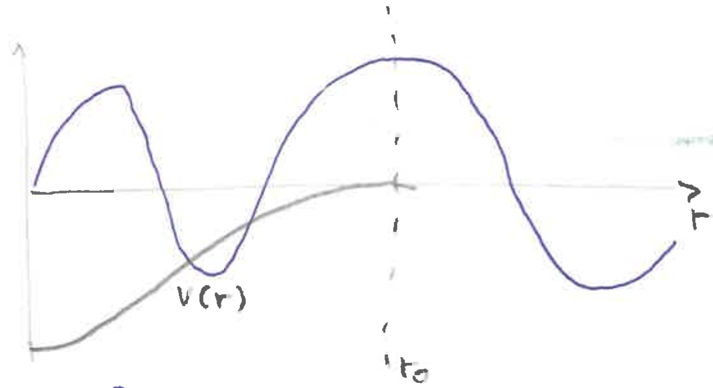
R-matrix method

- In the scattering we are looking for solutions of the Schrödinger equation with oscillatory asymptotic behaviour. The wf behavior is usually described by
  - phase shift δ
  - K-matrix $\operatorname{tg}\delta$
  - S-matrix $e^{2i\delta}$
  - T-matrix $e^{i\delta}\sin\delta$
  - Any other?



- Another way to define wf in outer region is B_ℓ or R_ℓ:

$$\left[-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}+2V(r)-k^2\right]u_\ell(r)=0$$

$$\left.\begin{aligned} u_\ell'(r_0) &= B_\ell^{(r_0)} u_\ell(r_0) \\ u_\ell(r_0) &= R_\ell(r_0)\, u_\ell'(r_0) \end{aligned}\right\} \quad R_\ell = B_\ell^{-1}$$

- **Question**: Is R_ℓ sufficient as a solution of the scattering problem

- Two cases:

1.) $V(r)=0$ for $r\geq r_0$: f_ℓ, g_ℓ are regular and irregular free solutions (ricatti-bessel, neumann)

$$\left.\begin{aligned} u_\ell(r_0) = R_\ell u_\ell'(r_0) &= A_\ell f_\ell(r_0) + B_\ell g_\ell(r_0) \\ \frac{1}{A_\ell} u_\ell(r_0) &\rightarrow f_\ell(r_0) + K_\ell g_\ell(r_0) \end{aligned}\right\} \quad K_\ell = -\frac{B_\ell}{A_\ell}$$

$$\frac{W(f_\ell,u_\ell)}{W(f_\ell,g_\ell)} = B_\ell \;;\; \frac{W(g_\ell,u_\ell)}{W(g_\ell,f_\ell)} = A_\ell = -\frac{W(g_\ell,u_\ell)}{W(f_\ell,g_\ell)} \Rightarrow K_\ell = -\frac{B_\ell}{A_\ell} = +\frac{W(f_\ell,u_\ell)}{W(g_\ell,u_\ell)} =$$

$$= \frac{f_\ell u_\ell' - f_\ell' u_\ell}{g_\ell u_\ell' - g_\ell' u_\ell} = \boxed{\frac{f_\ell - f_\ell' R_\ell}{g_\ell - g_\ell' R_\ell} = K_\ell}$$

2.) $V(r)\neq 0$ for $r\geq 0$ In this case one can choose an arbitrary value of $u_\ell(r_0)$ (choice of the normalization) and R_ℓ defines $u_\ell'(r_0) = R_\ell^{-1} u_\ell(r_0)$. Having value and the derivative allows to propagate the second-order dif. equation.

- History
  - first: non-variational derivation; Wigner-Eisenbud 1947 nuclear physics, resonancies. Sum-of-poles formula
  - second: variational derivation, 1948 Kohn. Resolvent form
  - third: eigenchannel formulation, Greene 1983, Szmytkowski 1997

Motivation: Is there a variational principle, similar to $E = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$, for continuum states? What is the stationary quantity? It canot be the energy as it is prescribed.

R-matrix (eigenchannel formulation)

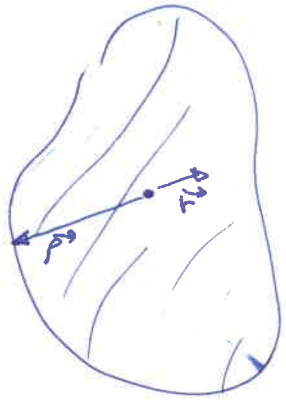
(3dim, 1particle) (R. Szmytkowski, J. Phys. A 30, 4413 (1997))

① Schrödinger equation

$$\boxed{(\hat H - E)\,\psi(E,\vec r) = 0}$$

in a finite volume V encompased by S, $V \subset \mathbb{R}^3$

$$\hat H = -\tfrac{1}{2}\nabla^2 + V(\vec r)$$



volume ~~vector~~ vectors .. $\vec r$
surface vectors $\vec \rho$

② Notation

$$\langle f|g\rangle \equiv \int_V d^3r\, f^*(\vec r)\, g(\vec r) \quad ; \quad (f|g) = \int_S d^2\rho\, f^*(\vec\rho)\, g(\vec\rho)$$

Definition $\delta^{(2)}(\vec\rho - \vec\rho\,')$: $\int_S d^2\rho'\, \delta^{(2)}(\vec\rho - \vec\rho\,')\, f(\vec\rho\,') = f(\vec\rho)$

Definition $D(E)$ space of functions, set of solutions $\psi(E,\vec r)$ solving $(\hat H - E)\psi(E,\vec r) = 0$

$D_S(E)$ surface values of $D(E)$, i.e. $\psi(E,\vec\rho)$

Lemma: for $\psi(E,\vec r)$ and $\psi'(E,\vec r\,')\in D(E)$:

$$\boxed{\langle \hat H\psi'|\psi\rangle - \langle\psi'|H|\psi\rangle = \tfrac{1}{2}(\psi'|\nabla_n\psi) - \tfrac{1}{2}(\nabla_n\psi'|\psi)}$$

∇_n ... normal gradient

Lesson 2

Winter 2019

Proof: Divergence theorem (Gauss – Ostrogradsky)

$$\int_V \vec{\nabla}\cdot\vec{F} = \int_S \vec{F}\cdot\vec{n}\, ds$$, we choose $\vec{F} = u\,\nabla v$

$$\int_V \left(u\nabla^2 v + \vec{\nabla}u\cdot\vec{\nabla}v\right) dv = \int_S u\,\underbrace{\vec{\nabla}v\cdot\vec{n}}_{\nabla_n v}\, ds$$

One of the Gauss identities

$$\boxed{\int_V \left(u\nabla^2 v - v\nabla^2 u\right) dv = \int_S \left(u\,\vec{\nabla}_n v - v\,\vec{\nabla}_n u\right) ds}$$

- Because ψ and ψ' are solutions of $(\hat{H} - E)\psi(E,\vec{r}) = 0$ we may write:

$$\boxed{(\psi' | \nabla_n \psi) = (\nabla_n \psi' | \psi)}$$

- Formal interpretation is, that operator ∇_n is Hermitian on class $D_S(E)$ with the scalar product $(\cdot|\cdot)$.

Definition on $D_S(E)$ we define a linear operators $\hat{B}(E)$ and $\hat{R}(E)$

$$\boxed{\begin{aligned} \nabla_n \psi(E,\vec{\rho}) &= \hat{B}(E)\,\psi(E,\vec{\rho}) \\ \psi(E,\vec{\rho}) &= \hat{R}(E)\,\nabla_n \psi(E,\vec{\rho}) \end{aligned}} \quad \hat{R}(E) = \hat{B}^{-1}(E)$$

- Logderivative operator $\hat{B}(E)$ and R-matrix operator $\hat{R}(E)$.

For a complete set of orthonormal functions $\phi_i(\vec{\rho})$ on S we may define matrix elements $(\phi_i|\hat{B}(E)|\phi_j)$, $(\phi_i|\hat{R}(E)|\phi_j)$ of the logderivative matrix, R-matrix, respectively.

Eigenstates and eigenvalues of $\hat{B}(E)$ and $\hat{R}(E)$

- Consider set of functions $\{\psi_i(E,r)\} \in D(E)$ that possess constant logderivative of the surface S

$$\begin{aligned} \nabla_n \psi_i(E,\vec{\rho}) - b_i(E)\,\psi_i(E,\vec{\rho}) &= 0 \\ \hat{B}(E)\,\psi_i(E,\vec{\rho}) &= b_i(E)\,\psi_i(E,\vec{\rho}) \end{aligned}$$

Surface values $\psi_i(E,\vec{\rho})$ are eigenvectors and $b_i(E)$ are eigenvalues of $\hat{B}(E)$

Because $\hat{B}(E)$ is Hermitian on $D_S(E)$, $b_i(E) \in \mathbb{R}$ and $\psi_i(E,\vec{\rho})$ are orthonormal on S.

$$\left. \begin{aligned} &(\psi_i|\psi_j) = \delta_{ij} \\ &\sum_i \psi_i(E,\vec{\rho})\,\psi_i(E,\vec{\rho}\,') = \delta^{(2)}(\vec{\rho}-\vec{\rho}\,') \end{aligned} \right\} \begin{aligned} &\text{orthonormal} \\ &\text{complete} \end{aligned}$$

Variational principle for $b(E)$

- Generalized construction of the VP (we omit the index "i" in $\psi_i(E,\vec{\rho})$)

(Gerjuoy 1983)

Lagrange functions instead of Lagrange multipliers

Functional

$$\boxed{F[\bar{b},\bar{\lambda},\bar{\Lambda},\bar{\psi}] = \bar{b} + (\bar{\lambda}|\partial_n\bar{\psi} - \bar{b}\bar{\psi}) + \langle\bar{\Lambda}|\hat{H}-E|\bar{\psi}\rangle}$$

- Instead of satisfaction of some scalar conditions we need ~~to~~ a satisfaction of differential equations. Instead of λ (condition) we apply $\langle\bar{\lambda}|\underbrace{L\bar{\psi}}_{0}\rangle$. Projection of "0" on any trial $\bar{\lambda}$ is sought to be zero. Non-countable number of the Lagrange "multipliers". In a similar manner as one gets the equations for λ_i for ~~the~~ the traditional "Lagrange-multipliers" system, we will get equations for functions $\bar{\lambda}(\vec{\rho})$ and $\bar{\Lambda}(\vec{r})$.

- For $\bar{\psi} \to \psi$ we get $F[b(E),\bar{\lambda},\bar{\Lambda},\psi] = b(E)$ regardless of $\bar{\lambda}(\vec{\rho})$ and $\bar{\Lambda}(\vec{r})$

- Our goal is to find such $\lambda(\vec{\rho}), \Lambda(\vec{r}), b(E)$ and $\psi(\vec{r})$ around which F becomes stationary with respect to small variations

$$\left| \begin{aligned} &\delta b = \bar{b} - b\,; \quad \delta\psi = \bar{\psi} - \psi \\ &\delta\lambda = \bar{\lambda} - \lambda\,; \quad \delta\Lambda = \bar{\Lambda} - \Lambda \end{aligned} \right| \qquad \text{i.e.} \quad \delta F[b,\lambda,\Lambda,\psi] = 0$$

Variation

$$\delta F[b,\lambda,\Lambda,\psi] = \delta b + (\delta\lambda|\partial_n\psi - b\psi) - \delta b(\lambda|\psi) + (\lambda|\partial_n\delta\psi - b\delta\psi) + \langle\delta\Lambda|\cancel{\hat{H}-E|\psi}\rangle + \langle\Lambda|\hat{H}-E|\delta\psi\rangle$$

$$\delta F[b,\lambda,\Lambda,\psi] = \delta b[1-(\lambda|\psi)] + (\lambda|\partial_n\delta\psi - b\delta\psi) + \langle\Lambda|\hat{H}-E|\delta\psi\rangle$$

$$\langle\Lambda|\hat{H}-E|\delta\psi\rangle = \langle(\hat{H}-E)\Lambda|\delta\psi\rangle + \tfrac{1}{2}(\partial_n\Lambda|\delta\psi) - \tfrac{1}{2}(\Lambda|\partial_n\delta\psi)$$

$$\boxed{\delta F[b,\lambda,\Lambda,\psi] = \delta b[1-(\lambda|\psi)] + (\tfrac{1}{2}\partial_n\Lambda - b\lambda|\delta\psi) + (\lambda - \tfrac{1}{2}\Lambda|\partial_n\delta\psi) + \langle(\hat{H}-E)\Lambda|\delta\psi\rangle}$$

Free variations of $\delta b, \delta\psi, \partial_n\delta\psi$ .... Requirement of the continuity of first derivatives is lifted

Resulting equations:

(1.) $\quad 1-(\lambda|\psi)=0$

(2.) $\quad (\hat{H}-E)\Lambda(\vec{r})=0$ in the volume V

(3.) $\quad \lambda(\vec{\rho})-\frac{\Lambda(\vec{\rho})}{2}=0$ on the surface S

(4.) $\quad \frac{1}{2}\nabla_n\Lambda(\vec{\rho})-b(E)\lambda(\vec{\rho})=0$ on the surface S

(3') $\quad \nabla_n\Lambda(\vec{\rho})-b(E)\Lambda(\vec{\rho})=0$

(4') $\quad \frac{1}{2}\Lambda(\vec{\rho})=\lambda(\vec{\rho})$

- Function $\Lambda(\vec{r})$ satisfies in V and on S the same equations (2) (3') as we require of $\psi(E,\vec{r})$. Therefore

$$\Lambda(\vec{r})=\gamma\,\psi(E,\vec{r})$$

Coefficient γ can be found through (4') and (1) as

$$\gamma=\frac{2}{(\psi|\psi)}$$

$$\boxed{\begin{aligned}\Lambda(\vec{r})&=\frac{2}{(\psi|\psi)}\psi(E,\vec{r})\\ \lambda(\vec{\rho})&=\frac{1}{(\psi|\psi)}\psi(E,\vec{\rho})\end{aligned}}$$

Stationarity of $F[\ ]$ requires in the stationary point!

Therefore, we can reduce the variational space so, that $\bar{\Lambda}(\vec{r})$ and $\bar{\lambda}(\vec{r})$ will not be independent variations but they will be bound to $\psi(E,\vec{r})$ exactly the same way as they are bound in the stationary point.

$$\bar{\Lambda}(\vec{r})=\frac{2}{(\bar{\psi}|\bar{\psi})}\bar{\psi}(E,\vec{r})$$
$$\bar{\lambda}(\vec{\rho})=\frac{1}{(\bar{\psi}|\bar{\psi})}\bar{\psi}(\vec{\rho})$$

Functional $\quad F[\bar{\psi}]=\dfrac{(\bar{\psi}|\nabla_n\bar{\psi})}{(\psi|\psi)}+2\dfrac{\langle\bar{\psi}|\hat{H}-E|\bar{\psi}\rangle}{(\psi|\psi)}=\dfrac{(\nabla_n\bar{\psi}|\bar{\psi})}{(\bar{\psi}|\bar{\psi})}+2\dfrac{\langle(\hat{H}-E)\bar{\psi}|\bar{\psi}\rangle}{(\bar{\psi}|\bar{\psi})}=F^*[\bar{\psi}]$

→ Functional $F[\ ]$ is real for any trial fction $\bar{\psi}$ (restriction to $\bar{\psi}\in D(E)$ is not needed)

→ Define $\bar{H}=\hat{H}+\frac{1}{2}\delta(S)\nabla_n$, where $\int_{R^3}dr^3 f(\vec{r})\delta(S)=\int_S dS\, f(\vec{\rho})$. Nonrestricted variational principle for the eigenvalues $b(E)$ of the $\hat{B}(E)$ operator:

$$\boxed{b(E)=\underset{\bar{\psi}}{\mathrm{stat}}\left\{2\frac{\langle\bar{\psi}|\bar{H}-E|\bar{\psi}\rangle}{(\bar{\psi}|\bar{\psi})}\right\}}\qquad \bar{H}=\hat{H}+\tfrac{1}{2}\delta(S)\nabla_n$$

Eigenchannel R-matrix ; channels decomposition

$$b(E) = 2\,\underset{\psi}{\mathrm{stat}} \frac{\langle\psi|\bar{H}-E|\psi\rangle}{(\psi|\psi)} = 2\frac{\langle\psi|\bar{H}-E|\psi\rangle}{\langle\psi|\delta(s)|\psi\rangle}$$ ... we omit $\bar{H}$ bar

$$\delta b = 0 = 2\,\frac{\langle\delta\psi|\bar{H}-E|\psi\rangle+\langle\psi|\bar{H}-E|\delta\psi\rangle}{\langle\psi|\delta(s)|\psi\rangle} - \underbrace{\frac{2\langle\psi|\bar{H}-E|\psi\rangle}{(\psi|\psi)^2}}_{\frac{b}{(\psi|\psi)}}\cdot\left[\langle\delta\psi|\delta(s)|\psi\rangle+\langle\psi|\delta(s)|\delta\psi\rangle\right]$$

$$0 = 2\langle\delta\psi|\bar{H}-E|\psi\rangle - b\langle\delta\psi|\delta(s)|\psi\rangle + \text{complex conjugate}$$

(1) $$\boxed{2(\bar{H}-E)|\psi\rangle = b\,\delta(s)|\psi\rangle \equiv b|\psi)}$$

(Greene 1983)

Volume basis $\{y_i\}$

$$\psi(\vec{r}) = \sum_j y_j(\vec{r})\,c_j$$

$$2\sum_j\langle y_i|\bar{H}-E|y_j\rangle c_j = b\sum_j\langle y_i|\delta|y_j\rangle c_j$$

Matrix eq: $$\boxed{\underline{\Gamma}(E)\,\underline{c} = \underline{\Lambda}\,\underline{c}\,\underline{b}}$$

$$\Gamma_{ij} = 2\langle y_i|\bar{H}-E|y_j\rangle = 2(H_{ij}-S_{ij}E)$$
$$\Lambda_{ij} = \langle y_i|\delta(s)|y_j\rangle = (y_i|y_j)$$
$$S_{ij} = \langle y_i|y_j\rangle$$

Matrix $\underline{\Lambda}$ is singular, because on the surface S, the ~~basis~~ volume basis $\{y_i\}$ is overcomplete.

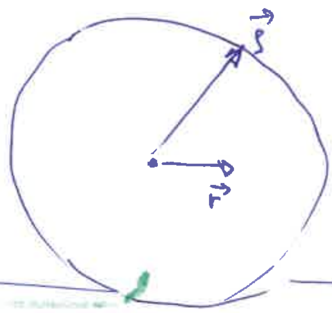
→ Define orthonormal basis on S: $\phi_\alpha(\vec{\rho})$, $(\phi_\alpha|\phi_\beta) = \delta_{\alpha\beta}$. This basis is called channels; Practical example:

V = volume of a sphere r_0

S = surface of the sphere r_0

$$\phi_\alpha = \frac{1}{r_0}Y_{lm}(\hat{r})$$

$$\alpha \equiv \{l,m\}$$



Eigensolutions of (1) will be projected onto ϕ_α on S:

$$\psi_i(E,\vec{\rho}) = \sum_\beta\phi_\beta(\vec{\rho})\,F_{\beta i}$$

$$\partial_n\psi_i(E,\vec{\rho}) = \sum_\beta\phi_\beta(\vec{\rho})\,F'_{\beta i}$$

$$(\psi_i|\psi_j) = \delta_{ij} = \sum_\alpha F^*_{\alpha i}F_{\alpha j} \Rightarrow \underline{\mathbb{1}_s = F^+F}$$

$\underline{F}$ is unitary

$|\phi^*_\alpha$ $$\psi_i(E,\vec{\rho}) = \hat{R}\,\partial_n\psi_i(E,\vec{\rho}) \longleftrightarrow \partial_n\psi_i(E,\vec{\rho}) = \hat{B}(E)\,\psi_i(E,\vec{\rho}) = b_i\,\psi_i(E,\vec{\rho})$$

$$\sum_\beta\phi_\beta(\vec{\rho})F_{\beta i} = \sum_\beta F'_{\beta i}\,\hat{R}\,\phi_\beta(\vec{\rho})$$

$$\boxed{F'_{\alpha i} = F_{\alpha i}\,b_i} \quad \boxed{\underline{F}' = \underline{F}\,\underline{b}}$$

$$F_{\alpha i} = \sum_\beta F'_{\beta i}\,(\phi_\alpha|\hat{R}|\phi_\beta)$$

$$\boxed{\underline{F} = \underline{R}\,\underline{F}'} \Longleftrightarrow \boxed{R = FF'^{-1}}$$

Eigenchannel R matrix (continued)

Projection coefficients of the basis $|y_i)$ on the surface channels $\phi_\alpha(\vec{\varsigma})$

$$y_i(\vec{\varsigma}) = \sum_\alpha \phi_\alpha(\vec{\varsigma})\, u^*_{i\alpha} \;;\quad \Lambda_{ij} = (y_i|y_j) = \sum_{\alpha\beta} u_{i\alpha} u^*_{j\beta} \underbrace{(\phi_\alpha|\phi_\beta)}_{\delta_{\alpha\beta}} = \sum_\alpha u_{i\alpha} u^*_{j\alpha}$$

$$\boxed{u^*_{i\alpha} = (\phi_\alpha|y_i) \Rightarrow u_{i\alpha} = (y_i|\phi_\alpha)}$$

$|\psi_i)$ are eigenstates of the Hermitian operator $\hat{B} \Rightarrow (\psi_i|\psi_j) = \delta_{ij} \Longleftrightarrow c^+\Lambda c = 1\!\!1$

$$\underbrace{cc^+}_{1}\underbrace{\Lambda cc^+}_{1} = cc^+ \rightarrow \boxed{(\Lambda c)^{-1} = c^+ \quad (A)}$$

(B)

One more identity: $F_{\alpha i} = (\phi_\alpha|\psi_i) = \sum_j (\phi_\alpha|y_j) c_{ji} = \sum_j c_{ji} u^*_{j\alpha}$; Matrix form: $\boxed{\underline{F} = \underline{U}^+ \underline{c}}$

Back to R matrix $\boxed{\underline{R} = \underline{F}\,\underline{F}'^{-1} \qquad F'_{\alpha i} = F_{\alpha i} b_i}$ $\underline{F}$ is unitary

$$R_{\alpha\beta} = \sum_i F_{\alpha i} (F'^{-1})_{i\beta} \;;\quad \delta_{\alpha\beta} \overset{\text{unitarity of } F}{=} \sum_i F^*_{\alpha i} F_{\beta i} = \sum_i \underbrace{F^*_{\alpha i} b_i}_{F'^*_{\alpha i}}\, \underbrace{b_i^{-1} F_{\beta i}}_{\Rightarrow (F'^{*-1})_{i\beta}} \;;\; \Rightarrow (F'^{-1})_{i\beta} = F^*_{\beta i} b_i^{-1}$$

$$R_{\alpha\beta} = \sum_i F_{\alpha i} F^*_{\beta i} b_i^{-1} \Longleftrightarrow \boxed{\underline{R} = \underline{F}\, \underline{b}^{-1} \underline{F}^+}$$

$\underline{b}^{-1}$ is diagonal

Eigenchannel form of R matrix

Transforming the eigenchannel form through (B) : $\underline{R} = \underline{F}\,\underline{b}^{-1}\underline{F}^+ = U^+ c\, b^{-1} c^+ U$

Identity from the eigenvalue equation:

$$\underline{\Gamma}\,\underline{c} = \underline{\Lambda}\,\underline{c}\,\underline{b}$$
$$\underline{c} = \underline{\Gamma}^{-1}\underline{\Lambda}\,\underline{c}\,\underline{b}$$
$$\underline{c}\,\underline{b}^{-1} = \underline{\Gamma}^{-1}\underline{\Lambda}\,\underline{c}$$
$$\underline{c}\,\underline{b}^{-1}\underline{c}^+ = \underline{\Gamma}^{-1}\underbrace{\underline{\Lambda}\,\underline{c}}_{(A)}\underbrace{\underline{c}^+}_{1\!\!1} = \Gamma^{-1}$$

$$\boxed{R = U^+ \underbrace{c\, b^{-1} c^+}_{\Gamma^{-1}} U = U^+ \Gamma^{-1} U}$$

$$\boxed{R_{\alpha\beta} = \sum_{ij} (\phi_\alpha|y_i)\, [2(\bar{H} - ES)]^{-1}_{ij}\, (y_j|\phi_\beta)}$$

Kohn's derivation 1948 generalized to 3D (Resolvent form)

Spectral decomposition, poles expansion, Wigner-Eisenbud form

Define: $\boxed{A_{ij} = \bar{H}_{ij} - S_{ij}E}$ Our goal is to compute A^{-1} through the spectral decomposition of $\bar{H}$

Eigenvalues and eigenvectors of $\bar{H} = H + \frac{1}{2}\delta(s)\partial_n$ ($\bar{H}$ is Hermitian inside the volume)

in generally non-orthogonal basis $|y_i\rangle$

$$\bar{H}\,|N_p\rangle = \mathcal{E}_p\,|N_p\rangle \qquad |N_p\rangle = \sum_j V_{jp}\,|y_j\rangle$$

$$\sum_j \langle y_i|\bar{H}|y_j\rangle V_{jp} = \mathcal{E}_\alpha \sum_j V_{jp} \underbrace{\langle y_i|y_j\rangle}_{S_{ij}}$$

$\leftarrow$ overlap matrix

Matrix form: $\boxed{\underline{\bar{H}}\;\underline{V} = \underline{S}\,\underline{V}\,\underline{\mathcal{E}}}$

$\underline{\mathcal{E}}$ is diagonal

Generalized eigenvalue problem (eigenvalue problem in an non-orthogonal basis)

Because $\langle N_p|N_q\rangle = \delta_{pq} = \sum_{ij} V^*_{ip} V_{jq} S_{ij} \iff \underline{V}^+\underline{S}\,\underline{V} = \underline{1}$ (A.)

$$\boxed{\underline{\bar{H}} = \underline{S}\,\underline{V}\,\underline{\mathcal{E}}\,\underline{V}^+\underline{S}}$$

to be compared with the case of the orthonormal basis, where $\underline{\bar{H}} = \underline{V}\,\underline{\mathcal{E}}\,\underline{V}^+$

This spectral decomposition ~~of~~ of $\hat{\bar{H}}$ allows the following:

$$\underline{A}^{-1} = (\underline{\bar{H}} - E\underline{S})^{-1} = [(\underline{S}\underline{V}\underline{\mathcal{E}}\underline{V}^+ - E\underline{1})\underline{S}]^{-1} = \underline{S}^{-1}(\underline{S}\underline{V}\underline{\mathcal{E}}\underline{V}^+ - E\,\underbrace{\underline{S}\underline{V}\underline{V}^+}_{1\ (A)})^{-1}$$

$$= \underline{S}^{-1}[\underline{S}\underline{V}(\underline{\mathcal{E}} - E)\underline{V}^+]^{-1} = \underline{S}^{-1}\underbrace{\underline{V}^{+-1}}_{(A)\ SV}(\underline{\mathcal{E}} - E)^{-1}\underbrace{(\underline{S}\underline{V})^{-1}}_{(A)\ V^+} = \underline{V}(\underline{\mathcal{E}} - \underline{E})^{-1}\underline{V}^+$$

$$\boxed{\underline{A}^{-1} = V(\mathcal{E} - E)^{-1}V^+}$$

$\rightarrow$ put inside the resolvent form of Kohn

$$R_{\alpha\beta} = \frac{1}{2}\sum_{ij}\sum_p \underbrace{\langle\phi_\alpha|\delta(s)|y_i\rangle V_{ip}}_{\text{with } \sum_i \text{ it gives } |N_p\rangle} \frac{1}{\mathcal{E}_p - E} \underbrace{V^*_{jp}\langle y_j|\delta(s)|\phi_\beta\rangle}_{\text{with } \sum_j \text{ we have } \langle N_p|}$$

$$\boxed{R_{\alpha\beta} = \frac{1}{2}\sum_p \frac{(\phi_\alpha|N_p)(N_p|\phi_\beta)}{\mathcal{E}_p - E}}$$

Wigner-Eisenbud form 1947

Expansion over the poles of $\bar{H}$

$(\phi_\alpha|N_p)$ ... surface amplitudes, projection of the p-th eigenfunction $|N_p\rangle$ onto the α-th surface channel