach apparatus* which measures any observable $\mathsf{H}_A(\mathsf{S})$—just as a traditional Stern-Gerlach apparatus measures the spin component $\mathbf{n}\cdot\mathsf{S}$ along the direction $\mathbf{n}$. The construction requires that arbitrary static electric and magnetic fields, consistent with Maxwell's equations, can be created in the laboratory. To construct an apparatus app(H_A) means to identify a spin Hamiltonian $\mathsf{H}(\mathbf{r},\mathsf{S})$ which splits an incoming beam of particles with spin s into subbeams corresponding to the eigenvalues A_n. The most general Hamiltonian acting on the Hilbert space $\mathcal{H}$ of a spin s reads

$$\mathsf{H}(\mathbf{r},\mathsf{S}) = \sum_{\nu=0}^{N^2-1} \Phi_\nu(\mathbf{r})\mathsf{T}_\nu \,, \tag{5}$$

with traceless (except for $\nu = 0$) symmetric expansion coefficients $\Phi_\nu(\mathbf{r})(\equiv \Phi^{(k)}_{j_1 j_2 \ldots j_k}(\mathbf{r}))$ which vary in space. Tune the electric and magnetic fields in such a way that the coefficients $\Phi_\nu(\mathbf{r})$ and its first derivative with respect to some spatial direction, r_1, say, satisfy

$$\Phi_\nu(\mathbf{r}=0) = \frac{\partial\Phi_\nu(\mathbf{r}=0)}{\partial r_1} = \mathsf{a}_n \,. \tag{6}$$

This is always possible with realistic fields satisfying Maxwell's equations. Then, the Hamiltonian in (5) has two important properties. (i) At the origin, $\mathbf{r} = 0$, it coincides with the matrix H_A. (ii) Suppose that a beam of particles with spin s enters the generalized Stern-Gerlach apparatus app(H_A) just described. At its center, particles in an eigenstate $|A_n\rangle$, say, will experience a force in the r_1 direction given (up to second order in distance from the center) by

$$F_1(\mathbf{r}=\mathbf{0}) = -\frac{\partial\langle A_n|\mathsf{H}(\mathbf{r}=0,\mathsf{S})|A_n\rangle}{\partial r_1} = -A_n \,, \qquad n = 1,\ldots,2s+1 \,. \tag{7}$$

Consequently, particles with a spin projected onto one of the eigenstates $|A_n\rangle$ of the operator H_A are separated spatially by this apparatus. The procedure is entirely analogous to that for a spin 1/2 where a familiar Stern-Gerlach apparatus is used (see [7] for details).

Ad 4: The 'projection postulate' of quantum mechanics describes the effect of measuring an observable $\widehat{B}$ on a system $\mathcal{S}$ by means of an apparatus app$(\widehat{B})$. If the system is prepared initially in a state with density matrix $\hat{\rho}$ one has:

$$\text{app}(\widehat{B}): \quad \hat{\rho} \quad \xrightarrow{p_n} \quad (B_n;\hat{\rho}_n) \,, \qquad p_n = \text{Tr}\,[\hat{\rho}\hat{\rho}_n] \,. \tag{8}$$

The action of the apparatus is, with probability p_n, to throw the system into an eigenstate $\hat{\rho}_n \equiv |B_n\rangle\langle B_n|$ of the observable $\widehat{B}$; the *outcome* of the measurement is given by the associated eigenvalue B_n. By the way, the notion of 'collapse' or 'projection' can be avoided by characterizing the process indirectly by refering to "repeatable measurements" [9].

The outcome of an *individual* measurement cannot be predicted due to the probabilistic character of quantum mechanics. Therefore, the *probabilities* p_n, resulting from (infinitely often) repeated measurements on identically prepared systems, represent the essential link between theory and experiment. They provide information about the state of the system conditioned by the selected observable. Thus, a measurement reveals (or confirms) properties of the *state* $\hat{\rho}$ of the system while the observable $\widehat{B}$ at hand is assumed to be known, including its eigenstates and eigenvalues. To put it differently, the observable defines the *scope* of the possible results of a measurement: the only possible outcomes are its eigenvalues B_n, and, directly after the measurement the system necessarily resides in the corresponding state $|B_n\rangle$.

As the occurrence of the eigenvalues is purely probabilistic, one needs to repeat the experiment until all values A_n have been obtained. If the spin s is prepared initially in a homogeneous mixture, $\hat{\rho} = \mathsf{E}/(2s+1)$, the $(2s+1)$ possible outcomes occur with equal probability. The probability not to have obtained one specific value A_n after $N_0 \gg N$ measurements equals $1/(2s+1)^{N_0}$, decreasing exponentially with N_0.

Ad 5: It would be very convenient now to 'read out' directly the quantum state $\hat{\rho}_n$ obtained from a single measurement with result A_n. However, due to the no-cloning theorem [10, 11], an unknown state cannot be determined if only one copy of it is available. Upon repeating the measurement a large number of times and keeping only those states with the *same* eigenvalue A_n, one produces an *ensemble* of systems prepared identically in the state $\hat{\rho}_n$. This is sufficient to reconstruct an unknown state since a density matrix $\hat{\rho}$ can be written as

$$\hat{\rho} = \frac{1}{N} \sum_{\mu=1}^{N^2} P_\mu \widehat{Q}^\mu \,, \qquad N = 2s+1 \,, \tag{9}$$

where the coefficient $P_\mu \equiv \langle \mathbf{n}_\mu | \hat{\rho} | \mathbf{n}_\mu \rangle$ is the probability to find the system in a coherent spin state $|\mathbf{n}_\mu\rangle$. The operators $\widehat{Q}^\mu, \mu = 1, \ldots, N^2$, form a basis for hermitian operators, similar to but different from the multipoles T_ν [12]. Thus, Eq. (9) parametrizes $\hat{\rho}$ by expectation values P_μ which can be measured by a standard Stern-Gerlach apparatus.-

In sum, the basic ingredient of quantum diagonalization is the 'collapse' of the wave function projecting any state onto a randomly selected eigenstate of the measured observable. Generalizations of this approach are expected to include the diagonalization of unitary matrices and the determination of roots of polynomials.

Usually, a measurement is thought to confirm or reveal some information about the state of the system. Here, on the contrary, the idea is to learn something about the

measured observable instead. Why is this possible? It is fundamental to realize that the *input* required to actually measure $\widehat{A}$ differs from the *output* of the experiment: for a measurement of $\widehat{A}$, the construction of an apparatus app($\widehat{A}$) is sufficient which is *possible without*knowing eigenvalues and eigenstates of $\widehat{A}$. Necessarily, after a measurement partial information about the spectral properties of the observable $\widehat{A}$ is available according to (8). This is due to the constraints (i) that the possible outcomes of measuring $\widehat{A}$ are its eigenvalues and (ii) that the system subsequently will occupy the corresponding eigenstate. Thus, if the eigenstates and eigenvalues of $\widehat{A}$ not known initially, one indeed acquires information about them by measuring $\widehat{A}$.

The quantum mechanical diagonalization appears to be neither an analog nor a digital calculation. It is not based on the representation of a mathematical equation in terms of a physical system which then would 'simulate' it. Similarly, no 'software program' is executed which would implement an diagonalization algorithm. One might best describe the measuring device app(H_A) as a 'special purpose machine' based on the projection postulate.

For the time being, the method introduced here is important from a conceptual but not a technological point of view. On the one hand, the diagonalization of matrices is not a hard problem such as factorization of large integer numbers; on the other, the actual implementation in the laboratory is challenging. It is important, however, that there is no physical principle which would forbid the construction of such a machine. Further, it is expected to be fruitful from a conceptual point of view since it provides a different perspective on the projection postulate [13]. Quantum diagonalization as introduced here shows that—in an unexpected way—standard quantum mechanics attributes *computational power* to the measurement of an observable. The fact that one can use a measurement to perform calculations might turn into an argument in favor of the 'reality' of the quantum mechanical projection postulate.

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