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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*: Hermitean $(N \times N)$ matrices can be diagonalized, in principle, by performing appropriate quantum mechanical measurements. 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 the underlying working principle is the 'collapse of the wavefunction' associated with a measurement, the procedure is neither a digital nor an analogue calculation—it defines thus a new example of a *quantum mechanical* method of computation.

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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 counter-intuitive but 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 factor large integers much more efficiently than any presently

known classical algorithm [3]. Throughout, these techniques make use of the *measurement* of quantum mechanical observables as an unquestioned tool. This is also true for many (but not all [4]) proposals of *quantum error correction* schemes [5, 6], necessary to let a 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. As shown below, it can be used to solve explicitly at least one specific computational task, namely to determine eigenvalues and, *a fortiori*, eigenstates 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 $\hat{A}$ 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 $\hat{A}\,|a_n\rangle = a_n|a_n\rangle$. 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 [7] 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 $\mathsf{A}_{kk'} = \langle k|\hat{A}|k'\rangle$ determine the operator $\hat{A}$ 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 $\hat{A}$ if the characteristic polynomial $P_A(\lambda)$ of the matrix A vanishes, $P_A(\lambda) = \det(\mathsf{A} - \lambda\mathsf{I}) = 0$, where I 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

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

provide the eigenvectors $|a_n\rangle$ in the basis $|k\rangle$. Analytic expressions for the eigenvalues a_n in terms of the matrix elements $\mathsf{A}_{kk'}$ exist only if $N \leqslant 4$. 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 (of a particle) is described correctly by non-relativistic quantum mechanics. This method exploits the 'collapse of the wavefunction' as a 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 in a condensed form first; subsequently, five comments explain various technical details.

Step 1. *Standard form of* A. Write the Hermitean $(N \times N)$ matrix A as a combination of linearly independent Hermitean *multipole* operators T_ν, $\nu = 0, \ldots, N^2 - 1$,

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

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

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

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

Step 3. *Setting up a measuring device*. Identify and construct an apparatus app(H_A) suitable to measure the observable H_A.

Step 4. *Determination of the eigenvalues*. Carry out measurements with the apparatus app(H_A) on a spin s prepared in a homogeneous mixture $\hat{\rho} = \mathsf{I}_s/(2s+1)$. The output of each individual

measurement will be one of the eigenvalues a_n of the matrix A. After sufficiently many repetitions, all eigenvalues will be known.

Step 5. *Determination of the eigenstates*. Calculate the eigenstates $|a_n\rangle$ of the matrix A by means of equation (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 zeros 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 expand on the background necessary to perform steps 1–5. Emphasis will be both on the construction of a device measuring a given Hermitean operator (step 3) and on the working of a quantum mechanical measurement (step 4).

Ad 1. Consider a Hilbert space $\mathcal{H}_s$ of dimension $N = (2s + 1)$ 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. Multipole operators $\mathsf{T}_{j_1 j_2 \cdots j_\sigma}$, are defined as the symmetrized products $\mathsf{S}_{j_1}\mathsf{S}_{j_2}\cdots\mathsf{S}_{j_\sigma}$, $j_i = 1, 2, 3$, and $\sigma = 0, 1, \ldots, 2s$, after subtracting off the trace, except for $\mathsf{T}_0 \equiv \mathsf{T}^{(0)} = \mathsf{I}_s$, the $(N \times N)$ unit matrix. The index σ labels $(2s + 1)$ classes with $(2\sigma + 1)$ elements transforming among themselves under rotations. Explicitly, the lowest multipoles read

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

For the sake of brevity, a collective index $\nu \equiv (\sigma; j_1, \ldots, j_k)$ is introduced now, taking on the values $\nu = 0, 1, \ldots, N^2 - 1$. The N^2 self-adjoint multipole operators $\mathsf{T}_\nu = \mathsf{T}^\dagger_\nu$ form a basis in the space of Hermitean operators acting on the N-dimensional Hilbert space $\mathcal{H}_s$ [8]. Two multipoles are orthogonal with respect to a scalar product defined as the trace of their product: $(1/N)\,\mathrm{Tr}\,[\mathsf{T}_\nu \mathsf{T}_{\nu'}] = \delta_{\nu\nu'}$.

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 $\hat{B}$ comes along with an apparatus app$(\hat{B})$ capable of measuring it [9]. For particle systems, setting up such a device remains a challenging task for an experimenter while the situation is more favourable for spin systems.

Swift and Wright [8] 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 $\boldsymbol{n}\cdot\mathsf{S}$ along the direction $\boldsymbol{n}$. 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 $\mathsf{H}(\boldsymbol{r}, \mathsf{S})$ 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 $\mathcal{H}_s$ of a spin s reads

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

with traceless mutltipoles (except for $\nu = 0$), and totally symmetric expansion coefficients $\Phi_\nu(\boldsymbol{r})(\equiv \Phi^{(\sigma)}_{j_1 j_2 \ldots j_\sigma}(\boldsymbol{r}))$ which vary in space. Tune the electric and magnetic fields in such a way that the coefficients $\Phi_\nu(\boldsymbol{r})$ and their first derivatives with respect to some spatial direction,

r_1, say, satisfy (in appropriately chosen units)

$$\Phi_\nu(\boldsymbol{r})|_{r=0} = \mathsf{a}_\nu \qquad \text{and} \qquad \left.\frac{\partial \Phi_\nu(\boldsymbol{r})}{\partial r_1}\right|_{r=0} = \mathsf{a}_\nu. \tag{6}$$

As shown explicitly in [8], this is always possible with realistic fields satisfying Maxwell's equations. Then, the Hamiltonian in (5) has two important properties. (i) At the origin, $\boldsymbol{r} = 0$, it coincides with the matrix H_A in equation (3). (ii) Suppose that a beam of particles with spin s enters the generalized Stern–Gerlach apparatus app(H_A) just described. At its centre, 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 centre) by

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

Consequently, this apparatus can spatially separate particles with a spin projected onto one of the eigenstates $|a_n\rangle$ of the operator H_A, with a separation proportional to the eigenvalue a_n. The working principle is entirely analogous to that of a familiar Stern–Gerlach apparatus for a spin 1/2 (see [8] for more details).

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

$$\text{app}(\hat{B}): \quad \hat{\rho} \quad \xrightarrow{p_n} \quad \big(b_n;\hat{\rho}_n\big) \qquad p_n = \text{Tr}\left[\hat{\rho}\hat{\rho}_n\right]. \tag{8}$$

In words, the action of the apparatus is, with probability p_n, to throw the system prepared in state $\hat{\rho}$ into an eigenstate $\hat{\rho}_n \equiv |b_n\rangle\langle b_n|$ of the observable $\hat{B}$; the *outcome* of the measurement will be the associated eigenvalue b_n. As a matter of fact, the notion of 'collapse' or 'projection' can be avoided if one characterizes the process indirectly by referring to 'repeatable measurements' [10].

As is well known, the outcome of an *individual* measurement cannot be predicted due to the probabilistic character of quantum mechanics, and it is necessary to repeat the experiment a number of times until *all* values a_n have been obtained. If the spin s is prepared initially in a homogeneous mixture, $\hat{\rho} = \mathsf{I}_s/(2s+1)$, the $(2s+1)$ possible outcomes will occur with equal probability. The probability *not* to have obtained one specific value a_n after $N_0 \gg N$ measurements equals $(2s/2s+1)^{N_0} \simeq \exp[-N_0/2s]$, decreasing exponentially with N_0.

Ad 5. It would be convenient 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 [11, 12], an unknown state cannot be determined if only one copy 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 in the state $\hat{\rho}_n$. This is sufficient to experimentally reconstruct an unknown state since a density matrix $\hat{\rho}$ can be written as

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

where the coefficient $P_\mu \equiv \langle \boldsymbol{n}_\mu|\hat{\rho}|\boldsymbol{n}_\mu\rangle$ is the probability to find the system in a coherent spin state $|\boldsymbol{n}_\mu\rangle$. As shown in [13], the operators [13] $\hat{Q}^\mu, \mu = 1,\ldots,N^2$, form a basis for Hermitean operators, similar to but different from the multipoles T_ν. Thus, equation (9) parametrizes $\hat{\rho}$ by expectation values P_μ which can be measured by a standard Stern–Gerlach apparatus.

Let us turn to the discussion of the idea underlying quantum diagonalization. Traditionally, a measurement is thought to confirm or reveal some information about the *state* of the system.

The probabilities p_n 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 $\hat{B}$ 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 $|b_n\rangle$.

In the present context, however, the idea is to extract information about the measured *observable*—not about the state $\hat{\rho}$. Why is this possible at all? It is fundamental to realize that the *input* needed to set up a measurement of $\hat{A}$ and to actually measure it is different from the *output* of the experiment. In order to measure the observable $\hat{A}$, the construction of an apparatus app($\hat{A}$) is sufficient—and its construction is indeed possible *without* knowing eigenvalues and eigenstates of $\hat{A}$ beforehand. After a measurement, however, partial information about the spectral properties of the observable $\hat{A}$ is available according to (8). This is due to the constraints (i) that the possible outcomes of measuring $\hat{A}$ are its eigenvalues and (ii) that the system subsequently will reside in the corresponding eigenstate. Thus, if the eigenstates and eigenvalues of $\hat{A}$ are *not* known initially, information about them indeed emerges by measuring $\hat{A}$.

The quantum mechanical diagonalization appears to be neither an analogue 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, even though the outcome will be read on an analogue scale. Further, *no* 'software program' is executed which would implement a 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 necessarily from 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 just as it is to set up a full-fledged quantum computer. It must be stressed, however, that there is no physical principle which would forbid to build such machines.

Further, quantum diagonalization is expected to be fruitful from a conceptual point of view since it provides a different perspective on the projection postulate [16]. It 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 favour of the 'reality' of the quantum mechanical projection postulate.

What is the relation of quantum diagonalization to other research in quantum computing? Various well-established quantum algorithms can be cast in a form which asks for the determination of eigenvalues of unitary operators [14] representing the action of a network on some initial state. The result of the calculation is encoded in the *phase* of the output state. Subsequently, measurements are necessary to read off the result but their role in the algorithm is different: the *calculation* has already been performed—and the measurement itself is *not* the working principle. Further, it has been pointed out in [15] how to use an ideal quantum computer to effectively simulate another quantum system. As indicated briefly, such a device would be a useful tool to measure arbitrary observables, in a spirit somewhat similar to the method presented here.

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

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