

# Hamiltonian Zoo

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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

$$H_{\text{Zeeman}} = -\frac{\mu_B (g_l \vec{L} + g_s \vec{S})}{\hbar} \cdot \vec{B} \quad (3)$$

#### 3. Complete magnetic dipole interaction

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

#### 4. Frosch-Foley

$$H_{\text{Frosch-Foley},1} = \frac{e\hbar}{2mc} \frac{2\mu \cdot \mathbf{L}}{r_1^3} + \frac{i2\mu_0}{\hbar} \mathbf{S} \cdot [\mathbf{p} \times \mathbf{A}] + \frac{2e^2\hbar}{4m^2c^3} \mathbf{S} \cdot [\epsilon' \times \mathbf{A}]. \quad (5)$$

$$H_{\text{Frosch-Foley},2} = aI_zL_z + b\vec{I} \cdot \vec{S} + cI_zS_z, \quad (6)$$

where

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

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

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

5. *Spin-orbit*

6. *Orbit-orbit*

7. *Spin-other-orbit (Gaunt)*

8. *Fermi Contact*

## C. Special Relativity

1. *Dirac*

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

2. *Klein-Gordon*

3. *Darwin ( $1e^-$ )*

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

4. *Darwin ( $2e^-$ )*

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

5. *Mass Velocity*

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

6. *Breit-Pauli*

7. *Dirac-Coulomb-Breit*

## D. Quantum Electrodynamics

1. *Aracki-Sucher*

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

2. *One-Loop*

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

3. *Schwinger-Dyson*

## E. Nuclear Motion

$$H_{\text{Nuc}} = -\frac{\hbar^2}{2} \sum_{i=1}^N \sum_{\alpha=1}^3 \frac{1}{M_i} \frac{\partial^2}{\partial R_{i\alpha}^2} + V(\mathbf{R}_1, \dots, \mathbf{R}_N) \quad (16)$$

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*

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

2. *1D Hydrogen chain Hubbard model*

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

### 3. 1D Hydrogen chain Hubbard model with $\mu$ term

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

### 4. With particle-hole symmetry

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

### 5. Bose-Hubbard (Boson Hubbard)

$$H = -t \sum_{\langle i,j \rangle} \hat{b}_i^{\dagger} \hat{b}_j + \frac{1}{2} U \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i \quad (21)$$

### 6. Fermi-Hubbard (Fermi Hubbard)

### 7. Bose-Fermi-Hubbard

### 8. Jaynes-Cummings-Hubbard

### 9. Tavis-Cummings-Hubbard

### 10. Periodic Anderson Model

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

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

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

where  $\omega_i$  is drawn from a uniform 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

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

## J. Spin lattices

### 1. XY model

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

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

## 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*

$$H_{\text{BCS}} = \sum_i \epsilon_i n_i + g \sum_{ij} c_{i\uparrow}^\dagger c_{-i\downarrow}^\dagger c_{-j\downarrow} c_{j\uparrow} \quad (27)$$

2. *Richardson-Gaudin*

3. *Exactly solvable pairing Hamiltonians*

*SU(2), Rank 1 algebra*

$$H_{\text{SU}(2)} = \sum_i \epsilon_i n_i - g \sum_{ij} P_i^+ P_j \quad (28)$$

*SO(5), Rank 2 algebra*

$$H_{\text{SO}(5)} = \sum_i \epsilon_i n_i - g \sum_{ijk} P_{ik}^+ P_{jk} \quad (29)$$

*SO(8), Rank 4 algebra*

$$H_{\text{SO}(8)} = \sum_i \epsilon_i n_i - g_T \sum_{ijk} P_{ik}^+ P_{jk} - g_S \sum_{ijk} D_{ik}^+ D_{jk} \quad (30)$$



#### 4. *t*-*J* model

### M. Models of Superfluidity

#### 1. *2D p-wave Fermi superfluid*

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

## 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*

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

## T. Miscellaneous

### 1. *Fertitta-Booth auxiliary Hamiltonian*

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

# Matrix Zoo

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

$$z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (34)$$

$$s_+ \equiv \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{x + iy}{2} \quad (35)$$

$$s_- \equiv \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \frac{x - iy}{2} \quad (36)$$

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

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

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

$$z_3 \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, x \equiv \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, y \equiv \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad (39)$$

$$\lambda_1 \equiv \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_2 \equiv \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_3 \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_4 \equiv \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad (40)$$

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

$$s_{3+} \equiv \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} = \frac{x_3 + iy_3}{2} \quad (42)$$

$$s_{3-} \equiv \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = \frac{x_3 - iy_3}{2} \quad (43)$$

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

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

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

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

$$\lambda_7 \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (48)$$

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

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

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

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

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

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

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

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

$$s_{4+} \equiv \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix} \equiv \frac{x_{3/2} + iy_{3/2}}{2} \equiv \frac{x_{4 \times 4} + iy_{4 \times 4}}{2} \quad (56)$$

$$s_{4-} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix} \equiv \frac{x_4 - iy_4}{2} \quad (57)$$

$$s_{4,1} \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{2} (z_2 + z_1 z_2 + z_1 - \mathbb{1}) \quad (58)$$

$$s_{4,2} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \quad (59)$$

$$s_{4,3} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \quad (60)$$

$$s_{4,4} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \quad (61)$$

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

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

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

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

$$\text{CNOT} \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = \frac{1}{2} (\mathbb{1} + z_1 + x_2 - z_1 x_2) \quad (66)$$

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

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

$$s_{5+} \equiv \begin{pmatrix} 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{6} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{6} & 0 \\ 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \equiv \frac{x_{5 \times 5} + iy_{5 \times 5}}{2} \equiv \frac{x_{(5)} + iy_{(5)}}{2} \quad (68)$$

$$s_{5-} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{6} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{6} & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \end{pmatrix} \equiv \frac{x_{5 \times 5} + iy_{5 \times 5}}{2} \equiv \frac{x_{(5)} + iy_{(5)}}{2} \quad (69)$$

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

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

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

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

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



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

$$|0_b 1_t\rangle\langle 1_b 0_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} (x\lambda_1 + iy\lambda_1 - ix\lambda_2 + y\lambda_2) \quad (75)$$

$$|1_b 0_t\rangle\langle 0_b 1_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} (x\lambda_1 - iy\lambda_1 + ix\lambda_2 + y\lambda_2) \quad (76)$$

$$|0_b 1_t\rangle\langle 1_b 0_t| + |1_b 0_t\rangle\langle 0_b 1_t| \equiv \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{2} (x\lambda_1 + y\lambda_2) \quad (77)$$

$$|2_t 0_b\rangle\langle 0_t 1_b| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \quad (78)$$

$$|2_t 0_b\rangle\langle 0_t 1_b| + |0_t 1_b\rangle\langle 2_t 0_b| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{2} (\lambda_5 y + \lambda_4 x) \quad (79)$$

$$|1_t 1_b\rangle\langle 2_t 1_b| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} (\lambda_6 - z\lambda_6 + i\lambda_7 - iz\lambda_7) = |1_b 1_t\rangle\langle 1_b 2_t| \quad (80)$$

$$|1_t 1_b\rangle\langle 2_t 1_b| + |2_t 1_b\rangle\langle 1_t 1_b| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} = \frac{1}{2} (\lambda_6 - z\lambda_6) \quad (81)$$

$$\equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} (z\lambda_1 + \lambda_1 - iz\lambda_2 - i\lambda_2) \quad (82)$$

$$\equiv \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} (z\lambda_1 + \lambda_1 + iz\lambda_2 + i\lambda_2) \quad (83)$$

$$\equiv \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{2} (z\lambda_1 + \lambda_1) \quad (84)$$

$$|0_b 2_t\rangle\langle 1_b 0_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} (x\lambda_4 + iy\lambda_4 - ix\lambda_5 + y\lambda_5) \quad (85)$$

$$|0_b 2_t\rangle\langle 1_b 0_t| + |1_b 0_t\rangle\langle 0_b 2_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{2} (x\lambda_4 + y\lambda_5) \quad (86)$$

$$\equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} (z\lambda_4 + \lambda_4 - iz\lambda_5 - i\lambda_5) \quad (87)$$

$$\equiv \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} (z\lambda_4 + \lambda_4) \quad (88)$$

$$|1_b 1_t\rangle\langle 1_b 2_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \quad (89)$$

$$|1_b 1_t\rangle\langle 1_b 2_t| + |1_b 2_t\rangle\langle 1_b 1_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} = \quad (90)$$

$$|1_{t,1}\rangle\langle 2_{t,1}|x_2 + |2_{t,1}\rangle\langle 1_{t,1}|x_2 \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} = \lambda_6 x_2 = -\frac{1}{2}z\lambda_1 + \frac{1}{2}\lambda_1 - \frac{1}{\sqrt{3}}x\lambda_8 + \frac{1}{3}x \neq x_2\lambda_6 \quad (91)$$

$$x_1|1_{t,2}\rangle\langle 2_{t,2}| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{2}x(\lambda_6 + i\lambda_7) \quad (92)$$

$$x_1|1_{t,2}\rangle\langle 2_{t,2}| + x_1|2_{t,2}\rangle\langle 1_{t,2}| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} = x\lambda_6 \quad (93)$$

$$|1_t 0_b\rangle\langle 2_t 0_b| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4}(x\lambda_6 + iy\lambda_6 - ix\lambda_7 + y\lambda_7) = \frac{1}{4}(\lambda_6 + \lambda_6 z + i\lambda_7 + i\lambda_7 z) \neq \frac{1}{4}(\lambda_6 + z\lambda_6 + i\lambda_7 + iz\lambda_7) \quad (94)$$

$$|0_b 1_t\rangle\langle 0_b 2_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \neq \frac{1}{4}(\lambda_6 + z\lambda_6 + i\lambda_7 + iz\lambda_7) = \frac{1}{4}(\lambda_6 + \lambda_6 z + i\lambda_7 + i\lambda_7 z) \quad (95)$$

$$|0_b 1_t\rangle\langle 0_b 2_t| + |0_b 2_t\rangle\langle 0_b 1_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{2} (\lambda_6 + \lambda_6 z) \quad (96)$$

## II. OTHER HAMILTONIANS

### A. Feynman Hamiltonian

# Wavefunction Zoo

### B. Electronic Structure Ansätze

#### 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

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**Functional Zoo**

**Function Zoo**

**Master Equation Zoo**

**Particle Zoo**

[https://en.wikipedia.org/wiki/Particle\\_zoo](https://en.wikipedia.org/wiki/Particle_zoo)

**Complexity Zoo** (founded by Scott Aaronson of UWaterloo)

[https://complexityzoo.uwaterloo.ca/Complexity\\_Zoo](https://complexityzoo.uwaterloo.ca/Complexity_Zoo)

**Algorithms Zoo** (founded by Stephen Jordan of NIST)

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