§1. Bootstrapping Method in QM (Arxiv 2108.08757)

Let $|E\rangle$ be the eigenvector of the Hamiltonian H.

$$H|E\rangle = E|E\rangle \qquad eq(1.1)$$

$\Rightarrow \langle E|[\mathcal{O}, H]|E\rangle = 0$ for any operator $\mathcal{O}$

Consider $H = \frac{1}{2m}p^2 + V(x)$ for 1-dimensional case.
Set $m = \hbar = 1$ in the following derivation, i.e.,

$$[x, p] = i \quad , \quad p \to -i\frac{\partial}{\partial x}$$

Now consider $\mathcal{O} = x^{s+1}p$

$$\Rightarrow \langle E|[x^{s+1}p, H]|E\rangle = 0 \qquad eq(1.2)$$

$$[x^{s+1}p, H]$$

$$= [x^{s+1}p, \tfrac{1}{2}p^2 + V(x)]$$

$$= \frac{1}{2}x^{s+1}p^3 + \underbrace{x^{s+1}p\,V(x)} \underbrace{- \frac{1}{2}p^2x^{s+1}p} - V(x)x^{s+1}p$$

$$= x^{s+1}V(x)p - ix^{s+1}V'(x)$$

where $V'(x) = \frac{\partial}{\partial x}V(x)$

$$= -\frac{1}{2}p[-i(s+1)x^s + x^{s+1}p]p$$

$$= -\frac{1}{2}(-i)(-i)(s+1)s\,x^{s-1}p + \frac{1}{2}i(s+1)x^sp^2 - \frac{1}{2}(-i)(s+1)x^sp^2 - \frac{1}{2}x^{s+1}p^3$$

$$\hookrightarrow = \frac{1}{2}s(s+1)x^{s-1}p - ix^{s+1}V'(x) + i(s+1)x^sp^2 \qquad eq(1.3)$$

Now consider $\mathcal{O} = x^s$

$$[x^s, \tfrac{1}{2}p^2 + V(x)]$$

$$= \tfrac{1}{2}x^s p^2 + x^s V(x) - \underbrace{\tfrac{1}{2}p^2 x^s}_{} - V(x) x^s$$

$$= -\tfrac{1}{2}(-i)s\,p\,x^{s-1} - \tfrac{1}{2}p x^s p$$

$$= -\tfrac{1}{2}(-i)(-i)s(s-1)x^{s-2} + \tfrac{1}{2}isx^{s-1}p$$

$$+ \tfrac{1}{2}isx^{s-1}p - \tfrac{1}{2}x^s p^2$$

$$= \tfrac{1}{2}s(s-1)x^{s-2} + isx^{s-1}p \qquad \text{eq (1.4)}$$

Combining equations (1.2), (1.3), (1.4):

$$\tfrac{1}{4}(s+1)s(s-1)\langle x^{s-2}\rangle - \langle x^{s+1}V'(x)\rangle + (s+1)\langle x^s p^2\rangle = 0 \qquad \text{eq (1.5)}$$

where $\langle \mathcal{O} \rangle \equiv \langle E|\mathcal{O}|E\rangle$

We now consider $\begin{cases} \langle E|x^s H|E\rangle = E\langle x^s\rangle \\ H = \tfrac{1}{2}p^2 + V(x) \end{cases}$

$$\Rightarrow \langle x^s p^2\rangle = 2E\langle x^s\rangle - 2\langle x^s V(x)\rangle \qquad \text{eq (1.6)}$$

Substitute $\langle x^s p^2\rangle$ term in (1.5) with (1.6), we get

$$\tfrac{1}{4}(s+1)s(s-1)\langle x^{s-2}\rangle - \langle x^{s+1}V'(x)\rangle + 2E(s+1)\langle x^s\rangle - 2(s+1)\langle x^s V(x)\rangle = 0$$

$$\text{eq (1.7)}$$

By substituting a specific potential $V(x)$, one can get the recursion of $\langle x^s\rangle$ represented in E.

Consider an operator $\mathcal{O} = \sum_{n=0}^{\infty} C_n X^n$, define

$$|\psi\rangle = \mathcal{O}|E\rangle$$

$\because \langle\psi|\psi\rangle \geq 0$

$\therefore \langle E|\mathcal{O}^\dagger\mathcal{O}|E\rangle = \langle\mathcal{O}^\dagger\mathcal{O}\rangle \geq 0$

$$\Rightarrow \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} C_m^* C_n X^{m+n} \geq 0 \qquad \text{eq (1.8)}$$

Construct a Hankel matrix M with the element at i-th row, j-th column is $M_{ij} = X^{i+j}$

$$\Rightarrow \begin{bmatrix} C_0^* & C_1^* & C_2^* & \cdots \end{bmatrix} \begin{bmatrix} X^0 & X^1 & X^2 & \\ X^1 & X^2 & & \\ X^3 & & \ddots & \\ & & & \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ \vdots \end{bmatrix} \geq 0 \qquad \text{eq (1.9)}$$

Equation (1.9) satisfies for any complex vector $\vec{C}$, so M is semi-positive definite. For every semi-positive definite matrix, the leading principle minors must be semi-positive! That is, the determinant of every submatrix on upper-left is semi-positive.

$$\forall K \in \mathbb{N}, \quad \det(M_{K\times K}) \geq 0 \qquad \text{eq (1.10)}$$

§ 2. One Dimensional Harmonic Potential

For 1-dimensional harmonic potential, define

$$V(x) = kx^2 \quad , \quad k>0 \qquad eq(2.1)$$

Plug in into eq(1.7) with $V'(x) = 2kx$

$$\Rightarrow \frac{1}{4}(s+1)s(s-1)\langle x^{s-2}\rangle - 2k\langle x^{s+2}\rangle + 2E(s+1)\langle x^s\rangle - 2k(s+1)\langle x^{s+2}\rangle = 0$$

$$\Rightarrow \langle x^{s+2}\rangle = \frac{E(s+1)}{k(s+2)}\langle x^s\rangle + \frac{(s+1)s(s-1)}{8k(s+2)}\langle x^{s-2}\rangle$$

Shift $s \to s-2$

$$\Rightarrow \langle x^s\rangle = \frac{s-1}{sk}E\langle x^{s-2}\rangle + \frac{(s-1)(s-2)(s-3)}{8ks}\langle x^{s-4}\rangle \qquad eq(2.2)$$

Let $|E\rangle$ be the normalized eigenfunction $\Rightarrow \langle E|E\rangle = 1$

$$\Rightarrow \langle x^0\rangle = \langle E|E\rangle = 1 \qquad eq(2.3)$$

Take $s=2 \Rightarrow \langle x^2\rangle = \frac{E}{2k}$

By parity, we know for odd s, $\langle x^s\rangle = 0$

§ 3. Coulomb Potential (Hydrogen Atom)

Consider the Coulomb potential

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r} = -\frac{k}{r} \qquad eq(3.1)$$

$$V'(r) = \frac{k}{r^2}$$

The Hamiltonian is

$$H = \frac{1}{2m_e} p_r^2 + \underbrace{\frac{l(l+1)\hbar^2}{2m_e r^2} - \frac{k}{r}} \qquad eq(3.2)$$

Can be viewed as effective potential

$$V_{eff}(r) \equiv \frac{l(l+1)}{2m_e r^2} - \frac{k}{r}$$

Set the electron mass $m_e = \hbar = 1$

$$\Rightarrow H = \frac{1}{2} p_r^2 + \frac{l(l+1)}{2r^2} - \frac{k}{r} \qquad eq(3.3)$$

Since p_r is the canonical momentum of r, i.e.,

$$\{r, p_r\} = 0$$

We have formulated it into an 1-dimensional problem!

Now plug in
$$\begin{cases} V_{eff}(r) = \dfrac{l(l+1)}{2r^2} - \dfrac{k}{r} \\[2ex] V'_{eff}(r) = -\dfrac{l(l+1)}{r^3} + \dfrac{k}{r^2} \end{cases}$$
into eq(1.7)

We can get the recursion relation

$$-E\langle r^s\rangle = \frac{k(2s+1)}{2(s+1)}\langle r^{s-1}\rangle + \left[\frac{1}{8}s(s-1) - \frac{s\ell(\ell+1)}{2(s+1)}\right]\langle r^{s-2}\rangle$$

eq (3.4)

Similarly, $\langle r^0\rangle = 1$

Take $s=0 \Rightarrow \langle r^{-1}\rangle = -\frac{2E}{k}$

Take $s=1 \Rightarrow \langle r^1\rangle = -\frac{3k}{4E} - \frac{\ell(\ell+1)}{2k}$

The energy eigenvalues $E^\ell_{n_r}$, $n_r \geq 0$

$$E^\ell_n = -\frac{\hbar^2}{2m_e a_0^2(n_r+\ell+1)^2}, \quad a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2} = \frac{\hbar^2}{m_e k}$$

Set $m_e = \hbar = 1 \Rightarrow a_0 = \frac{1}{k}$

$$\Rightarrow E^\ell_{n_r}(k) = -\frac{k^2}{2(n_r+\ell+1)^2}$$

eq (3.5)

n_r is the radial quantum number

$n = n_r + \ell + 1$ is the principal quantum number.

§4. Yukawa potential (First Order Approximated)

The Yukawa potential is

$$V(r) = -g^2 \frac{e^{-\alpha m r}}{r} \qquad eq\,(4.1)$$

With $g^2 = \frac{q_1 q_2}{4\pi\varepsilon_0}$, set $q_1 = q_2 = e$

$$\Rightarrow g^2 = \frac{e^2}{4\pi\varepsilon_0} = k$$

Also absorb m into α

$$\Rightarrow V(r) = -\frac{k}{r} e^{-\alpha r} \qquad eq\,(4.2)$$

$$\Rightarrow V'(r) = \frac{k}{r^2} e^{-\alpha r} + \frac{\alpha k}{r} e^{-\alpha r} \qquad eq\,(4.3)$$

Plug in into (1.7)

$$\Rightarrow \hbar(s+1)s(s-1)\langle r^{s-2}\rangle + 2E(s+1)\langle r^s\rangle \qquad eq\,(4.4)$$

$$-k\langle r^{s-1}e^{-\alpha r}\rangle - \alpha k\langle r^s e^{-\alpha r}\rangle + 2k(s+1)\langle r^{s-1}e^{-\alpha r}\rangle = 0$$

We do the Taylor expansion for $e^{-\alpha r}$ and keep the order to α

$$\Rightarrow e^{-\alpha r} = 1 - \alpha r + \mathcal{O}(\alpha^2) \qquad eq\,(4.5)$$

Discard the higher order terms $\mathcal{O}(\alpha^2)$

$$\Rightarrow \hbar(s+1)s(s-1)\langle r^{s-2}\rangle + 2E(s+1)\langle r^s\rangle - k\langle r^{s-1}\rangle + \alpha k\langle r^s\rangle$$

$$-\alpha k\langle r^s\rangle + 2k(s+1)\langle r^{s-1}\rangle - 2\alpha k(s+1)\langle r^s\rangle = 0$$

$$\Rightarrow -(E-\alpha k)\langle r^s\rangle = \frac{k(2s+1)}{2(s+1)}\langle r^{s-1}\rangle + \left[\frac{1}{8}s(s-1) - \frac{s\,l(l+1)}{2(s+1)}\right]\langle r^{s-2}\rangle \qquad eq(4.6)$$

Compare to eq(3.4), it is exactly the same recursion relation with energy shifted

$$E \to E-\alpha k$$

Similarly, $\langle r^0\rangle = 1$

Take $s=0 \Rightarrow \langle r^{-1}\rangle = -\frac{2}{k}(E-\alpha k)$

Take $s=1 \Rightarrow \langle r^1\rangle = -\frac{3k}{4(E-\alpha k)} - \frac{1}{2k}l(l+1)$

The approximated energy eigenvalues are given by

$$E^{l}_{n_r}(k) = -\frac{[k-\alpha(n_r+l+1)^2]^2}{2(n_r+l+1)^2} \qquad eq(4.7)$$

See ArXiv 1210.5886

For first order approximation of α, we see indeed

$$E^{l}_{n_r}(k) - \alpha k = -\frac{k^2}{2(n_r+l+1)^2} + \mathcal{O}(\alpha^2) \qquad eq(4.8)$$

Neglecting the higher order terms, we see that eq(4.8) is just the shifted eq(3.5)