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# Quantum-mechanical proof of a Redheffer inequality

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An alternate proof, with minor restrictions, of the "Weyl-type" inequality of Redheffer is given using tools of chemists' quantum mechanics and Hilbert space instead of mathematicians' real analysis.

Redheffer unveiled many different inequalities in an important paper in 1966 [1]. One of these, "of the Weyl-type", has applications in bounding expectation values in quantum mechanics [2,3]. In light of these applications, we present a quantum-mechanical proof of this inequality, with minor restrictions.

We begin with any two non-commuting self-adjoint operators, $A$ and $B$, and any function, $\psi$, in the domain of both $AB$ and $BA$:

$$\begin{aligned}\langle\psi|[A,B]|\psi\rangle &= \langle\psi \mid AB\psi\rangle - \langle\psi \mid BA\psi\rangle \\ &= \langle\psi \mid AB\psi\rangle - \langle(BA)^\dagger\psi \mid \psi\rangle \\ &= \langle\psi \mid AB\psi\rangle - \langle A^\dagger B^\dagger\psi \mid \psi\rangle \\ &= \langle\psi \mid AB\psi\rangle - \langle AB\psi \mid \psi\rangle \\ &= \langle\psi \mid AB\psi\rangle - \langle\psi \mid AB\psi\rangle^*, \end{aligned} \tag{1}$$

where $A^\dagger$ denotes the adjoint operator of $A$. From here we cannot reproduce Redheffer's result, although we can reach a simplification of it if we restrict our operators and function to be real. The expectation values in (1) are then real, and thus, $\langle\psi|[A,B]|\psi\rangle = 0$ despite the fact that $[A,B] \neq 0$.

We define the following self-adjoint operators, with reference to the radial domain $r \in [0,\infty)$ of the three-dimensional space, and their commutator

$$A = \Delta_r = \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}r^2\frac{\mathrm{d}}{\mathrm{d}r}, \qquad B = f(r) \text{ such that } f' \geqslant 0, \tag{2}$$

$$[A,B] = \left[\Delta_r, f(r)\right] = f'' + 2f'\frac{\mathrm{d}}{\mathrm{d}r} + 2r^{-1}f', \tag{3}$$

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where all the primes indicate differentiation with respect to $r$. Taking the expectation value of the commutator (3) with any function $\psi$ in the domain of $AB$ and $BA$ with the integration weight $r^2$ gives zero (let $g = f'$):

$$\int_0^\infty \big(g'r^2 + 2gr\big)\psi^2 \,\mathrm{d}r + 2\int_0^\infty \psi g\psi' r^2 \,\mathrm{d}r = 0. \tag{4}$$

The Schwartz inequality gives the following:

$$\begin{aligned} \left|\int_0^\infty \psi g\psi' r^2 \,\mathrm{d}r\right| &= \left|\int_0^\infty \psi g_1^{1/2} g_2^{1/2}\psi' r^2 \,\mathrm{d}r\right| \\ &\leqslant \left(\int_0^\infty g_1\psi^2 r^2 \,\mathrm{d}r\right)^{1/2}\left(\int_0^\infty g_2\big(\psi'\big)^2 r^2 \,\mathrm{d}r\right)^{1/2}, \end{aligned} \tag{5}$$

$$g = g_1^{1/2} g_2^{1/2}, \quad \text{where } g = f',\ g_1, g_2 \geqslant 0.$$

Combining (4) and (5) gives:

$$\left|\int_0^\infty \big(g'r^2 + 2rg\big)\psi^2 \,\mathrm{d}r\right| \leqslant 2\left(\int_0^\infty g_1\psi^2 r^2 \,\mathrm{d}r\right)^{1/2}\left(\int_0^\infty g_2\big(\psi'\big)^2 r^2 \,\mathrm{d}r\right)^{1/2}. \tag{6}$$

Making the substitutions $g_1 = hw^2/r^2$ and $g_2 = h/r^2$ (note that $h \geqslant 0$) in (6) we arrive at

$$\left|\int_0^\infty (hw)'\psi^2 \,\mathrm{d}r\right| \leqslant 2\left(\int_0^\infty hw^2\psi^2 \,\mathrm{d}r\right)^{1/2}\left(\int_0^\infty h\big(\psi'\big)^2 \,\mathrm{d}r\right)^{1/2}, \tag{7}$$

which is remark 7 in Redheffer's paper [1] except that we have integration over the entire domain of the variable $r$, while remark 7 holds for arbitrary limits. Letting $h = r^{2n}$, $w = r^{m-n}$, the following inequality (also given by Redheffer) is obtained:

$$\left|\int_0^\infty r^{m+n-1}\psi^2 \,\mathrm{d}r\right| \leqslant \frac{2}{m+n}\left(\int_0^\infty r^{2m}\psi^2 \,\mathrm{d}r\right)^{1/2}\left(\int_0^\infty r^{2n}\big(\psi'\big)^2 \,\mathrm{d}r\right)^{1/2}. \tag{8}$$

This is the form used in quantum mechanics to bound radial expectation values and one-electron kinetic energies. On the positive side our proof is much simpler to chemists than Redheffer's because it makes use of methods common to chemists; we avoid the mathematical notions of absolute continuity and suitability that Redheffer uses, although there are constraints on $\psi$ implicit in the domain considerations of $AB$ and $BA$. On the negative side our result is less versatile because the integration is over the entire domain of $r$. This must be so in our derivation because we require that the operators $A$ and $B$ must be self-adjoint. Changing the domain of an operator is equivalent to changing the operator, and thus changing the *adjoint* operator, so that the resulting operator and its adjoint may not be the same. This downside is of little consequence to chemists, however, since the main use of the Redheffer inequality is to bound expectation values for which the integration must be over all space.

Finally we note that in our derivation the only restriction on $h$ and $w$, which are derived from the operator $f$, is that $f\psi$ be in the domain of $A$. Redheffer restricts $h$ and $w$ to be integrable in remark 7 of [1]; however, this appears to be unnecessary since he proceeds to derive (8) from (7) in the same manner as above (he also applies the restriction $-m < n \leqslant m + 1$), in which $h$ and $w$ are *not* integrable.

## References

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