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Entropy when density operator has zero eigenvalues

In the class notes and the text [1] the Von Neumann entropy is defined as

$$S = -\operatorname{Tr} \rho \ln \rho. \tag{1.1}$$

In one of our problems I had trouble evaluating this, having calculated a density operator matrix representation

$$\rho = E \wedge E^{-1}, \tag{1.2}$$

where

$$E = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \tag{1.3}$$

and

$$\wedge = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}. \tag{1.4}$$

The usual method of evaluating a function of a matrix is to assume the function has a power series representation, and that a similarity transformation of the form $A = E \wedge E^{-1}$ is possible, so that

$$f(A) = E f(\wedge) E^{-1}, \tag{1.5}$$

however, when attempting to do this with the matrix of eq. (1.2) leads to an undesirable result

$$\ln \rho = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} \ln 1 & 0 \\ 0 & \ln 0 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \tag{1.6}$$

The $\ln 0$ makes the evaluation of this matrix logarithm rather unpleasant. To give meaning to the entropy expression, we have to do two things, the first is treating the trace operation as a higher precedence than the logarithms that it contains. That is

$$\begin{aligned} -\operatorname{Tr}(\rho \ln \rho) &= -\operatorname{Tr}(E \wedge E^{-1} E \ln \wedge E^{-1}) \\ &= -\operatorname{Tr}(E \wedge \ln \wedge E^{-1}) \\ &= -\operatorname{Tr}(E^{-1} E \wedge \ln \wedge) \\ &= -\operatorname{Tr}(\wedge \ln \wedge) \\ &= -\sum_k \wedge_{kk} \ln \wedge_{kk}. \end{aligned} \tag{1.7}$$

Now the matrix of the logarithm need not be evaluated, but we still need to give meaning to $\wedge_{kk} \ln \wedge_{kk}$ for zero diagonal entries. This can be done by considering a limiting scenerio

$$\begin{aligned} -\lim_{a \to 0} a \ln a &= -\lim_{x \to \infty} e^{-x} \ln e^{-x} \\ &= \lim_{x \to \infty} x e^{-x} \\ &= 0. \end{aligned} \tag{1.8}$$

The entropy can now be expressed in the unambiguous form

$$\boxed{S = -\sum_{\wedge_{kk} \neq 0} \wedge_{kk} \ln \wedge_{kk}.} \tag{1.9}$$

Bibliography

[1] Jun John Sakurai and Jim J Napolitano. *Modern quantum mechanics*. Pearson Higher Ed, 2014. 1