Hamiltonian Zoo

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and Whoever Else Contributes

No Matter Where They're From

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I. MODEL HAMILTONIANS

1. *Coulomb*

$$H_{\text{Coulomb}} = \frac{q_1 q_2}{4\pi\epsilon_0 r} \tag{1}$$

A. Electronic Structure

1. *Molecular Hamiltonian*

$$H_{\text{BO}} = -\sum_A \frac{1}{2M_A}\nabla_A^2 - \sum_i \frac{1}{2}\nabla_i^2 - \sum_{iA}\frac{Z_A}{r_{iA}} + \sum_{i>j}\frac{1}{r_{ij}} + \sum_{B>A}\frac{Z_A Z_B}{R_{AB}} \tag{2}$$

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2. Born-Oppenheimer Model

3. Watson Model

B. Fine and Hyperfine Structure

1. Stark

2. Zeeman

$$H_{\mathrm{Zeeman}} = -\frac{\mu_B \left(g_l \vec{L} + g_s \vec{S}\right)}{\hbar} \cdot \vec{B} \tag{3}$$

3. Complete magnetic dipole interaction

$$H_{\mathrm{Magnetic\,Dipole}} = \frac{g_I \mu_N \mu_B \mu_0}{2\pi} \left(\frac{1}{L_z} \sum_i \frac{\hat{l}_{zi}}{r_i^3} \vec{I} \cdot \vec{L} + \frac{2g_s}{S_z} \sum_i \frac{\hat{s}_{zi}}{r_i^3} \left(3 \left(\vec{I} \cdot \hat{r} \right) \left(\vec{S} \cdot \hat{r} \right) - \vec{I} \cdot \vec{S} \right) + \frac{g_s}{3S_z} \sum_i \hat{s}_{zi} \delta^3 \left(\vec{r}_i \right) \vec{I} \cdot \vec{S} \right) \tag{4}$$

4. Frosch-Foley

$$H_{\mathrm{Frosch-Foley,1}} = \frac{e\hbar}{2mc} \frac{2\mu \cdot \mathbf{L}}{r_1^3} + \frac{\mathrm{i}2\mu_0}{\hbar} \mathbf{S} \cdot [\mathbf{p} \times \mathbf{A}] + \frac{2e^2\hbar}{4m^2c^3} \mathbf{S} \cdot [\epsilon' \times \mathbf{A}]. \tag{5}$$

$$H_{\mathrm{Frosch-Foley,2}} = aI_zL_z + b\vec{I} \cdot \vec{S} + cI_zS_z, \tag{6}$$

where

$$a \equiv 2g_I\mu_0\mu_N \sum_i \left\langle \frac{1}{r_i^3} \right\rangle, \tag{7}$$

$$b \equiv 2g_I\mu_0\mu_N \sum_i \left\langle \frac{2e^2mc^2\mathcal{E}_r}{\left(E + eV + mc^2\right)^2} \frac{\left(1/2 \sin^2\chi + \cos^2\chi\right)}{r_i^2} - \frac{1}{2} \left(\frac{3\cos^2\chi - 1}{r_i^3} \right) \right\rangle, \text{ and} \tag{8}$$

$$c \equiv 2g_I\mu_0\mu_N \sum_i \left\langle \frac{2e^2mc^2\mathcal{E}_r}{\left(E + eV + mc^2\right)^2} \frac{\left(1/2 \sin^2\chi - \cos^2\chi\right)}{r_i^2} + \frac{3}{2} \left(\frac{3\cos^2\chi - 1}{r_i^3} \right) \right\rangle. \tag{9}$$

5. Spin-orbit

6. Orbit-orbit

7. Spin-other-orbit (Gaunt)

8. Fermi Contact

C. Special Relativity

1. Dirac

$$H = \beta mc^2 - eV + c\alpha \cdot (\mathbf{p} - \frac{e}{c}\mathbf{A}). \tag{10}$$

2. Klein-Gordon

3. Darwin ($1e^-$)

$$H_{\text{Darwin}-1} = \alpha_{\text{FS}}^2 \frac{\pi Z}{2} \sum_i \delta\left(\vec{r}_i\right) \tag{11}$$

4. Darwin ($2e^-$)

$$H_{\text{Darwin}-2} = \alpha_{\text{FS}}^2 \pi \sum_{i<j} \delta\left(\vec{r}_{ij}\right) \tag{12}$$

5. Mass Velocity

$$H_{\text{Mass}-\text{Velocity}} = -\alpha_{\text{FS}}^2 \frac{1}{8} \sum_i \nabla_i^4. \tag{13}$$

6. Breit-Pauli

7. Dirac-Coulomb-Breit

D. Quantum Electrodynamics

1. Aracki-Sucher

$$H_{\text{Aracki–Sucher}} = -\alpha_{\text{FS}}^3 \frac{7}{6\pi} \sum_{i>j} \lim_{a\to 0} \left(\frac{\theta\left(r_{ij} - a\right)}{r_{ij}^3} + 4\pi\left(\gamma + \ln a\right)\delta(\vec{r}_{ij}) \right) \tag{14}$$

2. One-Loop

$$H_{1\text{–loop}} = \alpha_{\text{FS}}^4 \pi Z^2 \left(\frac{427}{96} - \ln 2 \right) \sum_i \delta\left(\vec{r}_i\right) \tag{15}$$

3. Schwinger-Dyson

E. Nuclear Motion

$$H_{\text{Nuc}} = -\frac{\hbar^2}{2} \sum_{i=1}^{N} \sum_{\alpha=1}^{3} \frac{1}{M_i} \frac{\partial^2}{\partial R_{i\alpha}^2} + V\left(\boldsymbol{R}_1, \ldots, \boldsymbol{R}_N\right) \tag{16}$$

1. Rigid Rotor Harmonic Oscillator

2. Centrifugal distortion

3. Centrifugal distortion

F. Long-range Interactions

1. van der Waals

2. Lenard-Jones

3. Casimir-Polder

4. Resonance dipole-dipole

5. Meath

6. Axilrod-Teller

G. Hubbard Models

1. Non-interacting Hubbard model

$$H = \sum_{\mathbf{k}} \sum_{\sigma} \left(\varepsilon_{\mathbf{k}} - \mu\right) n_{\mathbf{k},\sigma} \tag{17}$$

2. 1D Hydrogen chain Hubbard model

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + U \sum_{i=1}^{N} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \quad t > 0, U > 0 \tag{18}$$

3. 1D Hydrogen chain Hubbard model with μ term

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + U \sum_{i=1}^{N} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_{i} \left(n_{i\uparrow} + n_{i\downarrow} \right) \tag{19}$$

4. With particle-hole symmetry

$$H = -t \sum_{\langle i,j \rangle} \sum_{\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + U \sum_{i=1}^{N} \left(\hat{n}_{i\uparrow} - \frac{1}{2} \right) \left(\hat{n}_{i\downarrow} - \frac{1}{2} \right) - \mu \sum_{i} \left(n_{i\uparrow} + n_{i\downarrow} \right) \tag{20}$$

5. Bose-Hubbard (Boson Hubbard)

$$H = -t \sum_{\langle i,j \rangle} \hat{b}^{\dagger}_{i} \hat{b}_{j} + \frac{1}{2} U \sum_{i} \hat{n}_{i} \left(\hat{n}_{i} - 1 \right) - \mu \sum_{i} \hat{n}_{i} \tag{21}$$

6. Fermi-Hubbard (Fermi Hubbard)

7. Bose–Fermi–Hubbard

8. Jaynes-Cummings-Hubbard

9. Tavis-Cummings-Hubbard

10. Periodic Anderson Model

$$\begin{aligned} H = & -t \sum_{\langle i,j \rangle} \sum_{\sigma} \left(\hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \hat{c}^{\dagger}_{j,\sigma} \hat{c}_{i,\sigma} \right) + V \sum_{\langle i,j \rangle} \sum_{\sigma} \left(c^{\dagger}_{j\sigma} d_{i\sigma} + d^{\dagger}_{i\sigma} c_{j\sigma} \right) \\ & + U \sum_{i=1}^{N} \left(\hat{n}_{di\uparrow} - \frac{1}{2} \right) \left(\hat{n}_{di\downarrow} - \frac{1}{2} \right) - \mu \sum_{i} \left(n_{di\uparrow} + n_{di\downarrow} + n_{ci\uparrow} + n_{ci\downarrow} \right), \end{aligned} \tag{22}$$

where $d_{i\sigma}$ is the annihilation operator for an electron in the localized band at site i, $c_{i\sigma}$ is the annihilation operator for an electron in the conduction band at site i, V is termed the hybridization and is the transition amplitude of an electron moving from the localized band at site i to the conduction band at site i or vice versa.

H. Disorder Models

1. Tight-binding Model with Onsite Disorder

$$H = \sum_i \omega_i \hat{c}_i^\dagger \hat{c}_i + t \sum_{\langle i,j \rangle} \hat{c}_i^\dagger \hat{c}_j, \tag{23}$$

where ω_i is drawn from a unifrom distribution of width W, the disorder strength, and the angular brackets indicate a sum over nearest-neighbours only.

2. Tight-binding Model with Continuous Off-diagonal Disorder

3. Tight-binding Model with Binary Off-diagonal Disorder

4. Long-range Disorder Models

I. Mean-field Hamiltonians

1. Clean Bose-Hubbard

$$H_{\mathrm{MF}} = \sum_i \left[-\mu \hat{n}_i + \frac{U}{2} \hat{n}_i (\hat{n}_i - 1) - zt(\psi^* \hat{b}_i + \psi \hat{b}_i^\dagger) + zt\psi^* \psi \right] \tag{24}$$

J. Spin lattices

1. XY model

$$H = -J \sum_i \left(\frac{1+\gamma}{2} \sigma_{x,i} \sigma_{x,i+1} + \frac{1-\gamma}{2} \sigma_{y,i} \sigma_{y,i+1} \right) - h \sum_i \sigma_{z,i} \tag{25}$$

$$H = -J \sum_i \left(\frac{1+\gamma}{2} x_i x_{i+1} + \frac{1-\gamma}{2} y_i y_{i+1} \right) - h \sum_i z_i \tag{26}$$

K. Open Quantum Systems

1. *Rabi model*

2. *Spin-Boson*

3. *Feynman-Vernon*

4. *Leggett-Caldeira*

5. *Ishizaki-Fleming*

6. *Jaynes-Cummings*

L. Models of Superconductivity

1. *BCS*

$$H_{\mathrm{BCS}} = \sum_i \epsilon_i n_i + g \sum_{ij} c^\dagger_{i\uparrow} c^\dagger_{-i\downarrow} c_{-j\downarrow} c_{j\uparrow} \tag{27}$$

2. *Richardson-Gaudin*

3. *Exactly solvable pairing Hamiltonians*

SU(2), Rank 1 algebra

$$H_{\mathrm{SU(2)}} = \sum_i \epsilon_i n_i - g \sum_{ij} P^+_i P_j \tag{28}$$

SO(5), Rank 2 algebra

$$H_{\mathrm{SO(5)}} = \sum_i \epsilon_i n_i - g \sum_{ijk} P^+_{ik} P_{jk} \tag{29}$$

SO(8), Rank 4 algebra

$$H_{\mathrm{SO(8)}} = \sum_i \epsilon_i n_i - g_T \sum_{ijk} P^+_{ik} P_{jk} - g_S \sum_{ijk} D^+_{ik} D_{jk} \tag{30}$$

4. t-J model

M. Models of Superfluidity

1. 2D p-wave Fermi superfluid

$$H_{2DFSF} = \sum_i \epsilon_i a_i^\dagger a_i + \frac{\mathrm{i}\Delta_i}{2}\left(a_i^\dagger a_{-i}^\dagger + \mathrm{H.c.}\right) \tag{31}$$

N. Spin models

1. Ising

2. Transverse Ising

3. XY

4. XYZ

O. Heisenberg

P. J1-J2 Model

Q. Majumdar-Ghosh

R. AKLT Model

S. Kitaev Models

1. Toric Code

2. Ocko-Yoshida

3. Honeycomb Model

$$H_{\text{Honeycomb}} = -J_x \sum_{x-\text{links}} x_i x_j - J_y \sum_{y-\text{links}} y_i y_j - J_z \sum_{z-\text{links}} z_i z_j \tag{32}$$

T. Miscellaneous

1. Fertitta-Booth auxiliary Hamiltonian

$$H_{\text{FB}} = \sum_{x=0}^{N_{\text{cells}}-1} \sum_{\alpha}^{N_{\text{Impurities}}} \sum_{k}^{N_{\text{aux}}} \nu_{\alpha k} \left(\hat{c}^{\dagger}_{\alpha+x} \hat{c}_{k+x} + \hat{c}^{\dagger}_{k+x} \hat{c}_{\alpha+x} \right) + \varepsilon_k \hat{c}^{\dagger}_{k+x} \hat{c}_{k+x} \tag{33}$$

Matrix Zoo

U. 2-level systems (spin-1/2 particles)

$$z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, y \equiv \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \tag{34}$$

$$s_+ \equiv \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{x + \mathrm{i}y}{2} \tag{35}$$

$$s_- \equiv \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \frac{x - \mathrm{i}y}{2} \tag{36}$$

$$s_\alpha \equiv \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{\mathbb{1} + z}{2} \equiv b \tag{37}$$

$$s_\beta \equiv \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{\mathbb{1} - z}{2} \tag{38}$$

V. 3-level systems (spin-1 particles)

$$z_3 \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, x_3 \equiv \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, y_3 \equiv \begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix} \tag{39}$$

$$\lambda_1 \equiv \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_2 \equiv \begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_3 \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_4 \equiv \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \tag{40}$$

$$\lambda_5 \equiv \begin{pmatrix} 0 & 0 & -\mathrm{i} \\ 0 & 0 & 0 \\ \mathrm{i} & 0 & 0 \end{pmatrix}, \lambda_6 \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \lambda_7 \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}, \lambda_8 \equiv \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} \tag{41}$$

$$s_{3+} \equiv \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} = \frac{x_3 + \mathrm{i} y_3}{2} \tag{42}$$

$$s_{3-} \equiv \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = \frac{x_3 - \mathrm{i} y_3}{2} \tag{43}$$

$$s_{3,1} \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \frac{\mathbb{1} + z}{2} \equiv t \tag{44}$$

$$s_{3,2} \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{45}$$

$$s_{3,3} \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \frac{\mathbb{1} - z}{2} \equiv t \tag{46}$$

$$|1\rangle\langle 2| \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} = \frac{1}{2} \left(\lambda_6 + \mathrm{i} \lambda_7 \right) \tag{47}$$

$$\lambda_7 \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{48}$$

$$\lambda_7 \lambda_5 = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_3 \lambda_7 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_7 \lambda_3 + \lambda_3 \lambda_7 = \lambda_1 \tag{49}$$

$$\lambda_7 \lambda_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} = -\lambda_6 \lambda_1, \lambda_2 \lambda_7 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = -\lambda_1 \lambda_6, \lambda_7 \lambda_2 + \lambda_2 \lambda_7 = -\lambda_4, \lambda_6 \lambda_1 + \lambda_1 \lambda_6 = \lambda_4 \tag{50}$$

$$\lambda_5^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = |\lambda_1| \tag{51}$$

$$\lambda_5\lambda_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \lambda_2\lambda_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_3\lambda_2 + \lambda_2\lambda_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = \lambda_6 \tag{52}$$

$$\lambda_2^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = |\lambda_3| \tag{53}$$

W. 4-level systems (spin-3/2 particles)

$$z_4 \equiv \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}, x_4 \equiv \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}, y_4 \equiv \begin{pmatrix} 0 & -\sqrt{3}\mathrm{i} & 0 & 0 \\ \sqrt{3}\mathrm{i} & 0 & 2 & 0 \\ 0 & 2 & 0 & -\sqrt{3}\mathrm{i} \\ 0 & 0 & \sqrt{3}\mathrm{i} & 0 \end{pmatrix} \tag{54}$$

$$\gamma^0 \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \gamma^1 \equiv \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & -1 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \gamma^2 \equiv \begin{pmatrix} 0 & 0 & 0 & -\mathrm{i} \\ 0 & 0 & \mathrm{i} & 0 \\ 0 & \mathrm{i} & 0 & 0 \\ -\mathrm{i} & 0 & 0 & 0 \end{pmatrix}, \gamma^3 \equiv \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \gamma^5 \equiv \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{55}$$

$$s_{4+} \equiv \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix} \equiv \frac{x_{3/2} + \mathrm{i}y_{3/2}}{2} \equiv \frac{x_{4\times 4} + \mathrm{i}y_{4\times 4}}{2} \tag{56}$$

$$s_{4-} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix} \equiv \frac{x_4 - \mathrm{i}y_4}{2} \tag{57}$$

$$s_{4,1} \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4}\left(z_2 + z_1 z_2 + z_1 + \mathbb{1}\right) \tag{58}$$

$$s_{4,2} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4}(\mathbb{1} + z_1 - z_2 - z_1 z_2) \tag{59}$$

$$s_{4,3} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4}(\mathbb{1} - z_1 + z_2 - z_1 z_2) \tag{60}$$

$$s_{4,4} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \frac{1}{4}(\mathbb{1} - z_1 - z_2 + z_1 z_2) \tag{61}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \frac{1}{2}\left(\mathbb{1} - z_1 + z_1 z_2 + z_2\right) \tag{62}$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \frac{1}{2}\left(\mathbb{1} - z_2 + z_1 z_2 + z_1\right) \tag{63}$$

$$|10\rangle\langle 01| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4}\left(x_1 x_2 - \mathrm{i} y_1 x_2 + \mathrm{i} x_1 y_2 + y_1 y_2\right) \tag{64}$$

$$|01\rangle\langle 10| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4}\left(x_1 x_2 - \mathrm{i} x_1 y_2 + \mathrm{i} y_1 x_2 + y_1 y_2\right) \tag{65}$$

$$\mathrm{CNOT} \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = \frac{1}{2}\left(\mathbb{1} + z_1 + x_2 - z_1 x_2\right) \tag{66}$$

X. 5-level systems (spin-2 particles)

$$z_5 \equiv \begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -2 \end{pmatrix}, x_5 \equiv \begin{pmatrix} 0 & 2 & 0 & 0 & 0 \\ 2 & 0 & \sqrt{6} & 0 & 0 \\ 0 & \sqrt{6} & 0 & \sqrt{6} & 0 \\ 0 & 0 & \sqrt{6} & 0 & 2 \\ 0 & 0 & 0 & 2 & 0 \end{pmatrix}, y_5 \equiv \begin{pmatrix} 0 & -2\mathrm{i} & 0 & 0 & 0 \\ 2\mathrm{i} & 0 & -\sqrt{6}\mathrm{i} & 0 & 0 \\ 0 & \sqrt{6}\mathrm{i} & 0 & -\sqrt{6}\mathrm{i} & 0 \\ 0 & 0 & \sqrt{6}\mathrm{i} & 0 & -2\mathrm{i} \\ 0 & 0 & 0 & 2\mathrm{i} & 0 \end{pmatrix} \tag{67}$$

$$s_{5+} \equiv \begin{pmatrix} 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{6} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{6} & 0 \\ 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \equiv \frac{x_{5\times5} + \mathrm{i}y_{5\times5}}{2} \equiv \frac{x_{(5)} + \mathrm{i}y_{(5)}}{2} \tag{68}$$

$$s_{5-} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{6} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{6} & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \end{pmatrix} \equiv \frac{x_{5\times5} + \mathrm{i}y_{5\times5}}{2} \equiv \frac{x_{(5)} + \mathrm{i}y_{(5)}}{2} \tag{69}$$

$$s_{5,1} \equiv \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \tag{70}$$

$$s_{5,2} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \tag{71}$$

$$s_{5,3} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \tag{72}$$

$$s_{5,4} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \tag{73}$$

$$s_{5,5} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} = \tag{74}$$

Y. 6-level systems (spin-3/2 particles)

$$x_6 \equiv \begin{pmatrix} 0 & \sqrt{5} & 0 & 0 & 0 & 0 \\ \sqrt{5} & 0 & \sqrt{8} & 0 & 0 & 0 \\ 0 & \sqrt{8} & 0 & \sqrt{9} & 0 & 0 \\ 0 & 0 & \sqrt{9} & 0 & \sqrt{8} & 0 \\ 0 & 0 & 0 & \sqrt{8} & 0 & \sqrt{5} \\ 0 & 0 & 0 & 0 & \sqrt{5} & 0 \end{pmatrix}, y_6 \equiv \begin{pmatrix} 0 & -\sqrt{5}i & 0 & 0 & 0 & 0 \\ \sqrt{5}i & 0 & -\sqrt{8}i & 0 & 0 & 0 \\ 0 & \sqrt{8}i & 0 & -\sqrt{9}i & 0 & 0 \\ 0 & 0 & \sqrt{9}i & 0 & -\sqrt{8}i & 0 \\ 0 & 0 & 0 & \sqrt{8}i & 0 & -\sqrt{5}i \\ 0 & 0 & 0 & 0 & \sqrt{5}i & 0 \end{pmatrix} \tag{75}$$

$$z_6 \equiv \begin{pmatrix} 5 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -3 & 0 \\ 0 & 0 & 0 & 0 & 0 & -5 \end{pmatrix} \tag{76}$$

$$s_{6+} \equiv \begin{pmatrix} 0 & \sqrt{5} & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{8} & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{9} & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{5} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, s_{6-} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ \sqrt{5} & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{8} & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{9} & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{5} & 5 \end{pmatrix} \tag{77}$$

$$|0_b 1_t\rangle\langle 1_b 0_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4}\left(x\lambda_1 + \mathrm{i}y\lambda_1 - \mathrm{i}x\lambda_2 + y\lambda_2\right) \tag{78}$$

$$|1_b 0_t\rangle\langle 0_b 1_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4}\left(x\lambda_1 - \mathrm{i}y\lambda_1 + \mathrm{i}x\lambda_2 + y\lambda_2\right) \tag{79}$$

$$|0_b 1_t\rangle\langle 1_b 0_t| + |1_b 0_t\rangle\langle 0_b 1_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{2}\left(x\lambda_1 + y\lambda_2\right) \tag{80}$$

$$|1_b 1_t\rangle\langle 0_b 1_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \tag{81}$$

$$|1_b1_t\rangle\langle 0_b1_t| + |0_b1_t\rangle\langle 1_b1_t| \equiv \begin{pmatrix} 0&0&0&0&0&0\\ 0&0&0&0&1&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&1&0&0&0&0\\ 0&0&0&0&0&0 \end{pmatrix} = \frac{1}{2}\left(\lambda_5 y + \lambda_4 x\right) \tag{82}$$

$$|1_b0_t\rangle\langle 1_b2_t| \equiv \begin{pmatrix} 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0 \end{pmatrix} = \frac{1}{4}\left(\lambda_6 - z\lambda_6 + \mathrm{i}\lambda_7 - \mathrm{i}z\lambda_7\right) = |1_b1_t\rangle\langle 1_b2_t| \tag{83}$$

$$|1_b0_t\rangle\langle 1_b2_t| + |1_b2_t\rangle\langle 1_b0_t| \equiv \begin{pmatrix} 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&1\\ 0&0&0&0&0&0\\ 0&0&0&1&0&0 \end{pmatrix} = \frac{1}{2}\left(\lambda_6 - \lambda_6 z\right) \tag{84}$$

$$|0_b1_t\rangle\langle 0_b0_t| \equiv \begin{pmatrix} 0&0&0&0&0&0\\ 1&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0 \end{pmatrix} = \frac{1}{4}\left(z\lambda_1 + \lambda_1 - \mathrm{i}z\lambda_2 - \mathrm{i}\lambda_2\right) \tag{85}$$

$$|0_b0_t\rangle\langle 0_b1_t| \equiv \begin{pmatrix} 0&1&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0 \end{pmatrix} = \frac{1}{4}\left(z\lambda_1 + \lambda_1 + \mathrm{i}z\lambda_2 + \mathrm{i}\lambda_2\right) \tag{86}$$

$$|0_b1_t\rangle\langle 0_b0_t| + |0_b0_t\rangle\langle 0_b1_t| \equiv \begin{pmatrix} 0&1&0&0&0&0\\ 1&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0 \end{pmatrix} = \frac{1}{2}\left(z\lambda_1 + \lambda_1\right) \tag{87}$$

$$|0_b2_t\rangle\langle 1_b0_t| \equiv \begin{pmatrix} 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&1&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0 \end{pmatrix} = \frac{1}{4}\left(x\lambda_4 + \mathrm{i}y\lambda_4 - \mathrm{i}x\lambda_5 + y\lambda_5\right) \tag{88}$$

$$|0_b 2_t\rangle\langle 1_b 0_t| + |1_b 0_t\rangle\langle 0_b 2_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{2}\left(x\lambda_4 + y\lambda_5\right) \tag{89}$$

$$|0_b 2_t\rangle\langle 0_b 0_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4}\left(z\lambda_4 + \lambda_4 - \mathrm{i}z\lambda_5 - \mathrm{i}\lambda_5\right) \tag{90}$$

$$|0_b 2_t\rangle\langle 0_b 0_t| + |0_b 0_t\rangle\langle 0_b 2_t| \equiv \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{2}\left(z\lambda_4 + \lambda_4\right) \tag{91}$$

$$|1_b 1_t\rangle\langle 1_b 2_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \tag{92}$$

$$|1_b 1_t\rangle\langle 1_b 2_t| + |1_b 2_t\rangle\langle 1_b 1_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} = \tag{93}$$

$$|1_{t,1}\rangle\langle 2_{t,1}|x_2 + |2_{t,1}\rangle\langle 1_{t,1}|x_2 \equiv \begin{pmatrix} 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&1\\ 0&0&0&0&1&0\\ 0&0&0&1&0&0\\ 0&0&1&0&0&0 \end{pmatrix} = \lambda_6 x_2 = -\frac{1}{2}z\lambda_1 + \frac{1}{2}\lambda_1 - \frac{1}{\sqrt{3}}x\lambda_8 + \frac{1}{3}x \neq x_2\lambda_6 \tag{94}$$

$$x_1|1_{t,2}\rangle\langle 2_{t,2}| \equiv \begin{pmatrix} 0&0&0&0&0&0\\ 0&0&0&0&0&1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&1&0&0&0\\ 0&0&0&0&0&0 \end{pmatrix} = \frac{1}{2}x\left(\lambda_6 + \mathrm{i}\lambda_7\right) \tag{95}$$

$$x_1|1_{t,2}\rangle\langle 2_{t,2}| + x_1|2_{t,2}\rangle\langle 1_{t,2}| \equiv \begin{pmatrix} 0&0&0&0&0&0\\ 0&0&0&0&0&1\\ 0&0&0&0&1&0\\ 0&0&0&0&0&0\\ 0&0&1&0&0&0\\ 0&1&0&0&0&0 \end{pmatrix} = x\lambda_6 \tag{96}$$

$$|0_b 2_t\rangle\langle 1_b 1_t| \equiv \begin{pmatrix} 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&1&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0 \end{pmatrix} = \frac{1}{4}\left(x\lambda_6 + \mathrm{i}y\lambda_6 - \mathrm{i}x\lambda_7 + y\lambda_7\right) = \frac{1}{4}\left(\lambda_6 + \lambda_6 z + \mathrm{i}\lambda_7 + \mathrm{i}\lambda_7 z\right) \neq \frac{1}{4}\left(\lambda_6 + z\lambda_6 + \mathrm{i}\lambda_7 + \mathrm{i}z\lambda_7\right) \tag{97}$$

$$|0_b 1_t\rangle\langle 0_b 2_t| \equiv \begin{pmatrix} 0&0&0&0&0&0\\ 0&0&1&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0 \end{pmatrix} = \frac{1}{4}\left(\lambda_6 + z\lambda_6 + \mathrm{i}\lambda_7 + \mathrm{i}z\lambda_7\right) \neq \frac{1}{4}\left(\lambda_6 + \lambda_6 z + \mathrm{i}\lambda_7 + \mathrm{i}\lambda_7 z\right) \tag{98}$$

$$|0_b 1_t\rangle\langle 0_b 2_t| + |0_b 2_t\rangle\langle 0_b 1_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{2}\left(\lambda_6 + z\lambda_6\right) \tag{99}$$

II. OTHER HAMILTONIANS

A. Feynman Hamiltonian

Wavefunction Zoo

B. Electronic Structure Ansatze

1. Hartree Product

2. Configuration Interaction

3. Coupled Cluster

CC(n)

Bruckner-CC(n)

EOM-CC(n)

EOM-IP-CC(n)

FS-CC(n)

DLPNO-CC(n)

MR-EOM

4. Geminals

AP1roG/pCCD

APIG

APSetG

APG

Potential Zoo

C. Diatomics

Harmonic Oscillator

Morse

Lenard-Jones

Morse/Long-range

Tiemann

Morse-Rosen

D. Triatomics

Jensen

Schwenke

PolyMLR

E. Torsion Potentials

Functional Zoo

Function Zoo

Master Equation Zoo

Particle Zoo

https://en.wikipedia.org/wiki/Particle_zoo

Complexity Zoo (founded by Scott Aarsonson of UWaterloo)

https://complexityzoo.uwaterloo.ca/Complexity_Zoo

Algorithms Zoo (founded by Stephen Jordan of NIST)

https://math.nist.gov/quantum/zoo/