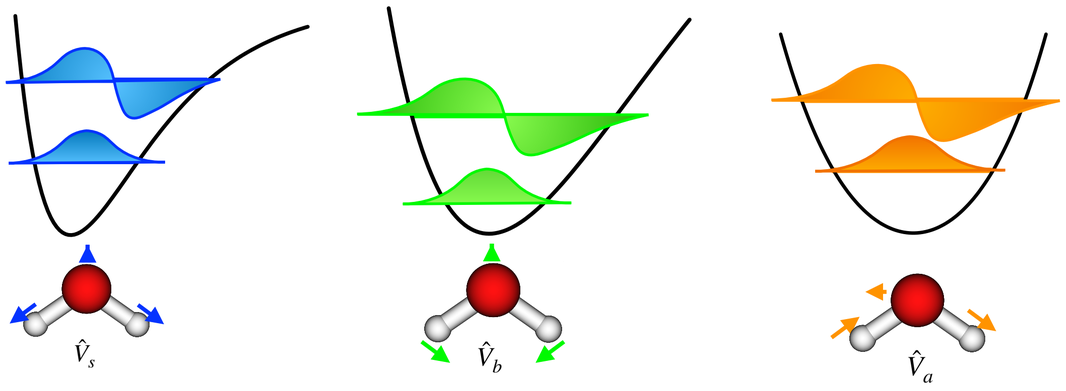
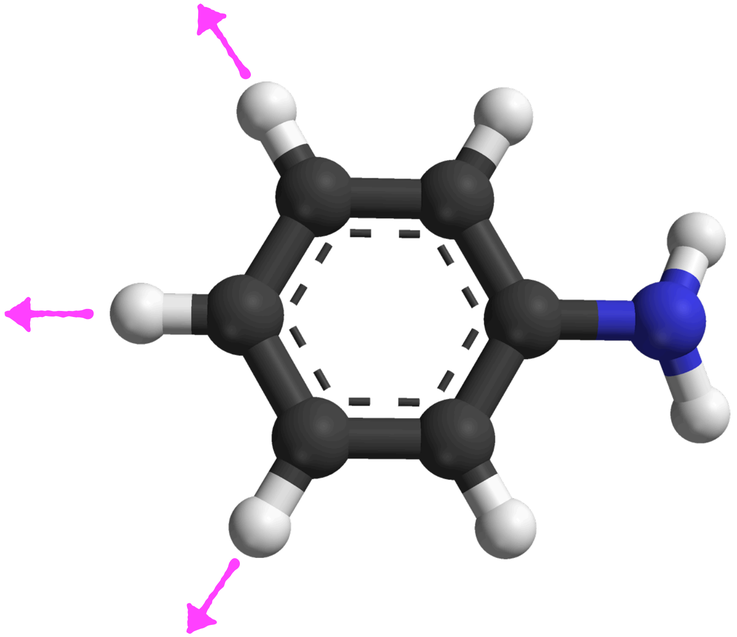
Stealing ideas from electronic structure to improve vibrational calculations

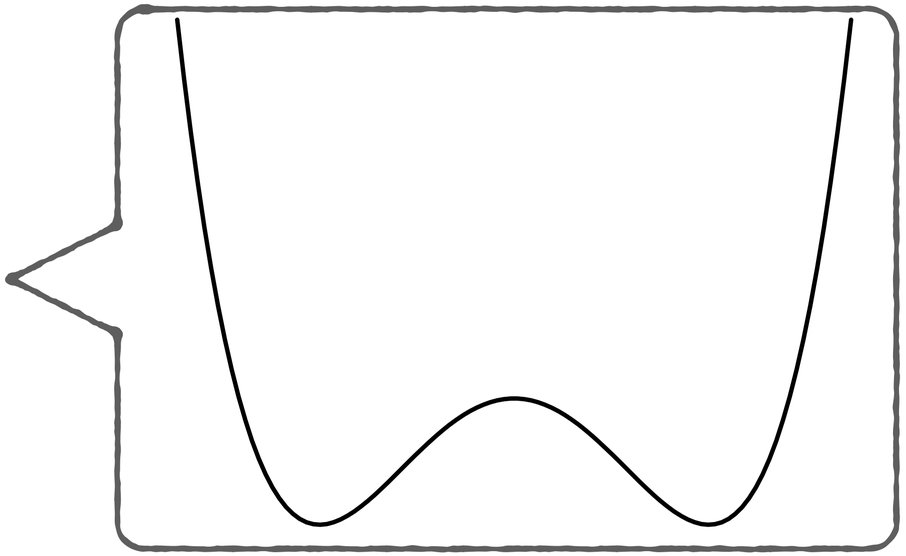
Part II. The Wavefunction



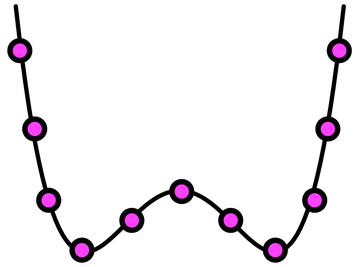
James H. Thorpe
Southern Methodist University
ISMS 2023

Motivation





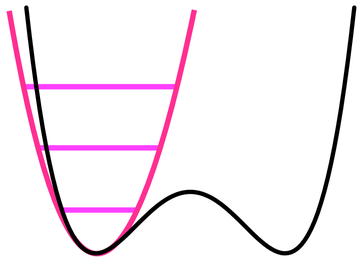
Variational



$$\begin{bmatrix} \hat{H} \end{bmatrix}\begin{bmatrix} C \end{bmatrix} = \begin{bmatrix} C \end{bmatrix}\begin{bmatrix} \varepsilon \end{bmatrix}$$

Bucknell *et al.*, *Mol. Phys.,* **28** (1974)

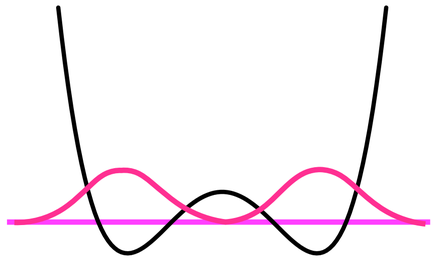
VPT



$$E^{(2)} = \langle\chi|\hat{H}^{(2)}|\chi\rangle + \sum_{\chi'} \frac{\langle\chi|\hat{H}^{(2)}|\chi'\rangle^2}{\epsilon^{(1)} - \epsilon^{(0)}}$$

I. M. Mills, *Mol. Spec.,* 115-140 (1972)

VMBT

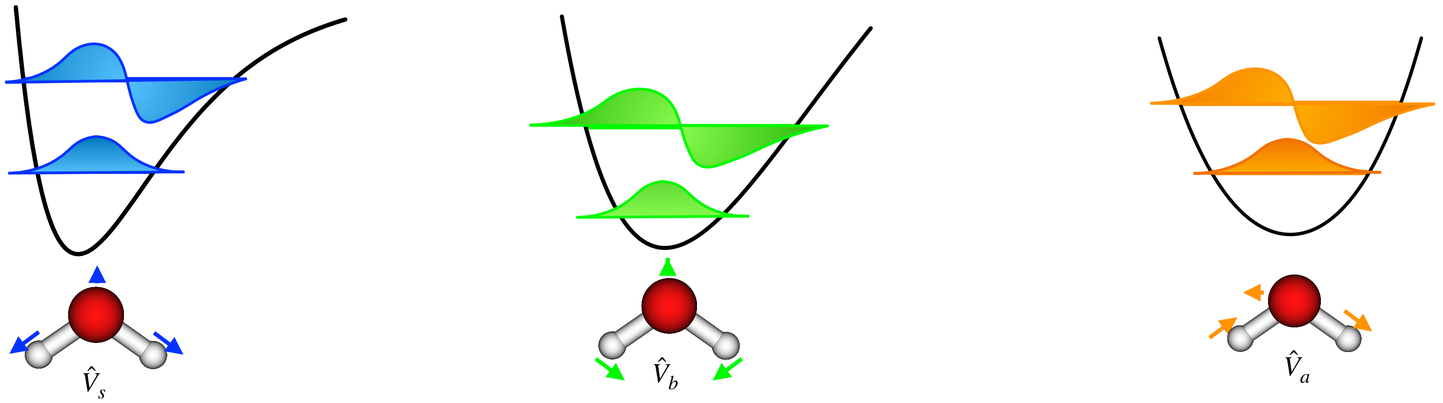


$$E = \langle 0|\hat{H}\hat{C}|0\rangle$$

J. M. Bowman, *JCP*, **68** (1978)

Part I. The Hamiltonian

Transformed the MultiMode (Many-Body) Hamiltonian to the GEN Hamiltonian



MultiMode

$$\hat{H}_1 = \sum_I H_I = \sum_I \sum_{m_I m_I'} h_{m_I'}^{m_I} \hat{b}_{m_I'}^{m_I}$$

$$\hat{H}_2 = \frac{1}{2} \sum_{IJ} H_{IJ} = \frac{1}{2} \sum_{IJ} \sum_{m_I m_I'} \sum_{m_J m_J'} h_{m_I' m_J'}^{m_I m_J} \hat{b}_{m_I'}^{m_I} \hat{b}_{m_J'}^{m_J}$$

$$\vdots$$

GEN

$$\tilde{F}_1 = \sum_I \tilde{F}_I = \sum_I \sum_{m_I m_I'} \tilde{f}_{m_I'}^{m_I} \hat{b}_{m_I'}^{m_I}$$

$$\tilde{G}_2 = \frac{1}{2} \sum_{IJ} \tilde{G}_{IJ} = \frac{1}{2} \sum_{IJ} \sum_{m_I m_I'} \sum_{m_J m_J'} \tilde{g}_{m_I' m_J'}^{m_I m_J} \hat{b}_{m_I'}^{m_I} \hat{b}_{m_J'}^{m_J}$$

$$\vdots$$

S. Carter, S. J. Culik, and J. M. Bowman, *TCA*, **100**, 191 (1998)
O. Christiansen, *JCP*, **120**, 2140 (2004)

J. H. Thorpe, *Dissertation* (2022)

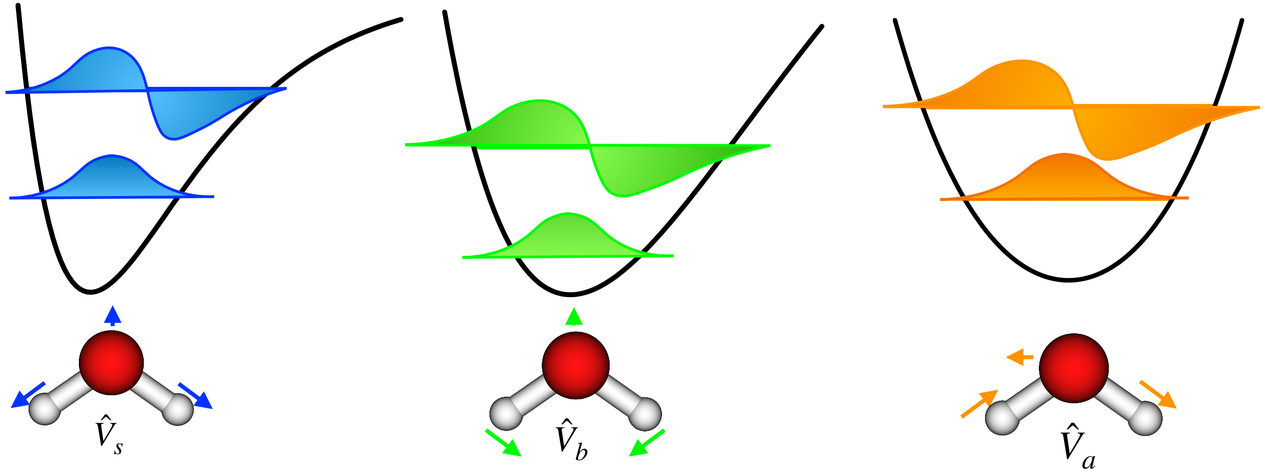
Part II. The Wavefunction

How do we construct useful wave functions with GEN Hamiltonian?

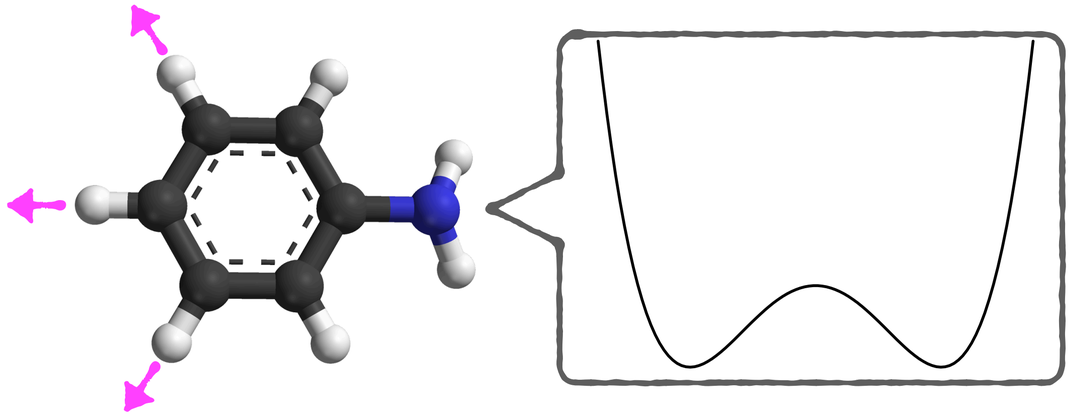
Vibrational CI

Simple, flexible, “fast”, VCI is commonplace in VMBT Calculations

$$\begin{bmatrix} \hat{H} \end{bmatrix} \begin{bmatrix} C \end{bmatrix} = \begin{bmatrix} C \end{bmatrix} \begin{bmatrix} \varepsilon \end{bmatrix}$$



$$\begin{array}{c} \\ \langle \Xi_0 | \\ \langle \Xi_S | \\ \langle \Xi_D | \end{array} \begin{array}{c} \begin{array}{ccc} |\Xi_0\rangle & |\Xi_S\rangle & |\Xi_D\rangle \end{array} \\ \begin{bmatrix} 0 & & \\ \tilde{F}_1 & \tilde{F}_1 + \tilde{G}_2 & \\ \tilde{G}_2 & \tilde{F}_1 + \tilde{G}_2 + \tilde{G}_3 & \begin{array}{c} \tilde{F}_1 + \tilde{G}_2 \\ +\tilde{G}_3 + \tilde{G}_4 \end{array} \end{bmatrix} \end{array} \begin{bmatrix} 1 \\ C_S \\ C_D \end{bmatrix}$$

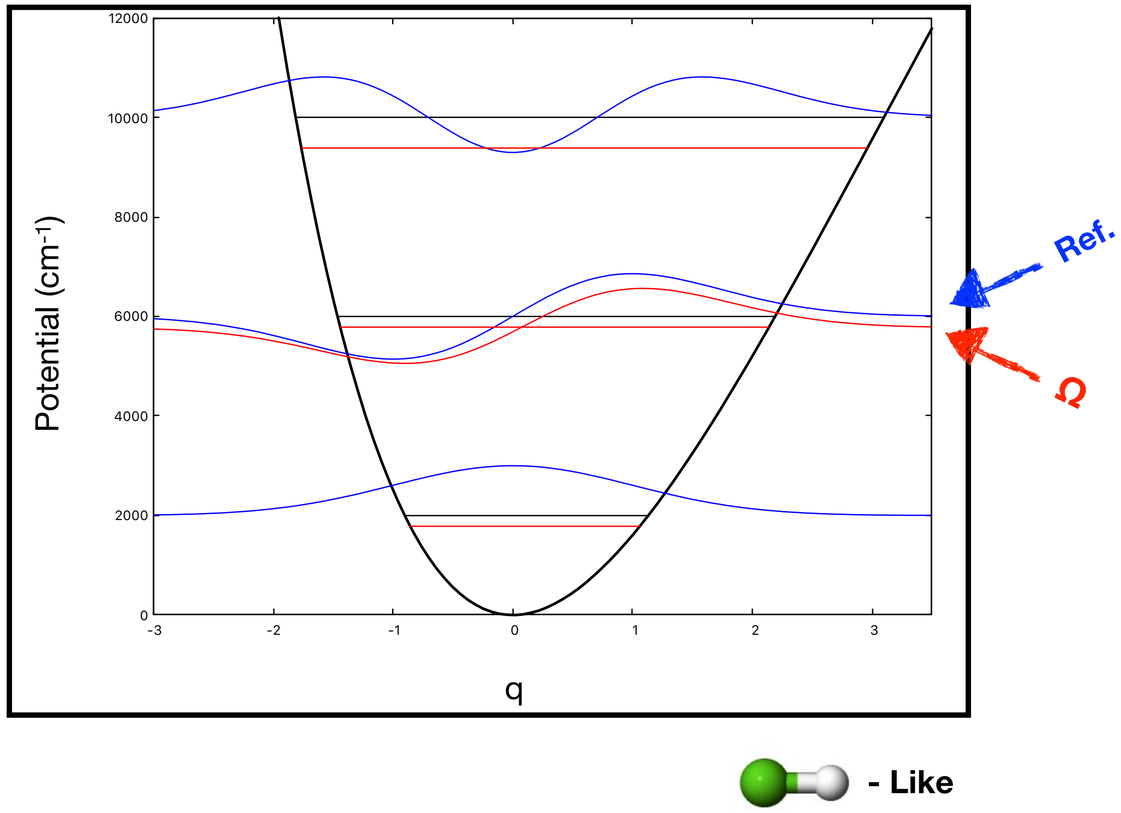


S. Carter, S. J. Culik, and J. M. Bowman, *TCA*, **100**, 191 (1998)

J. H. Thorpe, *Dissertation* (2022)

A Model System

Single Morse Oscillator, “VCIS” is a full-variational calculation



- Like

Basis Functions	v=0 VCIS	v=1 VCIS	Fundamental VCIS
Reference	2044.6	6224.5	4179.9
± 1	1988.0	5859.9	3871.9
± 2	1987.9	5844.3	3856.4
± 3	1976.3	5796.9	3820.5
± 4	1975.2	5779.1	3804.0
± 5	1975.1	5777.2	3802.1
± 6	1975.0	5775.8	3800.8
± 7	1975.0	5775.2	3800.2
± 8	1975.0	5775.1	3800.1
± 9	1975.0	5775.0	3800.0
± 10	1975.0	5775.0	3800.0
Exact	1975	5775	3800

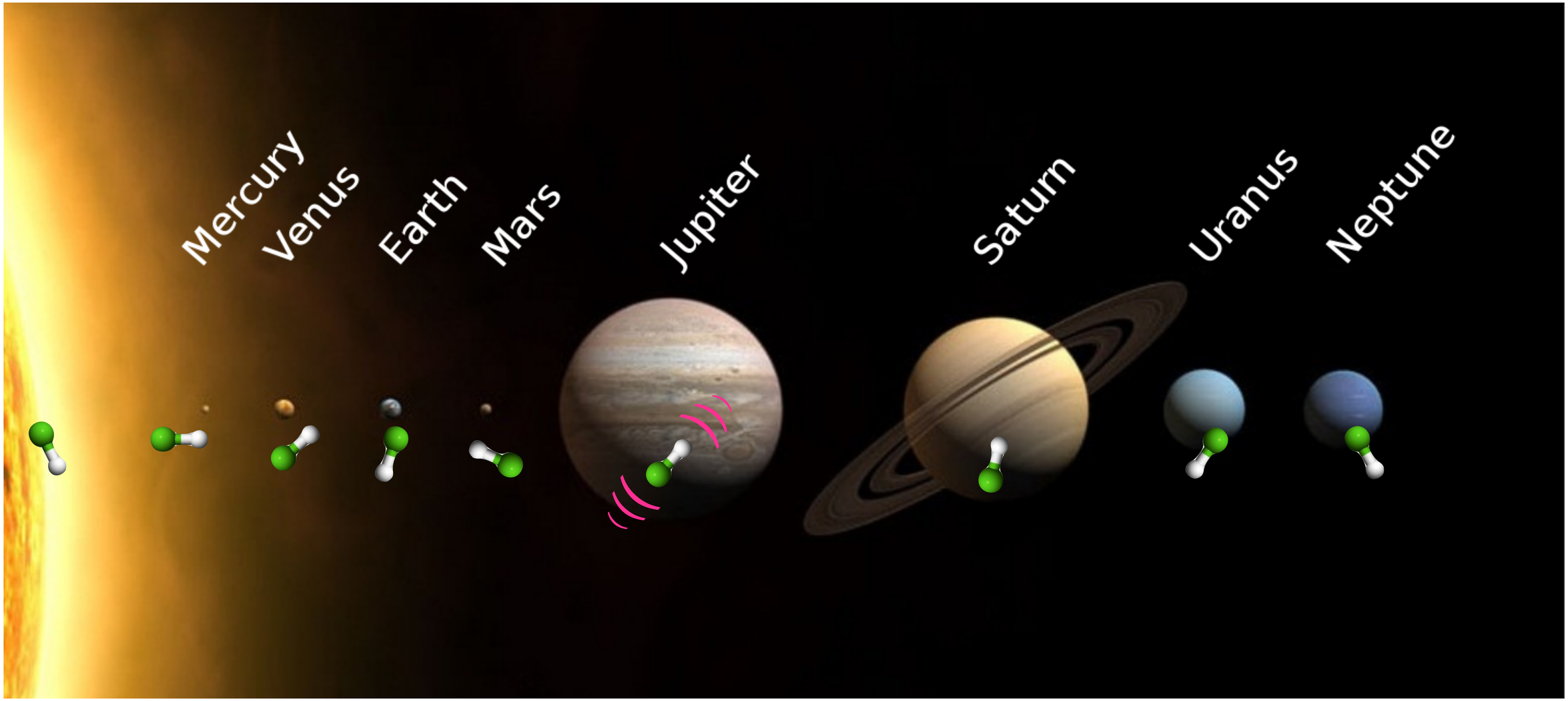
S. Carter, S. J. Culik, and J. M. Bowman, *TCA*, **100**, 191 (1998)

O. Christiansen, *JCP*, **120**, 2140 (2004)

J. H. Thorpe, *Dissertation* (2022)

A Problem

Nine uncoupled Morse Oscillators…



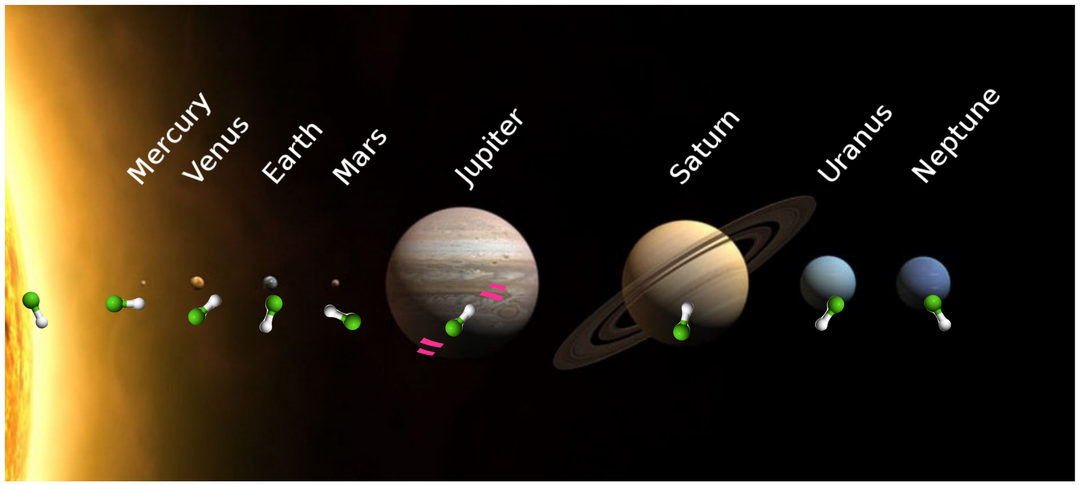
S. Carter, S. J. Culik, and J. M. Bowman, *TCA*, **100**, 191 (1998)

O. Christiansen, *JCP*, **120**, 2140 (2004)

J. H. Thorpe, *Dissertation* (2022)

A Problem

VCI has a problem — size consistency/extensivity



- Like

Basis Functions	v=0 VCIS	v=1 VCIS	Fundamental VCIS
Reference	18401.1	22581.0	4179.9
± 1	17936.9	21860.8	3923.9
± 2	17936.5	21850.9	3914.4
± 3	17845.3	21736.7	3891.4
± 4	17837.7	21717.9	3880.2
± 5	17837.6	21716.7	3879.1
± 6	17836.7	21715.0	3878.2
± 7	17836.6	21714.4	3877.8
± 8	17836.6	21714.4	3877.8
± 9	17836.6	21714.3	3877.7
± 10	17836.6	21714.3	3877.7
Exact	17775	21575	3800

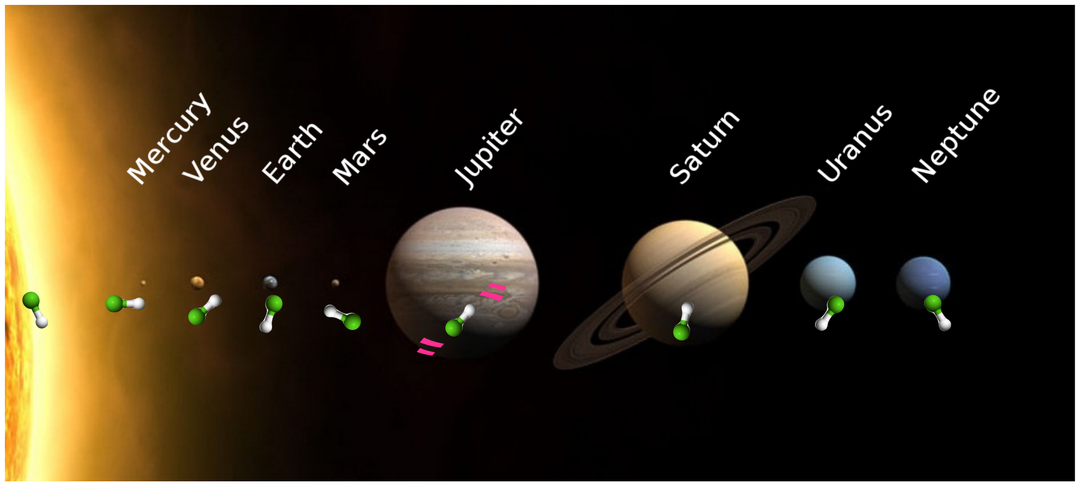
S. Carter, S. J. Culik, and J. M. Bowman, *TCA*, **100**, 191 (1998)

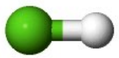
O. Christiansen, *JCP*, **120**, 2140 (2004)

J. H. Thorpe, *Dissertation* (2022)

Vibrational Coupled Cluster

VCCX is exact for ∞ uncoupled X-body vibrations




- Like

Basis Functions	v=0 VCCS	v=0 VCIS	v=1 VCCS	v=1 VCIS	Fundamental VCCS	Fundamental VCIS
			$(HF)_9$			
Reference	18401.1	18401.1	22581.0	22581.0	4179.9	4179.9
± 1	17892.2	17936.9	21764.1	21860.8	3871.9	3923.9
± 2	17890.9	17936.5	21747.3	21850.9	3856.4	3914.4
± 3	17787.1	17845.3	21607.7	21736.7	3820.5	3891.4
± 4	17776.5	17837.7	21580.4	21717.9	3804.0	3880.2
± 5	17776.3	17837.6	21578.4	21716.7	3802.1	3879.1
± 6	17775.2	17836.7	21576.0	21715.0	3800.8	3878.2
± 7	17775.0	17836.6	21575.2	21714.4	3800.2	3877.8
± 8	17775.0	17836.6	21575.1	21714.4	3800.1	3877.8
± 9	17775.0	17836.6	21575.0	21714.3	3800.0	3877.7
± 10	17775.0	17836.6	21575.0	21714.3	3800.0	3877.7
Exact	17775		21575		3800	

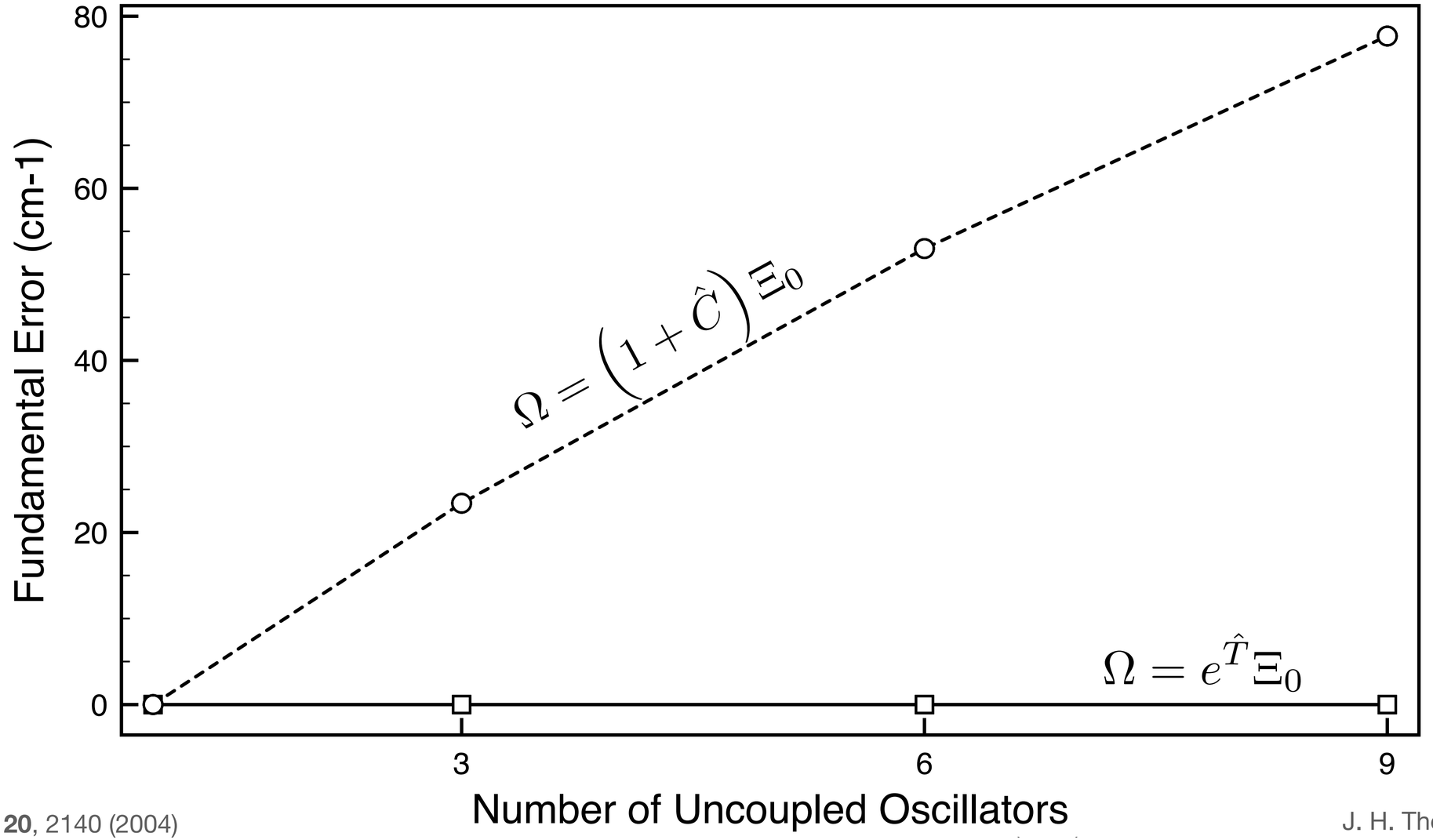
S. Carter, S. J. Culik, and J. M. Bowman, *TCA*, **100**, 191 (1998)

O. Christiansen, *JCP*, **120**, 2140 (2004)

J. H. Thorpe, *Dissertation* (2022)

Vibrational CI — A problem

A pretty extreme example, VCI usually great, but worth investigating



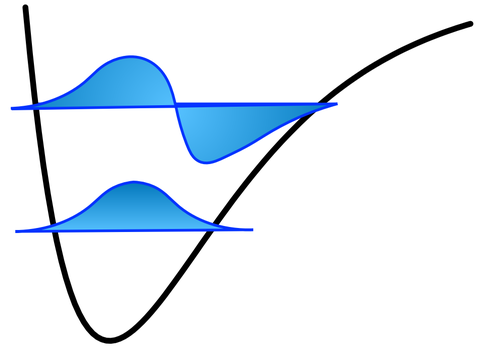
O. Christiansen, *JCP*, **120**, 2140 (2004)

J. H. Thorpe, *Dissertation* (2022)

What gives?

H̃S/VXXS

The working equations looks really similar…



H̃S/VCIS

$$\Omega = (1 + \hat{C}_1)\Xi_0$$

$$E = \sum_{v_I} \tilde{f}^{r_I}_{v_I} c^{v_I}_{r_I}$$

$$c^{v_I}_{r_I} = \frac{1}{\tilde{\epsilon}_{v_I}} (\tilde{f}^{v_I}_{r_I} + \sum_{v'_I} \tilde{f}^{v_I}_{r_I} c^{v'_I}_{r_I} - \tilde{\epsilon}_{v_I} c^{v_I}_{r_I} - E c^{v_I}_{r_I})$$

H̃S/VCCS

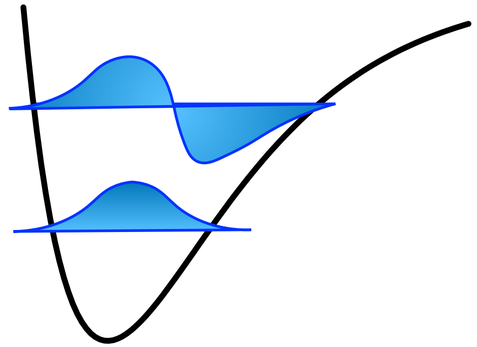
$$\Omega = e^{\hat{T}_1}\Xi_0$$

$$E = \sum_{v_I} \tilde{f}^{r_I}_{v_I} t^{v_I}_{r_I}$$

$$t^{v_I}_{r_I} = \frac{1}{\tilde{\epsilon}_{v_I}} (\tilde{f}^{v_I}_{r_I} + \sum_{v'_I} \tilde{f}^{v_I}_{r_I} t^{v'_I}_{r_I} - \tilde{\epsilon}_{v_I} t^{v_I}_{r_I} - t^{v_I}_{r_I} \sum_{v'_I} \tilde{f}^{r_I}_{v'_I} t^{v_I}_{r_I})$$

H̃S/VXXS

Diagrams reveal the cause of the problem!

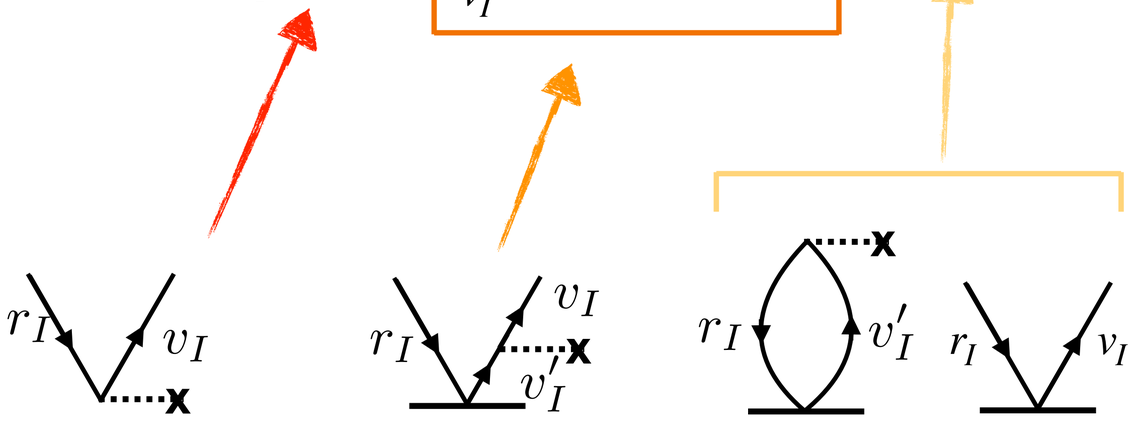


H̃S/VCIS

$$\Omega = (1 + \hat{C}_1)\Xi_0$$

$$E = \sum_{v_I} \tilde{f}^{r_I}_{v_I} c^{v_I}_{r_I}$$

$$c^{v_I}_{r_I} = \frac{1}{\tilde{\epsilon}_{v_I}}(\tilde{f}^{v_I}_{r_I} + \sum_{v'_I} \tilde{f}^{v_I}_{r_I} c^{v'_I}_{r_I} - \tilde{\epsilon}_{v_I} c^{v_I}_{r_I} - E c^{v_I}_{r_I})$$

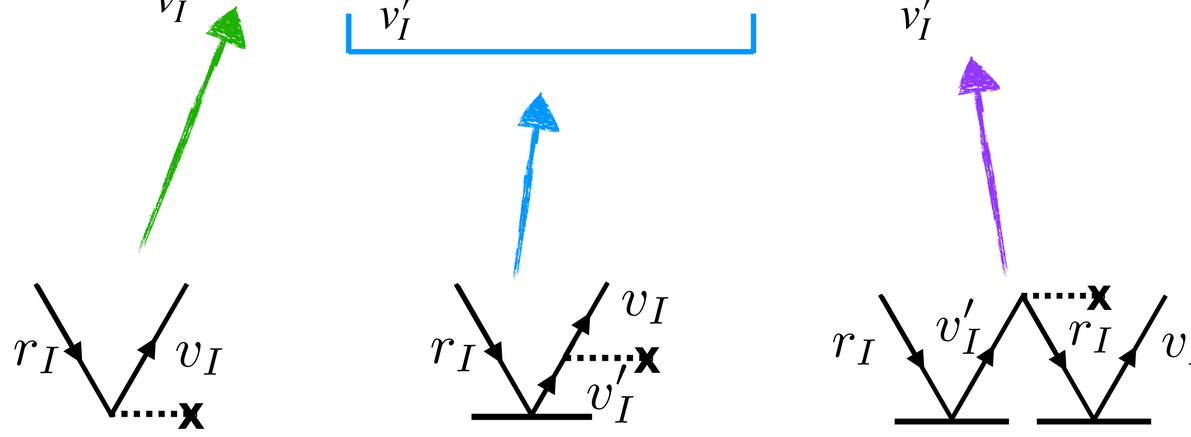


H̃S/VCCS

$$\Omega = e^{\hat{T}_1}\Xi_0$$

$$E = \sum_{v_I} \tilde{f}^{r_I}_{v_I} t^{v_I}_{r_I}$$

$$t^{v_I}_{r_I} = \frac{1}{\tilde{\epsilon}_{v_I}}(\tilde{f}^{v_I}_{r_I} + \sum_{v'_I} \tilde{f}^{v_I}_{r_I} t^{v'_I}_{r_I} - \tilde{\epsilon}_{v_I} t^{v_I}_{r_I} - t^{v_I}_{r_I} \sum_{v'_I} \tilde{f}^{r_I}_{v'_I} t^{v_I}_{r_I})$$

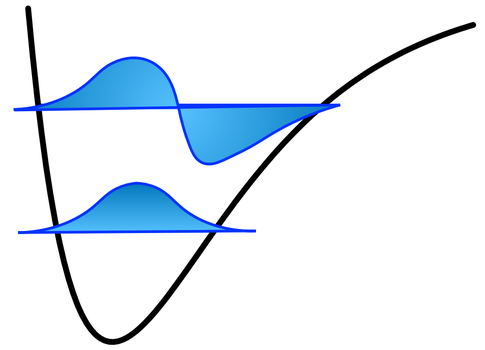


Takeaway #1

Diagrammatic techniques can be really useful in vibrational structure

Davidson-like correction

Can we “fix” this?

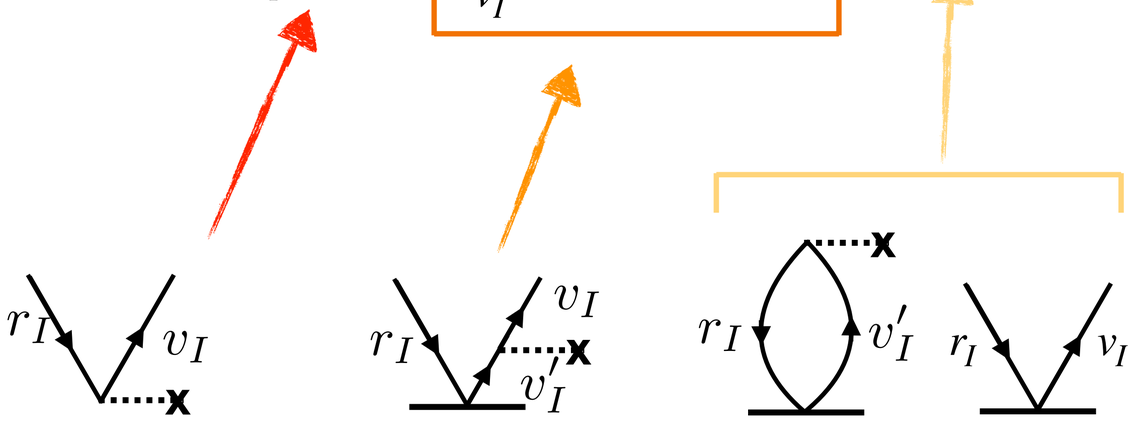


H̃S/VCIS

$$\Omega = (1 + \hat{C}_1)\Xi_0$$

$$E = \sum_{v_I} \tilde{f}^{r_I}_{v_I} c^{v_I}_{r_I}$$

$$c^{v_I}_{r_I} = \frac{1}{\tilde{\epsilon}_{v_I}}(\tilde{f}^{v_I}_{r_I} + \sum_{v'_I} \tilde{f}^{v_I}_{r_I} c^{v'_I}_{r_I} - \tilde{\epsilon}_{v_I} c^{v_I}_{r_I} - E c^{v_I}_{r_I})$$

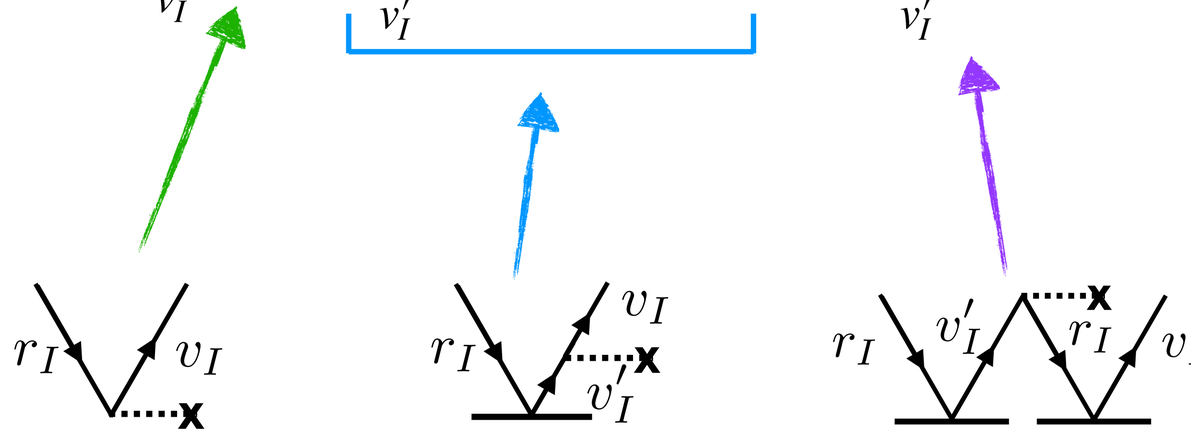


H̃S/VCCS

$$\Omega = e^{\hat{T}_1}\Xi_0$$

$$E = \sum_{v_I} \tilde{f}^{r_I}_{v_I} t^{v_I}_{r_I}$$

$$t^{v_I}_{r_I} = \frac{1}{\tilde{\epsilon}_{v_I}}(\tilde{f}^{v_I}_{r_I} + \sum_{v'_I} \tilde{f}^{v_I}_{r_I} t^{v'_I}_{r_I} - \tilde{\epsilon}_{v_I} t^{v_I}_{r_I} - t^{v_I}_{r_I} \sum_{v'_I} \tilde{f}^{r_I}_{v'_I} t^{v_I}_{r_I})$$



Davidson-like correction

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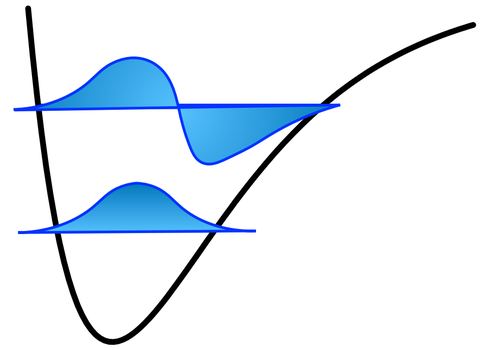
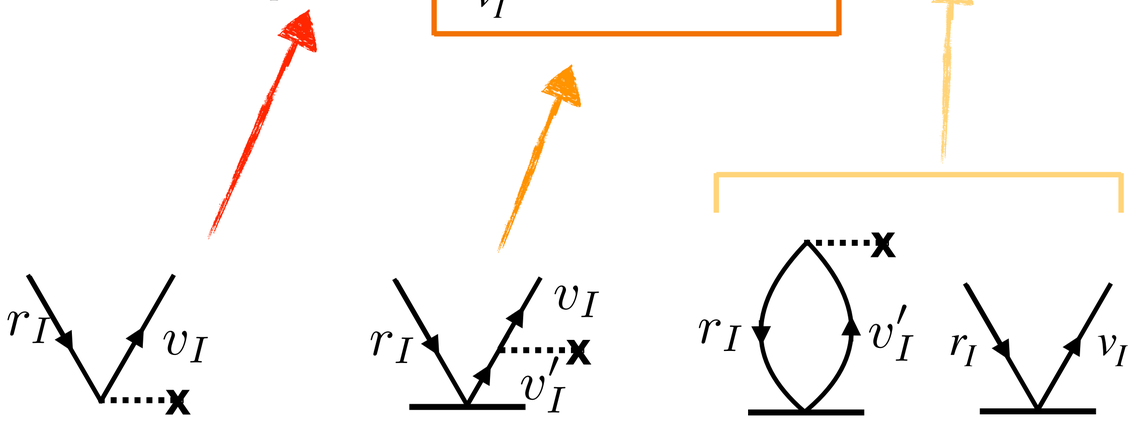


H̃S/VCIS

$$\Omega = (1 + \hat{C}_1)\Xi_0$$

$$E = \sum_{v_I} \tilde{f}^{r_I}_{v_I} c^{v_I}_{r_I}$$

$$c^{v_I}_{r_I} = \frac{1}{\tilde{\epsilon}_{v_I}}(\tilde{f}^{v_I}_{r_I} + \sum_{v'_I} \tilde{f}^{v_I}_{r_I} c^{v'_I}_{r_I} - \tilde{\epsilon}_{v_I} c^{v_I}_{r_I} - E c^{v_I}_{r_I})$$

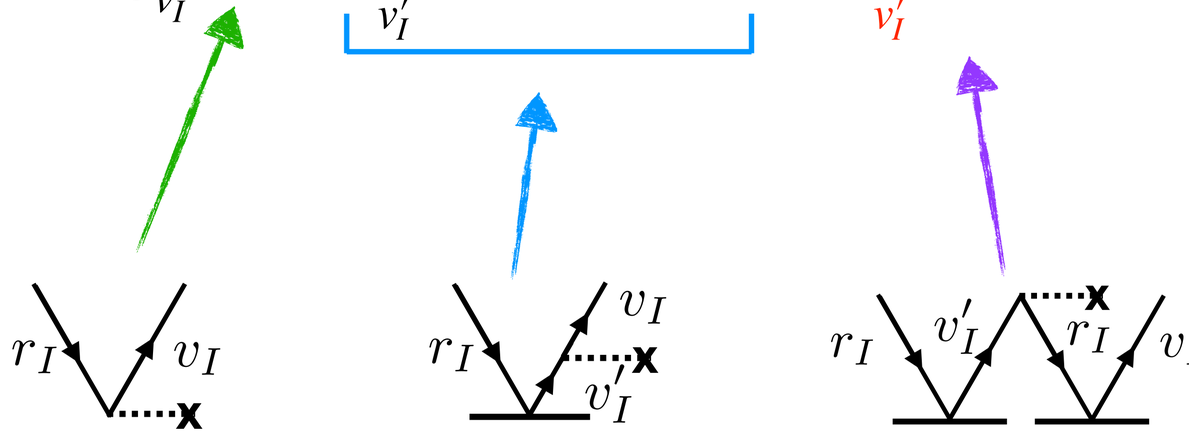


H̃S/VCCS

$$\Omega = e^{\hat{T}_1}\Xi_0$$

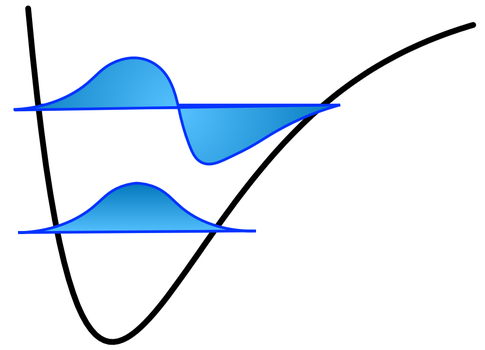
$$E = \sum_{v_I} \tilde{f}^{r_I}_{v_I} t^{v_I}_{r_I}$$

$$t^{v_I}_{r_I} = \frac{1}{\tilde{\epsilon}_{v_I}}(\tilde{f}^{v_I}_{r_I} + \sum_{v'_I} \tilde{f}^{v_I}_{r_I} t^{v'_I}_{r_I} - \tilde{\epsilon}_{v_I} t^{v_I}_{r_I} - t^{v_I}_{r_I} \sum_{v'_I} \tilde{f}^{r_I}_{v'_I} t^{v_I}_{r_I})$$



Davidson-like correction

Can we “fix” this?

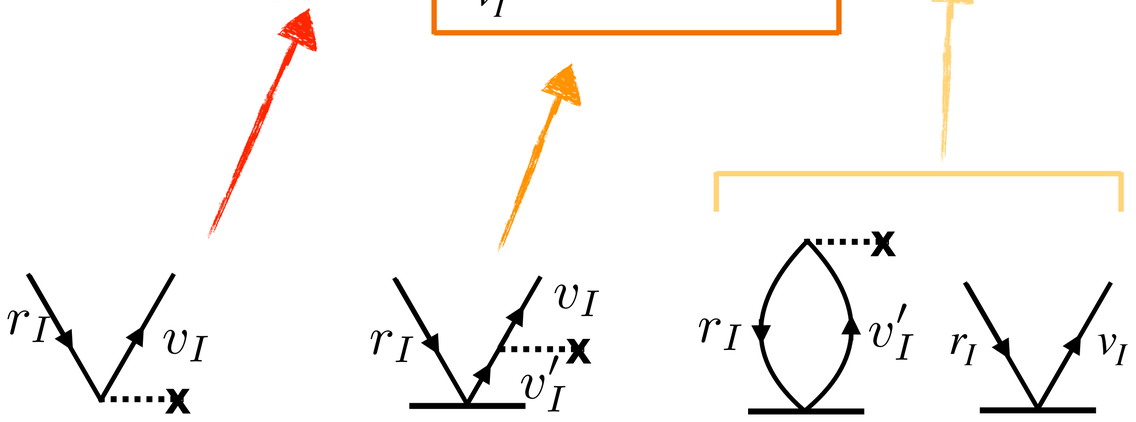


H̃S/VCIS

$$\Omega = (1 + \hat{C}_1)\Xi_0$$

$$E = \sum_{v_I} \tilde{f}^{r_I}_{v_I} c^{v_I}_{r_I}$$

$$c^{v_I}_{r_I} = \frac{1}{\tilde{\epsilon}_{v_I}}(\tilde{f}^{v_I}_{r_I} + \sum_{v'_I} \tilde{f}^{v_I}_{r_I} c^{v'_I}_{r_I} - \tilde{\epsilon}_{v_I} c^{v_I}_{r_I} - E c^{v_I}_{r_I})$$

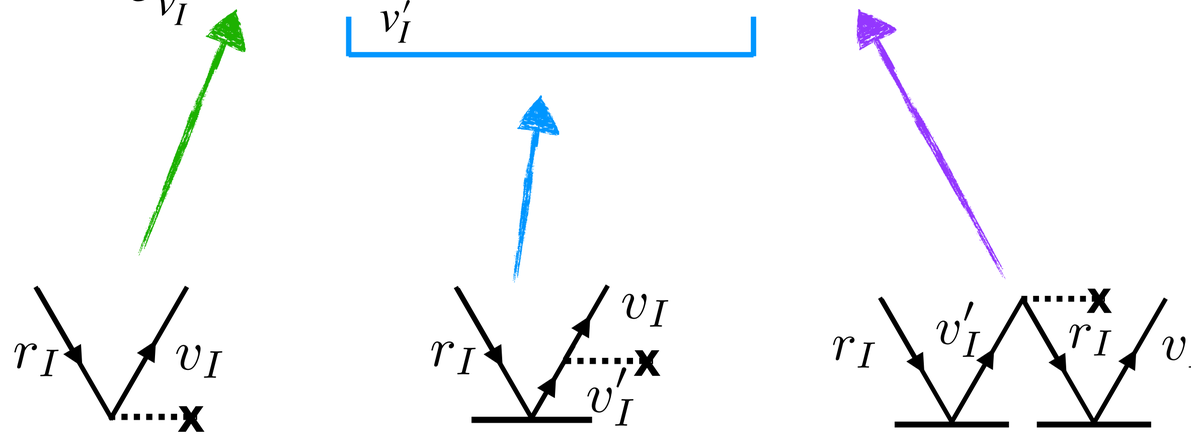


H̃S/VCCS

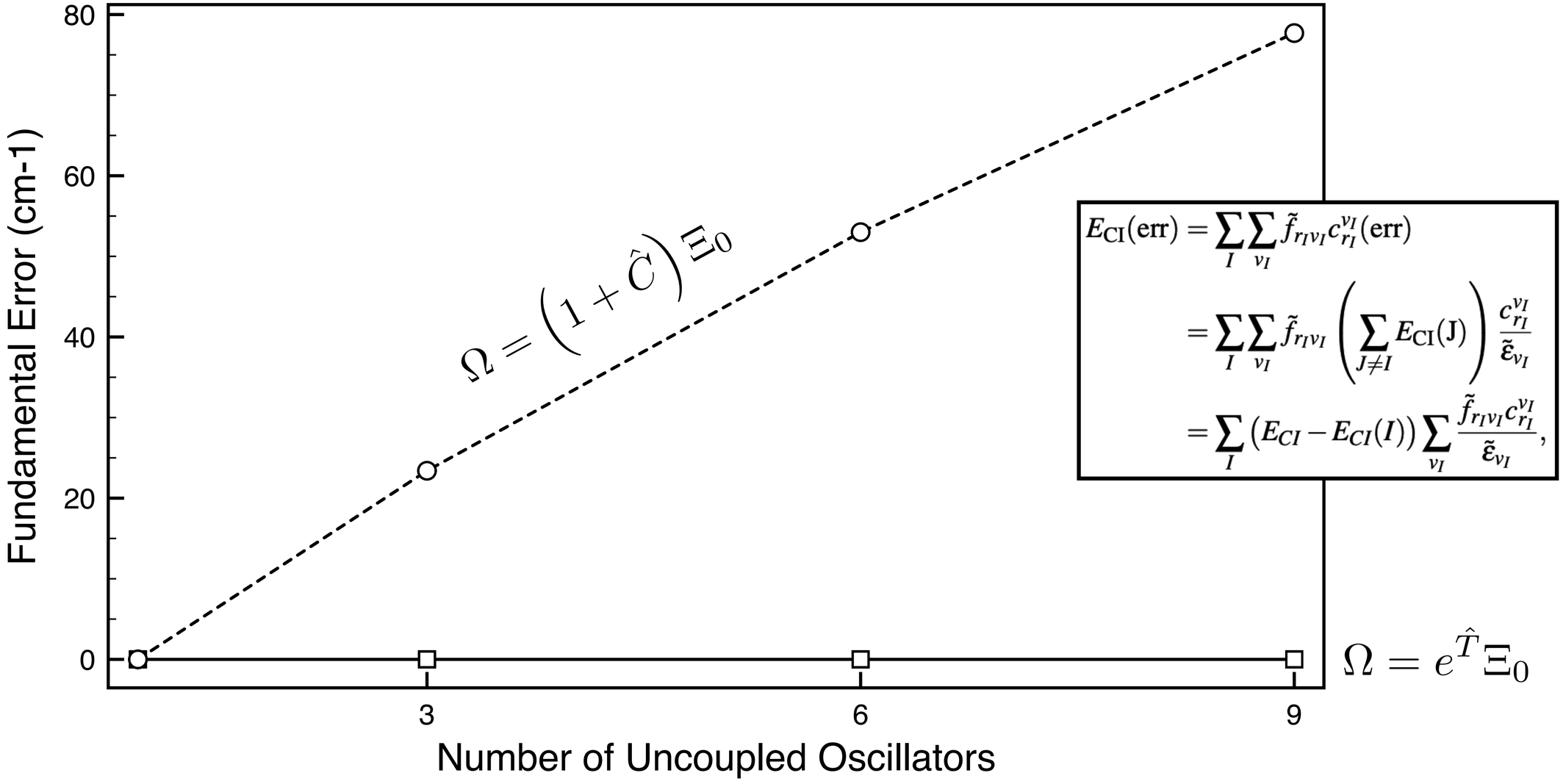
$$\Omega = e^{\hat{T}_1}\Xi_0$$

$$E = \sum_{v_I} \tilde{f}^{r_I}_{v_I} t^{v_I}_{r_I}$$

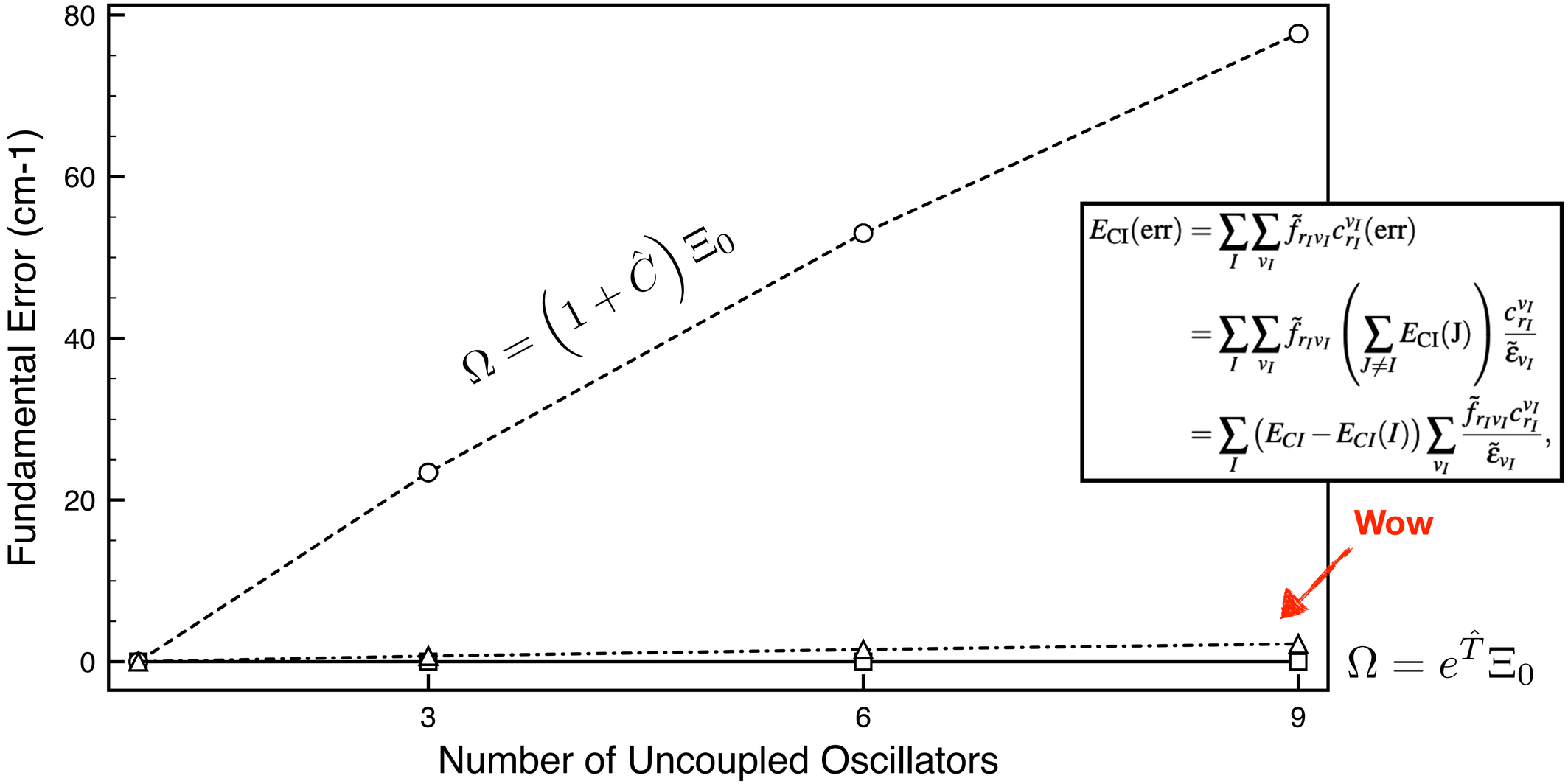
$$t^{v_I}_{r_I} = \frac{1}{\tilde{\epsilon}_{v_I}}(\tilde{f}^{v_I}_{r_I} + \sum_{v'_I} \tilde{f}^{v_I}_{r_I} t^{v'_I}_{r_I} - \tilde{\epsilon}_{v_I} t^{v_I}_{r_I} - E_I t^{v_I}_{r_I})$$



H̃S/VCIS “Davidson-like” Correction



H̃S/VCIS “Davidson-like” Correction



Takeaway #1

Diagrammatic techniques can be really useful in vibrational structure

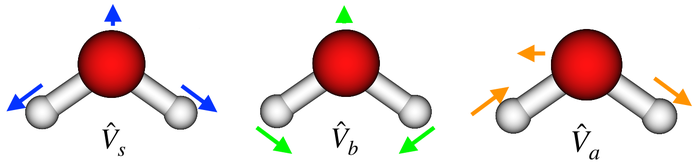
Takeaway #2

Comparing VCI unlinked diagrams to VCC gives a route to estimating (and correcting?) size-c./e. Errors

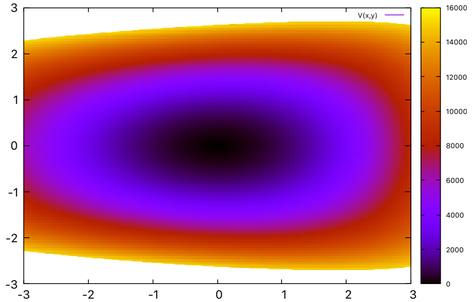
Backup

Workflow of a (VMBT) Simulation

Define coordinate system (q)

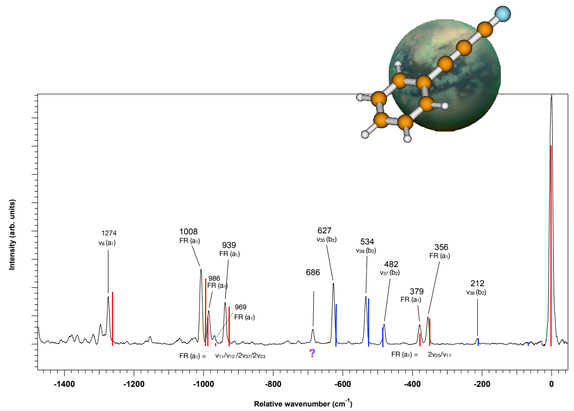


Generate Potential Energy Surface



Reference Hamiltonain/
Wavefunction/Basis

v	1975.000	5775.080	9378.594
0	-0.992	-0.119	-0.008
1	-0.118	0.933	0.323
2	-0.014	0.317	-0.752
3	-0.034	0.079	-0.504
4	-0.009	0.079	-0.198
5	-0.002	0.039	-0.154
6	-0.003	0.014	-0.100
7	-0.001	0.010	-0.048
8	-0.000	0.005	-0.029
9	-0.000	0.002	-0.015



Excited States and Spectra

Part I

Correlated Hamiltonian

$$\begin{aligned}\tilde{g}_{m_I m_J m_K n_I n_J n_K} &= g_{m_I m_J m_K n_I n_J n_K} - g_{m_I m_J r_K n_I n_J r_K}\delta_{m_K,n_K} \\ &- g_{m_I r_J n_K n_I r_J n_K}\delta_{m_J,n_J} - g_{r_I m_J n_K r_I n_J n_K}\delta_{m_I,n_I} \\ &+ g_{m_I r_J r_K n_I r_J r_K}\delta_{m_J,n_J}\delta_{m_K,n_K} + g_{r_I m_J r_K r_I n_J r_K}\delta_{m_I,n_I}\delta_{m_K,n_K} \\ &+ g_{r_I r_J m_K r_I r_J n_K}\delta_{m_I,n_I}\delta_{m_J,n_J} - g_{r_I r_J r_K r_I r_J r_K}\delta_{m_I,n_I}\delta_{m_J,n_J}\delta_{m_K,n_K}.\end{aligned}$$

Part II

Correlated Wavefunction/Energy

$\langle v_s |$ $\langle v_b |$ $\langle v_a |$

$\langle r_s |$ $\langle r_b |$ $\langle r_a |$

$| v_s \rangle$ $| v_b \rangle$ $| v_a \rangle$

$| r_s \rangle$ $| r_b \rangle$ $| r_a \rangle$

$\langle v_s |$ $\langle v_b |$ $\langle v_a |$

$\langle r_s |$ $\langle r_b |$ $\langle r_a |$

$| v_s \rangle$ $| v_b \rangle$ $| v_a \rangle$

$| r_s \rangle$ $| r_b \rangle$ $| r_a \rangle$

Basis Functions	v=0 VCCS	v=0 VCIS	v=0 VCIS*	v=1 VCCS	v=1 VCIS	v=1 VCIS*	Fundamental VCCS	Fundamental VCIS	Fundamental VCIS*
				$(HF)_1$					
Reference	2044.6	2044.6	2044.6	6224.5	6224.5	6224.5	4179.9	4179.9	4179.9
± 1	1988.0	1988.0	1988.0	5859.9	5859.9	5859.9	3871.9	3871.9	3871.9
± 2	1987.9	1987.9	1987.9	5844.3	5844.3	5844.3	3856.4	3856.4	3856.4
± 3	1976.3	1976.3	1976.3	5796.9	5796.9	5796.9	3820.5	3820.5	3820.5
± 4	1975.2	1975.2	1975.2	5779.1	5779.1	5779.1	3804.0	3804.0	3804.0
± 5	1975.1	1975.1	1975.1	5777.2	5777.2	5777.2	3802.1	3802.1	3802.1
± 6	1975.0	1975.0	1975.0	5775.8	5775.8	5775.8	3800.8	3800.8	3800.8
± 7	1975.0	1975.0	1975.0	5775.2	5775.2	5775.2	3800.2	3800.2	3800.2
± 8	1975.0	1975.0	1975.0	5775.1	5775.1	5775.1	3800.1	3800.1	3800.1
± 9	1975.0	1975.0	1975.0	5775.0	5775.0	5775.0	3800.0	3800.0	3800.0
± 10	1975.0	1975.0	1975.0	5775.0	5775.0	5775.0	3800.0	3800.0	3800.0
Exact	1975			5775			3800		

Fundamental		
VCCS	VCIS	VCIS*
4179.9	4179.9	4179.9
3871.9	3871.9	3871.9
3856.4	3856.4	3856.4
3820.5	3820.5	3820.5
3804.0	3804.0	3804.0
3802.1	3802.1	3802.1
3800.8	3800.8	3800.8
3800.2	3800.2	3800.2
3800.1	3800.1	3800.1
3800.0	3800.0	3800.0
3800.0	3800.0	3800.0
3800		

v=1		
VCCS	VCIS	VCIS*
$(HF)_1$		
6224.5	6224.5	6224.5
5859.9	5859.9	5859.9
5844.3	5844.3	5844.3
5796.9	5796.9	5796.9
5779.1	5779.1	5779.1
5777.2	5777.2	5777.2
5775.8	5775.8	5775.8
5775.2	5775.2	5775.2
5775.1	5775.1	5775.1
5775.0	5775.0	5775.0
5775.0	5775.0	5775.0
5775		

	v=0	
VCCS	VCIS	VCIS*
2044.6	2044.6	2044.6
1988.0	1988.0	1988.0
1987.9	1987.9	1987.9
1976.3	1976.3	1976.3
1975.2	1975.2	1975.2
1975.1	1975.1	1975.1
1975.0	1975.0	1975.0
1975.0	1975.0	1975.0
1975.0	1975.0	1975.0
1975.0	1975.0	1975.0
1975.0	1975.0	1975.0
1975		

Basis Functions
Reference
± 1
± 2
± 3
± 4
± 5
± 6
± 7
± 8
± 9
± 10
Exact

$$\begin{bmatrix} \hat{H} \end{bmatrix} \begin{bmatrix} C \end{bmatrix} = \begin{bmatrix} C \end{bmatrix} \boxed{\varepsilon}$$

$r_I \rightarrow$ Reference

$v_I \rightarrow$ Virtual

$m_I \rightarrow$ General

$\hat{b}^{m_I}_{m'_I} \rightarrow$ Subs. Opp.

$\hat{a}^{\dagger}_{v_I}, \hat{a}_{r_I} \rightarrow$ Create Opp.

$\hat{a}_{v_I}, \hat{a}^{\dagger}_{r_I} \rightarrow$ Annhl. Opp.

Basis Functions	v=0 VCCS	v=0 VCIS	v=0 VCIS*	v=1 VCCS	v=1 VCIS	v=1 VCIS*	Fundamental VCCS	Fundamental VCIS	Fundamental VCIS*
				$(HF)_9$					
Reference	18401.1	18401.1	18401.1	22581.0	22581.0	22581.0	4179.9	4179.9	4179.9
± 1	17892.2	17936.9	17891.1	21764.1	21860.8	21756.7	3871.9	3923.9	3865.7
± 2	17890.9	17936.5	17890.4	21747.3	21850.9	21744.0	3856.4	3914.4	3853.5
± 3	17787.1	17845.3	17787.6	21607.7	21736.7	21606.8	3820.5	3891.4	3819.2
± 4	17776.5	17837.7	17778.5	21580.4	21717.9	21583.7	3804.0	3880.2	3805.2
± 5	17776.3	17837.6	17778.4	21578.4	21716.7	21582.2	3802.1	3879.1	3803.8
± 6	17775.2	17836.7	17777.4	21576.0	21715.0	21580.2	3800.8	3878.2	3802.8
± 7	17775.0	17836.6	17777.3	21575.2	21714.4	21579.6	3800.2	3877.8	3802.3
± 8	17775.0	17836.6	17777.3	21575.1	21714.4	21579.5	3800.1	3877.8	3802.2
± 9	17775.0	17836.6	17777.2	21575.0	21714.3	21579.4	3800.0	3877.7	3802.2
± 10	17775.0	17836.6	17777.2	21575.0	21714.3	21579.4	3800.0	3877.7	3802.2
Exact	17775			21575			3800		

Basis Functions	v=0 VCCS	VCIS	VCIS*
Reference	18401.1	18401.1	18401.1
± 1	17892.2	17936.9	17891.1
± 2	17890.9	17936.5	17890.4
± 3	17787.1	17845.3	17787.6
± 4	17776.5	17837.7	17778.5
± 5	17776.3	17837.6	17778.4
± 6	17775.2	17836.7	17777.4
± 7	17775.0	17836.6	17777.3
± 8	17775.0	17836.6	17777.3
± 9	17775.0	17836.6	17777.2
± 10	17775.0	17836.6	17777.2
Exact	17775		

	v=1		
	VCCS	VCIS	VCIS*
$(HF)_9$			
	22581.0	22581.0	22581.0
	21764.1	21860.8	21756.7
	21747.3	21850.9	21744.0
	21607.7	21736.7	21606.8
	21580.4	21717.9	21583.7
	21578.4	21716.7	21582.2
	21576.0	21715.0	21580.2
	21575.2	21714.4	21579.6
	21575.1	21714.4	21579.5
	21575.0	21714.3	21579.4
	21575.0	21714.3	21579.4
	21575		

Fundamental		
VCCS	VCIS	VCIS*
4179.9	4179.9	4179.9
3871.9	3923.9	3865.7
3856.4	3914.4	3853.5
3820.5	3891.4	3819.2
3804.0	3880.2	3805.2
3802.1	3879.1	3803.8
3800.8	3878.2	3802.8
3800.2	3877.8	3802.3
3800.1	3877.8	3802.2
3800.0	3877.7	3802.2
3800.0	3877.7	3802.2
3800		

Many-Body Expansion : Wavefunction