CALCULATIONS FOR PRACTICAL WORK № 2 „SCHRÖDINGER EQUATION FOR H2"

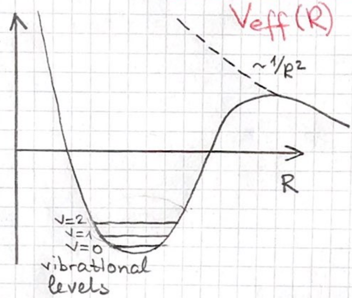
I. Time-independent Schrödinger eqn

Séparation of variables: $\Psi(\vec{R}) = \frac{1}{R}\psi(R)\,Y_{Jm}(\theta,\varphi)$

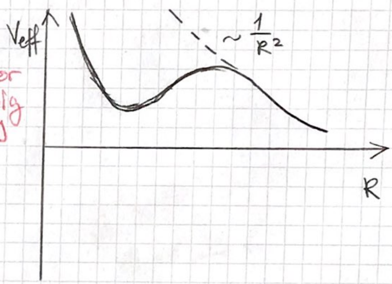
For the radial function: $\underline{H}\psi(R) = E\psi(R)$

$$\Big[-\frac{\hbar^2}{2\mu}\frac{d^2}{dR^2} + \underbrace{\underbrace{V(R)}_{\text{vibration}} + \underbrace{\frac{\hbar^2}{2\mu}\frac{J(J+1)}{R^2}}_{\text{centrifugal repulsion}}}_{V_{eff}(R)}\Big]\psi(R) = E\psi(R)$$

for small J



for big J



for each V, there is a rotational structure

$\exists$ 2 linearly independent solutions

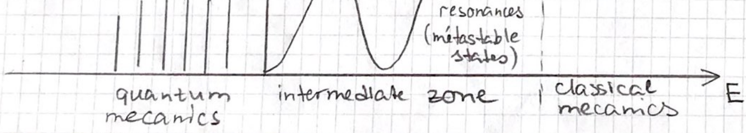
- $R \to 0$: $V(R)$ diverges $\Rightarrow$ one solution $= 0$ (regular solution) ← the single acceptable; other diverges
- $R \to \infty$: $V(R) \to 0 \Rightarrow -\frac{\hbar^2}{2\mu}\frac{d^2\psi(R)}{dR^2} = E\psi(R) \to \frac{d^2\psi}{dR^2} = k\psi$, $k = \sqrt{-\frac{2\mu E}{\hbar^2}}$

$E > 0$: $\psi(R)$ oscillating: $\sim Ae^{-ikR} + Be^{ikR}$

$E < 0$: $\psi(R) \sim Ae^{-kR} + Be^{kR}$ — physically meaningful if $B = 0$

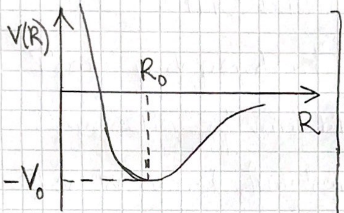
A, B depend on the initial conditions $\psi(0)=0$, $\psi'(0)=0$ (but also on $V(R)$ and E)

To get $B=0$, E takes discrete values



II. Numerical solution

II.1. Reduced variables



$r = \frac{R}{R_0} \rightarrow R = R_0 r$

$v(r) = \frac{V(R)}{V_0}$

$\equiv B$ (rotational constant)

$$\Rightarrow \left[-\frac{\hbar^2}{2\mu R_0^2}\frac{d^2}{dr^2} + v(r)V_0 + \frac{\hbar^2}{2\mu R_0^2}\frac{J(J+1)}{r^2} \right]\psi(r) = E\,\psi(r) \quad \Big/ :V_0$$

$b = \frac{B}{V_0}$, $e = \frac{E}{V_0}$

$$\downarrow$$

$$\boxed{\left[-b\frac{d^2}{dr^2} + v(r) + b\frac{J(J+1)}{r^2} \right]\psi(r) = e\,\psi(r)}$$

$-1 < e < 0$

II.2. Potential model

$$V(R) = V_0\left[e^{-2a\frac{R-R_0}{R_0}} - 2e^{-a\frac{R-R_0}{R_0}} \right]$$

Morse potential

$$\downarrow$$

$$\boxed{v(r) = e^{-2a(r-1)} - 2e^{-a(r-1)}}$$

$a \gg 1$

advantage: Sch. eq. can be solved analytically

$\exists\, J = 0$

$$\boxed{-b\psi''(r) + [v(r) - e]\psi(r) = 0} \quad (*)$$

$$-b\psi''(r) + \left[e^{-2a(r-1)} - 2e^{-a(r-1)} - e \right]\psi(r) = 0$$

$\exists\, x = e^{-a(r-1)} \rightarrow \frac{dx}{dr} = -a\,e^{-a(r-1)} = -ax \rightarrow dr = -\frac{dx}{ax}$

$$\psi'(r) \equiv \frac{d\psi(r)}{dr} = \frac{d\psi}{dx}(-ax) = -ax\frac{d\psi}{dx}$$

$$\psi''(r) \equiv (\psi'(r))'_r = -a\left(x\frac{d\psi}{dx}\right)'_r = -a\left(\underbrace{\frac{dx}{dr}}_{=-ax}\frac{d\psi}{dx} + x\frac{d^2\psi}{dx\,dr}\right) =$$

$$= -a\left(-ax\psi' + x\frac{d^2\psi}{dx^2}(-ax)\right) = a^2x\psi' + a^2x^2\psi''$$

$$\boxed{-ba^2x(\psi' + x\psi'') + [x^2 - 2x - e]\psi = 0}$$

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$\cancel{\ast}$ • Behavior for $r \to 0$ (i.e. $x = e^{a} \gg 1$)

$\exists\ \psi(x) \sim e^{-\alpha x}$

$$-ba^2 x\left(-\alpha \cancel{e^{-\alpha x}} + x\alpha^2 \cancel{e^{-\alpha x}}\right) + [x^2 - 2x - e]\cancel{e^{-\alpha x}} = 0$$

$$ba^2\alpha x - ba^2\alpha^2 x^2 + x^2 - 2x - e = 0$$

$$x^2(1 - a^2 b\alpha^2) + x(a^2 b\alpha - 2) - e = 0$$

$x \gg 1 \to$ the coefficient for x^2 must be $= 0$

$$a^2 b \alpha^2 = 1$$

$$\alpha^2 = \frac{1}{a^2 b}$$

$$\alpha = \frac{1}{a\sqrt{b}}$$

$$\boxed{\psi(x) \sim e^{-\frac{x}{a\sqrt{b}}}}$$

$\cancel{\ast}$ • Behavior for $r \to \infty$ (i.e. $x \to 0$)

$\exists\ \psi(x) \sim x^{\beta}$

$$-ba^2 x\left(\beta x^{\beta-1} + x\beta(\beta-1)x^{\beta-2}\right) + [x^2 - 2x - e]x^{\beta} = 0$$

$$-ba^2\left(\beta \cancel{x^{\beta}} + \beta(\beta-1)\cancel{x^{\beta}}\right) + [x^2 - 2x - e]\cancel{x^{\beta}} = 0$$

$$-ba^2\beta^2 + \underset{\downarrow\, 0}{x^2} - \underset{\downarrow\, 0}{2x} - e = 0$$

$$-ba^2\beta^2 = e$$

$$\beta^2 = -\frac{e}{ba^2}$$

$$\beta = \sqrt{\frac{-e}{a^2 b}}$$ $\leftarrow \exists$ for $e<0$

$$\boxed{\psi(x) \sim x^{\sqrt{\frac{-e}{a^2 b}}}}$$

Finally, for intermediate r values: ④

$$\exists \; \psi(x) = e^{-\alpha x} x^{\beta} \varphi(x)$$

$$\psi'(x) = \left(e^{-\alpha x} x^{\beta} \varphi(x)\right)'_x = \left(e^{-\alpha x} x^{\beta}\right)'_x \varphi(x) + e^{-\alpha x} x^{\beta} \varphi'(x) =$$

$$= \left[-\alpha e^{-\alpha x} x^{\beta} + e^{-\alpha x} \beta x^{\beta-1}\right] \varphi(x) + e^{-\alpha x} x^{\beta} \varphi'(x)$$

$$\psi''(x) = \left[-\alpha e^{-\alpha x} x^{\beta} + e^{-\alpha x} \beta x^{\beta-1}\right]'_x \varphi(x) + \left[-\alpha e^{-\alpha x} x^{\beta} + e^{-\alpha x} \beta x^{\beta-1}\right] \varphi'(x) +$$

$$+ \left[e^{-\alpha x} x^{\beta}\right]'_x \varphi'(x) + e^{-\alpha x} x^{\beta} \varphi''(x) =$$

$$= \left[\alpha^2 e^{-\alpha x} x^{\beta} - \alpha e^{-\alpha x} \beta x^{\beta-1} - \alpha e^{-\alpha x} \beta x^{\beta-1} + e^{-\alpha x} \beta(\beta-1) x^{\beta-2}\right] \varphi(x) +$$

$$+ \left[-\alpha e^{-\alpha x} x^{\beta} + e^{-\alpha x} \beta x^{\beta-1}\right] \varphi'(x) +$$

$$+ \left[-\alpha e^{-\alpha x} x^{\beta} + e^{-\alpha x} \beta x^{\beta-1}\right] \varphi'(x) + e^{-\alpha x} x^{\beta} \varphi''(x) =$$

$$= \left[\alpha^2 e^{-\alpha x} x^{\beta} - 2\alpha\beta e^{-\alpha x} x^{\beta-1} + \beta(\beta-1) e^{-\alpha x} x^{\beta-2}\right] \varphi(x) +$$

$$+ 2\left[-\alpha e^{-\alpha x} x^{\beta} + \beta e^{-\alpha x} x^{\beta-1}\right] \varphi'(x) +$$

$$+ e^{-\alpha x} x^{\beta} \varphi''(x)$$

$$-ba^2 x \Big\{ \underbrace{\left[-\alpha e^{-\alpha x} x^{\beta} + \beta e^{-\alpha x} x^{\beta-1}\right] \varphi(x) + e^{-\alpha x} x^{\beta} \varphi'(x)}_{\psi'} +$$

$$+ x\Big[\left(\alpha^2 e^{-\alpha x} x^{\beta} - 2\alpha\beta e^{-\alpha x} x^{\beta-1} + \beta(\beta-1) e^{-\alpha x} x^{\beta-2}\right)\varphi(x) + 2\left(-\alpha e^{-\alpha x} x^{\beta} + \beta e^{-\alpha x} x^{\beta-1}\right)\varphi'(x) + e^{-\alpha x} x^{\beta} \varphi''(x)\Big]\Big\} +$$

$$+ \left[x^2 - 2x - e\right] e^{-\alpha x} x^{\beta} \varphi(x) = 0 \qquad \Big| : e^{-\alpha x} x^{\beta}$$

$$-ba^2 x \left\{\left[-\alpha + \frac{\beta}{x}\right]\varphi(x) + \varphi'(x) + x\left[\left(\alpha^2 - 2\alpha\frac{\beta}{x} + \frac{\beta(\beta-1)}{x^2}\right)\varphi(x) + 2\left(-\alpha + \frac{\beta}{x}\right)\varphi'(x) + \varphi''(x)\right]\right\} + (x^2 - 2x - e)\varphi(x) = 0$$

$$-ba^2 \left\{\left[-\alpha x + \beta\right]\varphi(x) + x\varphi'(x) + \left[\left(\alpha^2 x^2 - 2\alpha\beta x + \beta(\beta-1)\right)\varphi(x) + 2\left(-\alpha x^2 + \beta x\right)\varphi'(x) + x^2\varphi''(x)\right]\right\} + (x^2 - 2x - e)\varphi(x) = 0$$

$$\left[-ba^2\left\{-\alpha x + \beta + \alpha^2 x^2 - 2\alpha\beta x + \beta(\beta-1)\right\} + x^2 - 2x - e\right]\varphi(x) +$$

$$+ \left[-ba^2\left\{x + 2\left(-\alpha x^2 + \beta x\right)\right\}\right]\varphi'(x) +$$

$$+ \left[-ba^2 x^2\right]\varphi''(x) = 0$$

$$\alpha = \frac{1}{a\sqrt{b}} \quad \text{and} \quad \beta = \frac{\sqrt{-e}}{a\sqrt{b}} \longrightarrow \boxed{-ba^2 = -\alpha^{-2}}$$

$$\beta a\sqrt{b} = \sqrt{-e}$$

$$\frac{\beta}{\alpha} = \sqrt{-e}$$

$$\boxed{-e = \frac{\beta^2}{\alpha^2}}$$

$$\left[-\alpha^{-2}\left(-\alpha x+\beta+\alpha^2x^2-2\alpha\beta x+\beta(\beta-1)\right)+x^2-2x+\frac{\beta^2}{\alpha^2}\right]\varphi(x)+$$

$$+\left[-\alpha^{-2}\left(x+2\left(-\alpha x^2+\beta x\right)\right)\right]\varphi'(x)+\left[-\alpha^{-2}x^2\right]\varphi''(x)=0 \qquad *(-\alpha^2)$$

$$\Big[\underbrace{\left(-\alpha x+\cancel{\beta}+\alpha^2x^2-2\alpha\beta x+\beta^2-\cancel{\beta}\right)-\alpha^2\left(x^2-2x+\frac{\beta^2}{\alpha^2}\right)}\Big]\varphi(x)+\left[x-2\alpha x^2+2\beta x\right]\varphi'(x)+x^2\varphi''(x)=0$$

$$-\alpha x+\cancel{\alpha^2x^2}-2\alpha\beta x+\cancel{\beta^2}-\cancel{\alpha^2x^2}+2\alpha^2x-\cancel{\beta^2}$$

$$\alpha x(-1-2\beta+2\alpha)$$

$$\alpha\cancel{x}(-1-2\beta+2\alpha)\varphi(x)+\cancel{x}[1-2\alpha x+2\beta]\varphi'(x)+x^{\cancel{2}}\varphi''(x)=0$$

$$\boxed{x\varphi''+[1+2(\beta-\alpha x)]\varphi'+\alpha(-1-2\beta+2\alpha)\varphi=0}$$

$$\exists\ \varphi(x)=\sum_{n=0}^{\infty}a_nx^n$$

$$\varphi'(x)=\sum_{n=1}^{\infty}na_nx^{n-1} \quad ; \quad \varphi''(x)=\sum_{n=2}^{\infty}n(n-1)a_nx^{n-2}$$

$$\sum_{n=2}n(n-1)a_nx^{n-1}+\underbrace{[1+2(\beta-\alpha x)]\sum_{n=1}na_nx^{n-1}}_{\sum_{n=1}^{\infty}na_nx^{n-1}(1+2\beta)-2\alpha\sum_{n=1}^{\infty}na_nx^n}+\alpha(-1-2\beta+2\alpha)\sum_{n=0}a_nx^n=0$$

$$\sum_{n=2}^{\infty}\left[n(n-1)a_n+na_n(1+2\beta)\right]x^{n-1}+\sum_{n=1}^{\infty}\left[-2\alpha na_n+\alpha a_n(-1-2\beta+2\alpha)\right]x^n=0$$

→ the coefficient for each power of x must be $=0$

$n=2,\dots$

$$n(n-\cancel{1}+\cancel{1}+2\beta)a_n+\left[-2\alpha(n-1)a_{n-1}+\alpha a_{n-1}(-1-2\beta+2\alpha)\right]=0$$

$$n(n+2\beta)a_n+\alpha a_{n-1}(2-2n-1-2\beta+2\alpha)=0 \quad (\to 1)$$

$$n(n+2\beta)a_n+\alpha a_{n-1}(1-2(n+\beta-\alpha))=0$$

$$n(n+2\beta)a_n=\alpha a_{n-1}\left[2(n+\beta-\alpha)-1\right]$$

$$\frac{a_n}{a_{n-1}}=\frac{\alpha[2(n+\beta-\alpha)-1]}{n(n+2\beta)}\xrightarrow[n\to\infty]{}\frac{\alpha 2n}{n^2}=\frac{2\alpha}{n}$$

$$a_n=\frac{2\alpha}{n}a_{n-1}=\frac{2\alpha}{n}\cdot\frac{2\alpha}{n-1}a_{n-2}=\frac{2\alpha}{n}\frac{2\alpha}{n-1}\frac{2\alpha}{n-2}\cdots\frac{2\alpha}{1}a_0=\frac{(2\alpha)^n}{n!}a_0$$

$$\varphi(x)=\sum^{\infty}a_0\frac{(2\alpha)^n}{n!}x^n=a_0\sum^{\infty}\frac{(2\alpha x)^n}{n!}=a_0e^{2\alpha x}$$

Normally, $n = 0, 1, 2, \ldots$
so that instead considering $\frac{a_n}{a_{n-1}}$

we must consider

$$\frac{a_{n+1}}{a_n} = \frac{\alpha[2(n+1+\beta-\alpha)-1]}{(n+1)(n+1+2\beta)}$$

To get the rhs of our eqn equal to zero,
we must have

$$2(n+1+\beta-\alpha)-1 = 0$$

$$2+2(n+\beta-\alpha)-1 = 0$$

$$2(n+\beta-\alpha) = -1$$

$$n+\beta-\alpha = -\frac{1}{2}$$

$$n = \alpha-\beta-\frac{1}{2}$$

$$n = \frac{1}{a\sqrt{b}} - \frac{\sqrt{-e}}{a\sqrt{b}} - \frac{1}{2}$$

← maximal value: $n \leq \frac{1}{a\sqrt{b}} - \frac{1}{2}$
for $e \approx 0$

$$2a\sqrt{b}\,n = 2(1-\sqrt{-e}) - a\sqrt{b}$$

$$2(1-\sqrt{-e}) = a\sqrt{b}(2n+1)$$

$$1-\sqrt{-e} = a\sqrt{b}\left(n+\frac{1}{2}\right)$$

$$1-a\sqrt{b}\left(n+\frac{1}{2}\right) = \sqrt{-e}$$

$$\boxed{e = -\left[1-a\sqrt{b}\left(n+\frac{1}{2}\right)\right]^2}$$

II.3. Propagation

$$\psi_i' \approx \frac{\psi_i - \psi_{i-1}}{h}$$

$$\psi_i'' \approx \frac{\psi_{i+1}' - \psi_i'}{h} = \frac{\psi_{i+1} - \psi_i - \psi_i + \psi_{i-1}}{h^2} = \frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{h^2}$$

So, the Schr. eq. in reduced variables (* with rot. term added):

$$-b\,\psi''(r) + \left(v(r) + \frac{bJ(J+1)}{r^2} - e\right)\psi(r) = 0$$

becomes

$$-\frac{b}{h^2}\left(\psi_{i+1} - 2\psi_i + \psi_{i-1}\right) + \left(v_i + \frac{bJ(J+1)}{r_i^2} - e\right)\psi_i = 0$$

$$-b\left(\psi_{i+1} - 2\psi_i + \psi_{i-1}\right) + h^2\left(v_i + \frac{bJ(J+1)}{r_i^2} - e\right)\psi_i = 0$$

$$\psi_{i+1} - 2\psi_i + \psi_{i-1} = \frac{h^2}{b}\left(v_i + \frac{bJ(J+1)}{r_i^2} - e\right)\psi_i$$

$$\boxed{\psi_{i+1} = \left[\frac{h^2}{b}\left(v_i + \frac{bJ(J+1)}{r_i^2} - e\right) + 2\right]\psi_i - \psi_{i-1}}$$ propagation to the right

$$\boxed{\psi_{i-1} = \left[\frac{h^2}{b}\left(v_i + \frac{bJ(J+1)}{r_i^2} - e\right) + 2\right]\psi_i - \psi_{i+1}}$$ propag. to the left

Determination of a and b for the model potential

$$E_v = -V_0\left[1-a\sqrt{b}\left(v+\frac{1}{2}\right)\right]^2 = V_0\left[-1+2a\sqrt{b}\left(v+\frac{1}{2}\right)-a^2b\left(v+\frac{1}{2}\right)^2\right]$$

$$E_0 = -V_0\left[1-\frac{a\sqrt{b}}{2}\right]^2 = V_0\left[-1+a\sqrt{b}-\frac{1}{4}a^2b\right]$$

For the experimental values:

$$E_1 = V_0\left(-1+3a\sqrt{b}-\frac{9}{4}a^2b\right)$$

$$E_2 = V_0\left(-1+5a\sqrt{b}-\frac{25}{4}a^2b\right)$$

$$\begin{cases} E_1-E_0 = 4159.48\,\mathrm{cm}^{-1} = V_0\left(\cancel{-1}+3a\sqrt{b}-\frac{9}{4}a^2b+\cancel{1}-a\sqrt{b}+\frac{1}{4}a^2b\right) = \\ \quad = V_0\left(2a\sqrt{b}-2a^2b\right) \\ E_2-E_0 = 8083.20\,\mathrm{cm}^{-1} = V_0\left(-1+5a\sqrt{b}-\frac{25}{4}a^2b+1-a\sqrt{b}+\frac{1}{4}a^2b\right) = \\ \quad = V_0\left(4a\sqrt{b}-6a^2b\right) \end{cases}$$

* $2(E_1-E_0)-(E_2-E_0) = V_0\left[\cancel{4a\sqrt{b}}-4a^2b-\cancel{4a\sqrt{b}}+6a^2b\right] = V_0 2a^2b = 2a^2\underbrace{B}_{\text{rot. const}}$

$$\boxed{a = \sqrt{\frac{2(E_1-E_0)-(E_2-E_0)}{2B}} = \dots}$$ your calculation

* $\frac{E_2-E_0}{E_1-E_0} = \frac{4a\sqrt{b}-6a^2b}{2a\sqrt{b}-2a^2b} = \frac{2a\sqrt{b}-3a^2b}{a\sqrt{b}-a^2b} = \frac{2-3a\sqrt{b}}{1-a\sqrt{b}}$

$$(E_2-E_0)(1-a\sqrt{b}) = (E_1-E_0)(2-3a\sqrt{b})$$

$$(E_2-E_0)-a\sqrt{b}(E_2-E_0) = 2(E_1-E_0)-3a\sqrt{b}(E_1-E_0)$$

$$(E_2-E_0)-2(E_1-E_0) = a\sqrt{b}\left[(E_2-E_0)-3(E_1-E_0)\right]$$

$$\sqrt{b} = \frac{(E_2-E_0)-2(E_1-E_0)}{a\left[(E_2-E_0)-3(E_1-E_0)\right]}$$

$$\boxed{b = \left[\quad\right]^2 = \dots}$$ your calculation

$$\boxed{V_0 = \frac{B}{b} = \dots}$$ your calculation

STUDY OF THE Q-BRANCH

* the centrifugal potential as a perturbation:

$$-b\psi''(r) + \left(v(r) + \frac{bJ(J+1)}{r^2}\right)\psi(r) = e\psi(r)$$

Perturbation theory:

$$-b\psi''(r) + \left(v(r) + bJ(J+1)\left(1 + \left(\frac{1}{r^2} - 1\right)\right)\right)\psi(r) = e\psi(r)$$

$$\underbrace{\left[\underbrace{-b\frac{\partial^2}{\partial r^2} + v(r)}_{\text{vibrationnel}} + \underbrace{bJ(J+1)}_{\text{rotationnel}}\right.}_{p_0\ (J=0)} \left.\underbrace{+ bJ(J+1)\left(\frac{1}{r^2} - 1\right)}_{p_1}\right]\psi(r) = e\psi(r)$$

$$(p_0 + p_1)\psi(r) = e\psi(r)$$

$\boxed{p_0\psi_v^0(r) = e_v^0\psi_v^0(r)}$ — eigen energies and functions found (order „zero")

$$\psi(r) = \psi^0(r) + \psi^1(r) + \dots$$

$$e = e^0 + e^1 + \dots$$

order „0"

$$p_0(\psi^0 + \psi^1) + p_1(\psi^0 + \psi^1) = e^0(\psi^0 + \psi^1) + e^1(\psi^0 + \psi^1)$$

1st order: $\boxed{p_0\psi^1 + p_1\psi^0 = e^0\psi^1 + e^1\psi^0}$

and $\psi^1 = \sum_v a_v \psi_v^0$, the 1st order becomes, for each v of ψ

$$p_0\sum_{v'} a_{v'}\psi_{v'}^0 + p_1\psi_v^0 = e_v^0\sum_{v'} a_{v'}\psi_{v'}^0 + e^1\psi_v^0 \quad \Big| \cdot \psi_{v''}^0 \text{ et } \int dr$$

"$e_{v'}^0\psi_{v'}^0$"

On the left!

$$\sum_{v'} a_{v'} e_{v'}^0 \underbrace{\int \psi_{v'}^0 \psi_{v''}^0 dr}_{\delta_{v'v''}} + \int \psi_{v''}^0 p_1 \psi_v^0 dr = e_v^0 \sum_{v'} a_{v'} \underbrace{\int \psi_{v'}^0 \psi_{v''}^0 dr}_{\delta_{v'v''}} + e^1 \underbrace{\int \psi_v^0 \psi_{v''}^0 dr}_{\delta_{vv''}}$$

non-vanishing $v, v' = v''$

$$a_{v''} e_{v''}^0 + \int \psi_{v''}^0 p_1 \psi_v^0 dr = e_v^0 a_{v''} + e^1 \delta_{vv''}$$

If $v'' = v$, so $e^1 = \int \psi_v^0 p_1 \psi_v^0 dr$ ☆

If $v'' \neq v$, so $a_{v''}(e_v^0 - e_{v''}^0) = \int \psi_{v''}^0 p_1 \psi_v^0 dr$

$$a_{v''} = \int \psi_{v''}^0 p_1 \psi_v^0 dr \,/\, (e_v^0 - e_{v''}^0)$$

$\circledast$: $e_1 = \int \Psi_v^0 \left[bJ(J+1)\left(\frac{1}{r^2} - 1\right)\right] \Psi_v^0 \, dr =$ 10

$$= bJ(J+1) \langle v | \frac{1}{r^2} - 1 | v \rangle$$

$$e_{v,j} = e^0_v + \underbrace{bJ(J+1) \langle v | \frac{1}{r^2} | v \rangle}_{b_v}$$