THE EFFECTIVE POTENTIAL $1/u$

We define u as the solution of:

$$\hat{H}u = -\frac{\hbar^2}{2m}\ \Delta u + Vu = 1\ . \tag{1}$$

Inspired by Agmon's work [1, 2], any function V satisfying

$$\langle\psi|\hat{H}|\psi\rangle \geq \langle\psi|\hat{V}|\psi\rangle\ \ , \tag{2}$$

for any quantum state ψ can be used to define a distance whose exponential governs the decay of the eigenfunction in the places where the potential V is larger than the state energy E (the "barriers" of V). We give here a sketch of the proof showing that $W = 1/u$, where u is as in Eq. 1, satisfies this inequality. To do so, we write $\psi = u\varphi$, which yields:

$$\begin{aligned}
\langle\psi|\hat{H}|\psi\rangle &= \langle u\varphi|\ \hat{p}^2 + \hat{V}\ |u\varphi\rangle = \langle u\varphi|\ \hat{p}^2\,(u\varphi) + Vu\varphi\rangle \\
&= \langle u\varphi\ |\ \varphi\ \hat{p}^2 u + u\ \hat{p}^2\varphi + 2\hat{p}u\ \hat{p}\varphi + Vu\varphi\rangle \\
&= \langle u\varphi\ |\ \varphi + u\ \hat{p}^2\varphi + 2\ \hat{p}u\ \hat{p}\varphi\rangle \\
&= \langle u\varphi|\frac{1}{u}\ u\varphi\rangle + \langle u\varphi|\frac{1}{u}\ \left(u^2\ \hat{p}^2\varphi + 2u\ \hat{p}u\ \hat{p}\varphi\right)\rangle \\
&= \langle\psi|\hat{W}|\psi\rangle + \langle\varphi|\hat{p}\left(u^2\hat{p}\varphi\right)\rangle \\
&= \langle\psi|\hat{W}|\psi\rangle + \langle\hat{p}\varphi|\widehat{u^2}|\hat{p}\varphi\rangle \\
&= \langle\psi|\hat{W}|\psi\rangle + \left\langle u\ \hat{p}\frac{\psi}{u}\ \middle|\ u\ \hat{p}\frac{\psi}{u}\right\rangle \geq \langle\psi|\hat{W}|\psi\rangle\ \ .
\end{aligned}$$

This proves that $1/u$ can be used as an effective confining potential to build an Agmon distance governing the exponential decay of the wavefunctions.

[1] S. Agmon, *Lectures on exponential decay of solutions of second-order elliptic equations: bounds on eigenfunctions of N-body Schrödinger operators*, Mathematical Notes, Vol. 29 (Princeton University Press, Princeton, New Jersey, 1982).

[2] S. Agmon, Lecture Notes in Mathematics **1159**, 1 (1985).