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From: *C. M. Caves*
Subject: **Constructing an orthonormal basis from an arbitrary basis**
1996 May 23

Consider an arbitrary set of basis vectors $|\phi_k\rangle$ (linearly independent vectors that span a vector space). There are many ways—e.g., Gram-Schmidt orthogonalization—to construct an orthonormal basis from this arbitrary basis. The aim here is to give a procedure that is *democratic* in the sense that it treats all the vectors $|\phi_k\rangle$ on the same footing.

Define the operator

$$\hat{G} \equiv \sum_k |\phi_k\rangle\langle\phi_k| \; . \tag{1}$$

This operator is manifestly positive, because

$$\langle\psi|\hat{G}|\psi\rangle = \sum_k |\langle\phi_k|\psi\rangle|^2 \geq 0 \; , \tag{2}$$

and thus has a positive square root $\hat{G}^{1/2}$. Moreover, it is easy to show that $\hat{G}$ is positive definite. Any vector $|\psi\rangle$ can be expanded (uniquely) as

$$|\psi\rangle = \sum_k c_k|\phi_k\rangle \; , \tag{3}$$

which implies that

$$\langle\psi|\psi\rangle = \sum_k c_k\langle\psi|\phi_k\rangle \; . \tag{4}$$

Suppose that a vector $|\psi\rangle$ satisfies

$$0 = \langle\psi|\hat{G}|\psi\rangle = \sum_k |\langle\phi_k|\psi\rangle|^2 \; . \tag{5}$$

This implies that $\langle\phi_k|\psi\rangle = 0$ for all k. Hence, from (4), we have that $\langle\psi|\psi\rangle = 0$, which implies that $|\psi\rangle = 0$. Thus $\hat{G}$ is positive definite, which means that its square root has an inverse $\hat{G}^{-1/2}$.

Now notice that

$$\hat{1} = \hat{G}^{-1/2}\hat{G}\hat{G}^{-1/2} = \sum_k |\psi_k\rangle\langle\psi_k| \; , \tag{6}$$

where

$$|\psi_k\rangle \equiv \hat{G}^{-1/2}|\phi_k\rangle \; . \tag{7}$$

Any vectors $|\psi_k\rangle$ that satisfy the completeness condition (6) span the space, for an arbitrary vector $|\psi\rangle$ can be expanded as

$$|\psi\rangle = \sum_k |\psi_k\rangle\langle\psi_k|\psi\rangle \; . \tag{8}$$

Moreover, the linear independence of the original basis vectors $|\phi_k\rangle$ implies immediately that the vectors $|\psi_k\rangle$ are linearly independent. Linearly independent vectors that satisfy the completeness condition are orthonormal, for the uniqueness of the expansion

$$|\psi_l\rangle = \sum_k |\psi_k\rangle\langle\psi_k|\psi_l\rangle \tag{9}$$

implies that

$$\langle\psi_k|\psi_l\rangle = \delta_{kl} \ . \tag{10}$$

Thus the vectors $|\psi_k\rangle$ make up an orthonormal basis.

I learned this procedure from Ben Schumacher, who extracted it from the ρ-distortion technique introduced by Hughston, Jozsa, and Wootters. The procedure could be used, for example, to convert a basis of nonorthogonal vectors localized on phase space into an orthonormal basis of localized vectors.