Large D limit for excited states of a hydrogen atom

I. FORMULATION OF THE PROBLEM

We are going to prove that as $D \to \infty$,

$$E \sim V_{\min}, \tag{1}$$

where E is the energy and $V_{\min}$ is the minimum of the function

$$V_{\text{eff}}(r) = \frac{n^2}{2r^2} - \frac{1}{r} \tag{2}$$

at $r > 0$. In equation (2), n is the principal quantum number.

A. Definition of principal quantum number in D dimensions

In three dimensions, the principal quantum number of a given quantum state is usually defined as a sum of "orbital quantum number" and "radial quantum number" plus one, i.e.

$$n = l + n_r + 1, \tag{3}$$

or alternatively just as $1/\sqrt{-2E}$. If we adopt the latter definition of the principal quantum number in D dimensions, i.e.

$$n = \frac{1}{\sqrt{-2E}}, \tag{4}$$

then there is nothing to prove, since obviously the function (2) has a minimum

$$V_{\min} = -\frac{1}{2n^2} = E \tag{5}$$

at the point

$$r_{\min} = n^2. \tag{6}$$

We adopt here the following equivalent definition of the quantum number n,

$$n = l + n_r + \frac{D-1}{2}, \tag{7}$$

where n_r is the number of positive roots of the radial wavefunctions, and l is some sort of generalization of orbital quantum number to D dimensions.

To avoid complications related to angular momentum in arbitrary dimensions, we consider here only the case of zero angular momentum ($l = 0$) by solving the problem inside a subspace of radially-symmetric wavefunctions. Without knowledge of the form of exact solution, we find in Section IV that asymptotically at large D, $E/V_{\min} \to 1$, or more precisely $E/V_{\min} - 1 \sim o(1/n)$. In fact, if we would know the energy exactly, we could see that $E = V_{\min}$, but the strength of current approach is the proof *without* solving the equation exactly.

II. RADIAL SCHRÖDINGER EQUATION

We assume that the function $\psi(r)$ depends only on one variable which is radius $r = \left(\boldsymbol{r}^2\right)^{1/2}$. Derivatives of the wave function are as follows,

$$\begin{aligned} \frac{\partial\psi(r)}{\partial r_i} &= \frac{r_i}{r}\psi'(r), \\ \frac{\partial^2\psi(r)}{\partial r_i^2} &= \frac{1}{r}\psi'(r) + \frac{r_i^2}{r^2}\left(\psi''(r) - \frac{1}{r}\psi'(r)\right). \end{aligned} \tag{8}$$

Using (8), the kinetic energy is expressed as

$$-\frac{\boldsymbol{\nabla}^2}{2}\psi(r) = -\frac{1}{2}\sum_{i=1}^{D}\frac{\partial^2\psi(r)}{\partial r_i^2} = -\frac{1}{2}\left[\psi''(r) + \frac{D-1}{r}\psi'(r)\right]. \tag{9}$$

Thus, the Schrödinger equation is reduced to a differential equation in one variable r,

$$-\frac{1}{2}\left[\psi''(r)+\frac{D-1}{r}\psi'(r)\right]-\frac{1}{r}\psi(r)=E\psi(r), \tag{10}$$

where we use units where $\hbar=m=1$.

It is convenient to introduce "radial" function $P(r)=r^{\frac{D-1}{2}}\psi(r)$ and to rewrite equation (10) in an equivalent form without linear derivatives,

$$-\frac{1}{2}\frac{d^2P}{dr^2}+\left[\frac{(D-1)(D-3)}{8r^2}-\frac{1}{r}-E\right]P(r)=0. \tag{11}$$

Using equation (7), we express D through n as $D=2n-2n_r+1$ and find that

$$\frac{(D-1)(D-3)}{8r^2}=\frac{(n-n_r)(n-n_r-1)}{2r^2}. \tag{12}$$

III. SCALING TRANSFORMATION

Let us perform scaling transformation $r=n^2(1+n^{-1/2}x)$. Scaled wave function y is defined as

$$y(x)=P\left(n^2(1+n^{-1/2}x)\right). \tag{13}$$

Then,

$$\frac{d^2P}{dr^2}=n^{-3}\frac{d^2y}{dx^2}, \tag{14}$$

where l.h.s. is calculated at the point $r=n^2(1+n^{-1/2}x)$.

We rewrite

$$\frac{(n-n_r)(n-n_r-1)}{2r^2}-\frac{1}{r}-E=\frac{(r-n^2)^2}{2n^2r^2}-\frac{(2n_r+1)n}{2r^2}+\frac{n_r(n_r+1)}{2r^2}-\widetilde{E}, \tag{15}$$

where

$$\widetilde{E}=E+\frac{1}{2n^2}. \tag{16}$$

Now, we express each term in equation (15) through a new variable x,

$$\frac{(r-n^2)^2}{2n^2r^2} = n^{-3}\frac{x^2}{2(1+n^{-1/2}x)^2}, \tag{17}$$

$$-\frac{(2n_r+1)n}{2r^2} = -n^{-3}\frac{2n_r+1}{2(1+n^{-1/2}x)^2}, \tag{18}$$

$$-\frac{n_r(n_r+1)}{2r^2} = n^{-4}\frac{n_r(n_r+1)}{2(1+n^{-1/2}x)^2}. \tag{19}$$

After multiplying equation (11) by n^3 and using (13) - (19), we find

$$\left[-\frac{1}{2}\frac{d^2}{dx^2} + \frac{x^2}{2(1+n^{-1/2}x)^2} - \frac{n_r+1/2}{(1+n^{-1/2}x)^2} + n^{-1}\frac{n_r(n_r+1)}{2(1+n^{-1/2}x)^2} - \epsilon\right] y(x) = 0, \tag{20}$$

where

$$\epsilon \equiv n^3\widetilde{E} = n^3E + \frac{n}{2} = -\frac{n}{2}\left(\frac{E}{V_{\min}} - 1\right). \tag{21}$$

IV. LARGE-n LIMIT OF SCALED SCHRÖDINGER EQUATION

In the limit of $n \to \infty$, equation (20) reads

$$\left[-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2 - (n_r+1/2) - \epsilon_\infty\right] y_\infty(x) = 0. \tag{22}$$

It is the equation for a harmonic oscillator shifted by a constant $-(n_r+1/2)$ on the energy scale. It is known that the oscillator's energy eigenvalue equals to $n_r+1/2$. After adding the extra constant $-(n_r+1/2)$, we obtain $\epsilon_\infty = 0$. Thus, we proved that

$$n\left(\frac{E}{V_{\min}} - 1\right) \to 0, \tag{23}$$

i.e. $E/V_{\min} - 1 \sim o(1/n)$.

Note that in this scaling, the large-n limit is a regular function which is an eigenfunction of the harmonic oscillator (not a δ-function).