

# Hamiltonian Zoo

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*No Matter Where They're From*

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## I. MODEL HAMILTONIANS

### 1. *Coulomb*

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

### A. Electronic Structure

#### 1. *Born-Oppenheimer Model*

#### 2. *Watson Model*

### B. Fine and Hyperfine Structure

#### 1. *Stark*

#### 2. *Zeeman*

$$H_{\text{Zeeman}} = -\frac{\mu_B (g_l \vec{L} + g_s \vec{S})}{\hbar} \cdot \vec{B} \quad (2)$$

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### 3. Complete magnetic dipole interaction

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

4. *Frosch-Foley*

5. *Spin-orbit*

6. *Orbit-orbit*

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

8. *Fermi Contact*

### C. Special Relativity

1. *Dirac*

2. *Klein-Gordon*

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

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

5. *Mass Velocity*

6. *Breit-Pauli*

7. *Dirac-Coulomb-Breit*

### D. Quantum Electrodynamics

1. *Aracki-Sucher*

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

2. *One-Loop*

3. *Schwinger-Dyson*

**E. Nuclear Motion**

$$H_{\text{Nuc}} = -\frac{\hbar^2}{2} \sum_{i=1}^N \sum_{\alpha=1}^3 \frac{1}{M_i} \frac{\partial^2}{\partial R_{i\alpha}^2} + V(\mathbf{R}_1, \dots, \mathbf{R}_N) \quad (5)$$

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. *Bose-Hubbard (Boson Hubbard)*

2. *Fermi-Hubbard (Fermi Hubbard)*

3. *Jaynes-Cummings-Hubbard*

## **H. Open Quantum Systems**

1. *Rabi model*

2. *Spin-Boson*

3. *Feynman-Vernon*

4. *Leggett-Caldeira*

5. *Ishizaki-Fleming*

## 2. Richardson-Gaudin

### 3. Exactly solvable pairing Hamiltonians

*SU(2), Rank 1 algebra*

$$H_{\text{SU}(2)} = \sum_i \epsilon_i n_i - g \sum_{ij} P_i^+ P_j \quad (7)$$

*SO(5), Rank 2 algebra*

$$H_{\text{SO}(5)} = \sum_i \epsilon_i n_i - g \sum_{ijk} P_{ik}^+ P_{jk} \quad (8)$$

*SO(8), Rank 4 algebra*

$$H_{\text{SO}(8)} = \sum_i \epsilon_i n_i - g_T \sum_{ijk} P_{ik}^+ P_{jk} - g_S \sum_{ijk} D_{ik}^+ D_{jk} \quad (9)$$

## 4. *t*-J model

## J. Models of Superfluidity

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

$$H_{2DFS F} = \sum_i \epsilon_i a_i^\dagger a_i + \frac{i\Delta_i}{2} (a_i^\dagger a_{-i}^\dagger + \text{H.c.}) \quad (10)$$

# Matrix Zoo

**K. Ising**

**L. Heisenberg**

**M. J1-J2 Model**

**N. Majumdar-Ghosh**

**O. AKLT Model**

**P. Kitaev Models**

*1. Toric Code*

*2. Ocko-Yoshida*

*3. Honeycomb Model*

$$H_{\text{Honeycomb}} = -J_x \sum_{x\text{-links}} x_i x_j - J_y \sum_{y\text{-links}} y_i y_j - J_z \sum_{z\text{-links}} z_i z_j \quad (11)$$

**Q. 2-level systems (spin- $1/2$  particles)**

$$z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, y \equiv \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (12)$$

$$s_+ \equiv \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{x + iy}{2} \quad (13)$$

$$s_- \equiv \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \frac{x - iy}{2} \quad (14)$$

$$s_\alpha \equiv \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{\mathbb{1} + z}{2} \equiv b \quad (15)$$

$$s_\beta \equiv \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{\mathbb{1} - z}{2} \quad (16)$$



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

$$z_3 \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, x \equiv \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, y \equiv \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad (17)$$

$$\lambda_1 \equiv \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_2 \equiv \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_3 \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_4 \equiv \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad (18)$$

$$\lambda_5 \equiv \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \lambda_6 \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \lambda_7 \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \lambda_8 \equiv \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} \quad (19)$$

$$s_{3+} \equiv \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} = \frac{x_3 + iy_3}{2} \quad (20)$$

$$s_{3-} \equiv \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = \frac{x_3 - iy_3}{2} \quad (21)$$

$$s_{3,1} \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \frac{\mathbb{1} + z}{2} \equiv t \quad (22)$$

$$s_{3,2} \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (23)$$

$$s_{3,3} \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \frac{\mathbb{1} - z}{2} \equiv t \quad (24)$$

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

$$z_4 \equiv \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}, x_4 \equiv \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}, y_4 \equiv \begin{pmatrix} 0 & -\sqrt{3}i & 0 & 0 \\ \sqrt{3}i & 0 & 2 & 0 \\ 0 & 2 & 0 & -\sqrt{3}i \\ 0 & 0 & \sqrt{3}i & 0 \end{pmatrix} \quad (25)$$

$$\gamma^0 \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \gamma^1 \equiv \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & -1 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \gamma^2 \equiv \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix}, \gamma^3 \equiv \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \gamma^5 \equiv \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad (26)$$

$$s_{4+} \equiv \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix} \equiv \frac{x_{3/2} + iy_{3/2}}{2} \equiv \frac{x_{4 \times 4} + iy_{4 \times 4}}{2} \quad (27)$$

$$s_{4-} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix} \equiv \frac{x_4 - iy_4}{2} \quad (28)$$

$$s_{4,1} \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{2} (z_2 + z_1 z_2 + z_1 - \mathbb{1}) \quad (29)$$

$$s_{4,2} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \quad (30)$$

$$s_{4,3} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \quad (31)$$

$$s_{4,4} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \quad (32)$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \frac{1}{2} (\mathbb{1} - z_1 + z_1 z_2 + z_2) \quad (33)$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \frac{1}{2} (\mathbb{1} - z_2 + z_1 z_2 + z_1) \quad (34)$$

$$|10\rangle\langle 01| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} (x_1 x_2 - \mathrm{i} y_1 x_2 + \mathrm{i} x_1 y_2 + y_1 y_2) \quad (35)$$

$$|10\rangle\langle 01| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} (x_1 x_2 - \mathrm{i} x_1 y_2 + \mathrm{i} y_1 x_2 + y_1 y_2) \quad (36)$$

$$\text{CNOT} \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} = \frac{1}{2} (\mathbb{1} + z_1 + x_2 - z_1 x_2) \quad (37)$$

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

$$z_5 \equiv \begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -2 \end{pmatrix}, x_5 \equiv \begin{pmatrix} 0 & 2 & 0 & 0 & 0 \\ 2 & 0 & \sqrt{6} & 0 & 0 \\ 0 & \sqrt{6} & 0 & \sqrt{6} & 0 \\ 0 & 0 & \sqrt{6} & 0 & 2 \\ 0 & 0 & 0 & 2 & 0 \end{pmatrix}, y_5 \equiv \begin{pmatrix} 0 & -2i & 0 & 0 & 0 \\ 2i & 0 & -\sqrt{6}i & 0 & 0 \\ 0 & \sqrt{6}i & 0 & -\sqrt{6}i & 0 \\ 0 & 0 & \sqrt{6}i & 0 & -2i \\ 0 & 0 & 0 & 2i & 0 \end{pmatrix} \quad (38)$$

$$s_{5+} \equiv \begin{pmatrix} 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{6} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{6} & 0 \\ 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \equiv \frac{x_{5 \times 5} + iy_{5 \times 5}}{2} \equiv \frac{x_{(5)} + iy_{(5)}}{2} \quad (39)$$

$$s_{5-} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{6} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{6} & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \end{pmatrix} \equiv \frac{x_{5 \times 5} + iy_{5 \times 5}}{2} \equiv \frac{x_{(5)} + iy_{(5)}}{2} \quad (40)$$

$$s_{5,1} \equiv \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \quad (41)$$

$$s_{5,2} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \quad (42)$$

$$s_{5,3} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \quad (43)$$

$$s_{5,4} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \quad (44)$$

$$s_{5,5} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} = \quad (45)$$

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

$$|0_b 1_t\rangle\langle 1_b 0_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} (z\lambda_1 + \lambda_1 - iz\lambda_2 - i\lambda_2) \quad (46)$$

$$|1_b 0_t\rangle\langle 0_b 1_t| \equiv \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} (z\lambda_1 + \lambda_1 + iz\lambda_2 + i\lambda_2) \quad (47)$$

$$|0_b 1_t\rangle\langle 1_b 0_t| + |1_b 0_t\rangle\langle 0_b 1_t| \equiv \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{2} (z\lambda_1 + \lambda_1) \quad (48)$$

$$|0_b 2_t\rangle\langle 1_b 0_t| \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} (z\lambda_4 + \lambda_4 - iz\lambda_5 - i\lambda_5) \quad (49)$$

## 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

*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/>