Lesson 1

Winter 2019

Variational principles in the scattering theory

- Commonly known Rayleigh-Ritz method for the discrete spectrum
$$[E] = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$
- The energy is prescribed for the continuum states
- RR method gives an approximation for ψ and for E
- Variational principles do not provide eigenstates and eigenenergies, just their approximations
- Why VP's then?

1.) Kohn VP

2.) Schwinger method

3.) R-matrix

(1) Kohn variational principle (initially by Hulten 1944)

$$\underbrace{\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + 2V(r) - k^2\right]}_{L_l(E)} u_l(r) = 0$$

- Functional

$$I_l = \int_0^\infty \bar{u}_l(r)\, L_l(E)\, \bar{u}_l(r) \quad \ldots \text{ for real trial solutions } \bar{u}_l(r)$$

A.) $\bar{u}_l(0) = 0$

B.) $\bar{u}_l(r) \xrightarrow{r\to\infty} F_l(kr) + \bar{\lambda}\, G_l(kr)$ … $F_l(kr), G_l(kr)$ linearly independent free solutions for $V(r)=0$

$u_l(r) \xrightarrow{r\to\infty} F_l(kr) + \lambda\, G_l(kr)$

- Functional $I_l = 0$ for trial $\bar{u}_l = u_l$

– ~~Th Variat~~

Variation of I_ℓ around the exact solution, i.e. $\overline{u_\ell}(r) = u_\ell(r) + \delta u_\ell(r)$

A.) $\delta u_\ell(r) = 0$

B.) $\delta u_\ell(r) \xrightarrow{r\to\infty} \delta\lambda \, G_\ell(kr)$

$$\delta I_\ell = \int_0^\infty \delta u_\ell L_\ell u_\ell + \underbrace{\int_0^\infty u_\ell L_\ell \delta u_\ell}_{A} + \int_0^\infty \delta u_\ell L_\ell \delta u_\ell \quad ; \quad \boxed{W(F,G) = FG' - F'G}$$

A) kinetic energy $-\frac{d^2}{dr^2}$ is a single non-symmetric (non-hermitian) operator on class of functions $u_\ell(r)$, $\delta u_\ell(r)$

$$-\int_0^R u_\ell \frac{d^2}{dr^2}\delta u_\ell = -\left[u_\ell \frac{d}{dr}\delta u_\ell\right]_0^R + \int_0^R \frac{du_\ell}{dr}\frac{d\delta u_\ell}{dr} = \underbrace{-\left[u_\ell \frac{d}{dr}\delta u_\ell\right]_0^R + \left[\frac{du_\ell}{dr}\delta u_\ell\right]_0^R}_{W(\delta u_\ell, u_\ell)\big|_{R\to\infty} = \delta\lambda k W(G,F)}$$

$$-\int_0^R \frac{d^2 u_\ell}{dr^2}\delta u_\ell$$

$$\delta I_\ell = 2\underbrace{\int_0^R \delta u_\ell L_\ell u_\ell}_{0} + \delta\lambda k \underbrace{W(G,F)}_{-W(F,G)\equiv -W} + \int_0^\infty \delta u_\ell L_\ell \delta u_\ell$$

$$\boxed{\delta I_\ell = -\delta\lambda k W(F,G) + \int_0^\infty \delta u_\ell L_\ell \delta u_\ell}$$

Kato identity

$$\boxed{[\lambda] = \overline{\lambda} + \frac{1}{kW}\int_0^\infty \overline{u_\ell} L_\ell \overline{u_\ell}}$$

General Kohn VP

Choice of the asymptotics F_ℓ, G_ℓ:

1.) $F_\ell(kr) = \sin\left(kr - \frac{\ell\pi}{2}\right)$

$G_\ell(kr) = \cos(kr - \ell\pi/2)$

$u_\ell(r) \xrightarrow{r\to\infty} \sin(kr - \ell\pi/2) + \lambda\cos(kr - \ell\pi/2)$

$\boxed{W(F_\ell, G_\ell) = -1, \quad \lambda = \operatorname{tg}\delta_\ell}$ $\quad [\operatorname{tg}\delta_\ell] = \overline{\operatorname{tg}\delta_\ell} - \frac{1}{k}\int_0^\infty \overline{u_\ell} L_\ell \overline{u_\ell}$ $\quad$ Kohn

2.) $\boxed{W_\ell(F_\ell, G_\ell) = +1, \quad \lambda = \operatorname{cotg}\delta_\ell}$

$F_\ell(kr) = \cos(kr - \ell\pi/2)$

$G_\ell(kr) = \sin(kr - \ell\pi/2)$

$[\operatorname{cotg}\delta_\ell] = \overline{\operatorname{cotg}\delta_\ell} + \frac{1}{k}\int_0^\infty \overline{u_\ell} L_\ell \overline{u_\ell}$ $\quad$ Rubinow (Inverse Kohn VP)

3.) Whole procedure needs to be repeated

$u_\ell(r) \xrightarrow{r\to\infty} \sin(kr - \ell\pi/2 + \delta)$ $\quad [\delta_\ell] = \overline{\delta_\ell} + \frac{1}{k}\int_0^\infty \overline{u_\ell} L_\ell \overline{u_\ell}$ $\quad$ Hulthén

Kohn variational method: solution in a basis

- Assume that $V(r)$ is negligible beyond R.

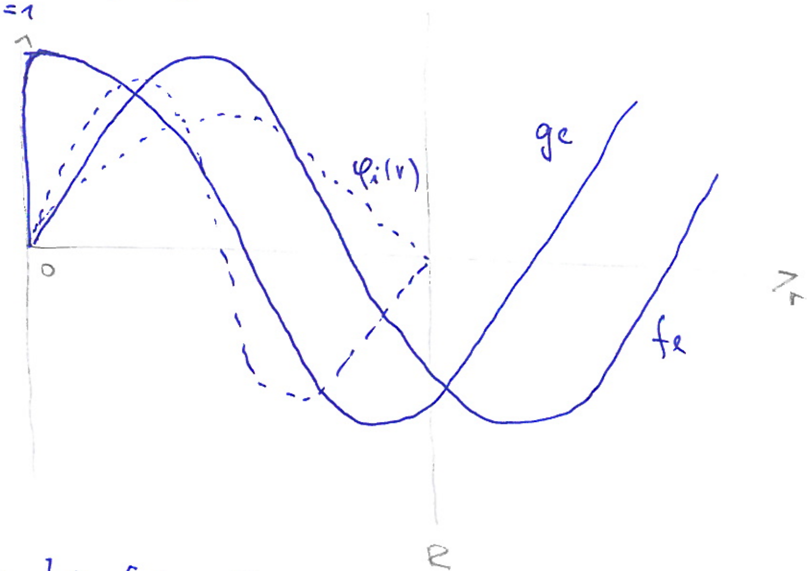
$$\bar{u}_\ell(r) = f_\ell(kr) + \bar{\lambda}\, g_\ell(kr) + \sum_{i=1}^{N} c_i \varphi_i(r)$$

basis consists of $N+2$ elements

A.) $\varphi_i(0) = 0$

B.) $\varphi_i(r) = 0$ for $r \geq R$

C.) $f_\ell(0) = g_\ell(0) = 0$



$$[\lambda] = \bar{\lambda} + \frac{1}{kW}\int_0^\infty \Big[f_\ell(kr) + \bar{\lambda} g_\ell(kr) + \sum_i c_i \varphi_i\Big] L_\ell \Big[f_\ell + \bar{\lambda} g_\ell + \sum_i c_i \varphi_i\Big]$$

Variations:

1.) $$\frac{\partial[\lambda]}{\partial \bar{\lambda}} = 0 = 1 + \frac{1}{kW}\int_0^R g_\ell L_\ell \bar{u}_\ell + \frac{1}{kW}\int_0^R \bar{u}_\ell L_\ell g_\ell$$

$$= 1 + \frac{2}{kW}\int_0^\infty g_\ell L_\ell \bar{u}_\ell + \frac{1}{kW}\underbrace{W(g_\ell, \bar{u}_\ell)}_{-W(f_\ell, g_\ell)}\Big|_{R\to\infty}$$

$$\Rightarrow \int_0^R g_\ell L_\ell \bar{u}_\ell = 0$$

2.) $$\frac{\partial[\lambda]}{\partial c_j} = 0 \Rightarrow \int \varphi_j L_\ell \bar{u}_\ell = 0$$

$\varphi_0 \equiv g_\ell$, $c_0 \equiv \bar{\lambda}$ gives

$$\rightarrow \int_0^\infty \varphi_j L_\ell \Big(f_\ell + \sum_{i=0}^{N} c_i \varphi_i\Big) = 0 \quad \rightarrow \quad \boxed{\begin{aligned} \underline{M}\,\underline{c} + \underline{S} &= 0 \\ \underline{c} &= -\underline{M}^{-1} S \end{aligned}}$$

M is energy dependent

$$M_{ij} = \int_0^R \varphi_i L_\ell \varphi_j$$

$$S_i = \int_0^\infty \varphi_i L_\ell f_\ell$$

- inversions cause Kohn anomalies for real f_ℓ and g_ℓ
- Problem is solved for $g_\ell = i\,(F_\ell(kr) - i\, G_\ell(kr))$ – komplex Kohn method

2. Schwinger variational principle

- Originated in Schwinger lectures at Harvard, published 1947
- Variational method based on L-S equation

Identities

(we will work with the retarded Green's operator $G_0^{(+)}$)

A. $|\psi_k^{(+)}\rangle = |\varphi_k\rangle + G_0^{(+)} V |\psi_k^{(+)}\rangle$

$$|k^+\rangle = |k\rangle + G_0^{(+)} V |k^+\rangle$$

B. $$\langle k'^-| = \langle k'| + \langle k'^-| V G_0^{(+)}$$

$\langle k'^-|V$ (A) $\Rightarrow$

$$\langle k'^-|V|k^+\rangle = \underbrace{\langle k'^-|V|k\rangle}_{\langle k'|T|k\rangle} + \langle k'^-|V G_0^{(+)} V|k^+\rangle$$

C. $$\langle k'|T|k\rangle = \langle k'^-|V - V G_0^{(+)} V|k^+\rangle$$

→ $|k^+\rangle$ and $\langle k'^-|$ are the exact solutions

→ $|\bar{k}^+\rangle$ and $\langle \bar{k}'^-|$ are the trial solutions

New identity

from C we have

$$\langle k'|T|k\rangle = \langle \bar{k}'^- - k'^-|V - V G_0^{(+)} V|\bar{k}^+ - k^+\rangle - \langle \bar{k}'^-|V - V G_0^{(+)} V|\bar{k}^+\rangle +$$
$$+ \langle \bar{k}'^-|\underbrace{V - V G_0^{(+)} V|k^+\rangle}_{(A)\ V|k\rangle} + \underbrace{\langle k'^-|V - V G_0^{(+)} V}_{(B)\ \langle k'|V}|\bar{k}^+\rangle$$

Therefore:

$$\boxed{\langle k'|T|k\rangle = \langle \bar{k}'^-|V|k\rangle + \langle k'|V|\bar{k}^+\rangle - \langle \bar{k}'^-|V - V G_0^{(+)} V|\bar{k}^+\rangle + \langle \Delta k'^-|V - V G_0^{(+)} V|\Delta k^+\rangle}$$

Still an identity

$|\Delta k^+\rangle = |\bar{k}^+ - k^+\rangle$

$\langle \Delta k'^-| = \langle \bar{k}'^- - k'^-|$

Let's assume $\langle \bar{k}'^-|$ and $|\bar{k}^+\rangle$ are exact:

$$\langle k'|T|k\rangle = \langle k'|T|k\rangle + \langle k'|T|k\rangle - \langle k'|T|k\rangle + \phi$$

$$\boxed{[\langle k'|T|k\rangle] = \langle \bar{k}'^-|V|k\rangle + \langle k'|V|\bar{k}^+\rangle - \langle \bar{k}'^-|V - V G_0^{(+)} V|\bar{k}^+\rangle + \mathcal{O}(\Delta k^2)}$$

Linear form of the Schwinger variational principle

A note: Is it possible to form VP instead of $t = t + t - t$ in form of $t = \frac{t \cdot t}{t}$?

Is $\langle k' | T | k \rangle = \frac{\langle k' | V | \bar{k}^+ \rangle \langle \bar{k}'^- | V | k \rangle}{\langle \bar{k}'^- | V - V G_0^{(+)} V | \bar{k}^+ \rangle}$ variationally stable?

Substitutions in the Schwinger VP stimulated by reduction of multi-dimensionality of $\langle \bar{k}'^- | V G_0^{(+)} V | \bar{k}^+ \rangle$ integral.

1.) $|q^+\rangle \equiv V |\bar{k}^+\rangle$ $\quad [\langle k' | T | k \rangle] = \langle k' | q^+ \rangle + \langle q'^- | k \rangle - \langle q'^- | V^{-1} - G_0^{(+)} | q^+ \rangle$

$\langle q'^- | \equiv \langle \bar{k}'^- | V$

may be a problem

2.) Partial substitution (compromise)

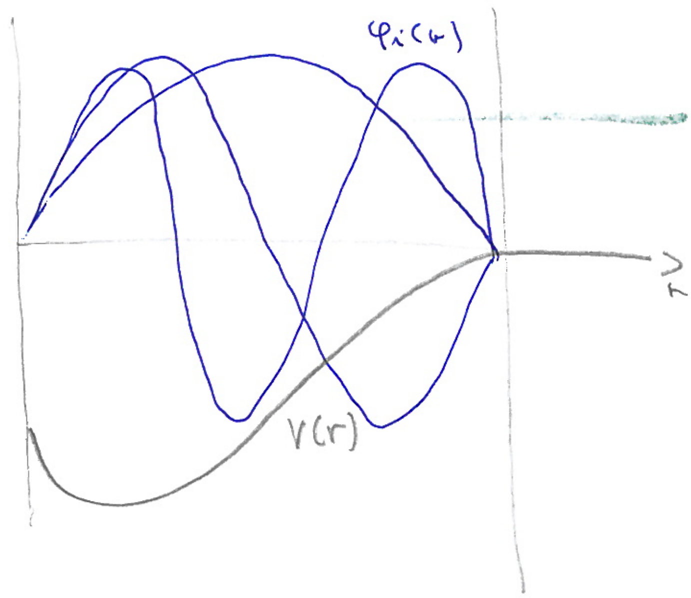
$\langle q'^- | \equiv \langle \bar{k}'^- | V$

$[\langle k' | T | k \rangle] = \langle k' | V | \bar{k}^+ \rangle + \langle q'^- | k \rangle - \langle q'^- | \mathbb{1} - G_0^{(+)} V | \bar{k}^+ \rangle$

Schwinger variational method: solution in a basis

A Comparison with the Kohn VP:

- L^2 basis is sufficient for finite range V, because $\langle \bar{k}'^- |$ and $| \bar{k}^+ \rangle$ are always multiplied by V
- No boundary conditions in the basis because $G_0^{(+)}$ is taking care of that



Basis set $\quad |\bar{k}^+\rangle = \sum_i b_i |\varphi_i\rangle$

$|\bar{k}'^-\rangle = \sum_j c_j |\varphi_j\rangle$

Lesson 7

Winter 2019

$$[\langle k'|T|k\rangle] = \sum_i b_i \langle k'|V|\varphi_i\rangle + \sum_j c_j \langle \varphi_j|V|k\rangle - \sum_{ij} b_i c_j \langle \varphi_j|V - VG_0^{(+)}V|\varphi_i\rangle$$

1.) $\dfrac{\partial[\langle k'|T|k\rangle]}{\partial b_i} = 0$: $\langle k'|V|\varphi_i\rangle = \sum_j c_j \langle \varphi_j|V - VG_0^{(+)}V|\varphi_i\rangle$

2.) $\dfrac{\partial[\langle k'|T|k\rangle]}{\partial c_j} = 0$: $\langle \varphi_j|V|k\rangle = \sum_i \langle \varphi_j|V - VG_0^{(+)}V|\varphi_i\rangle b_i$

Define $(D^{-1})_{ji} = \langle \varphi_j|V - VG_0^{(+)}V|\varphi_i\rangle$

1.) $c_j = \sum_i \langle k'|V|\varphi_i\rangle D_{ij}$

2.) $b_i = \sum_j D_{ij} \langle \varphi_j|V|k\rangle$

After substitution into all the 3 term become identical to each other

$$\boxed{[\langle k'|T|k\rangle] = \sum_{ij} \langle k'|V|\varphi_i\rangle D_{ij} \langle \varphi_j|V|k\rangle}$$

- Independent of the normalization $|k^+\rangle$ and $|k'^-\rangle$
- Most of L^2 bases work fine
- Following Schwinger-Lanczos method in which the basis $|\varphi_i\rangle$ is generated step-by-step for an optimal set with small number of #elements.