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

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

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- 2. Born-Oppenheimer Model
 - 3. Watson Model

B. Fine and Hyperfine Structure

- 1. Stark
- 2. Zeeman

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

3. Complete magnetic dipole interaction

$$H_{\text{Magnetic Dipole}} = \frac{g_{I}\mu_{N}\mu_{B}\mu_{0}}{2\pi} \left(\frac{1}{L_{z}} \sum_{i} \frac{\hat{l}_{zi}}{r_{i}^{3}} \vec{I} \cdot \vec{L} + \frac{2g_{s}}{S_{z}} \sum_{i} \frac{\hat{s}_{zi}}{r_{i}^{3}} \left(3\left(\vec{I} \cdot \hat{r}\right)\left(\vec{S} \cdot \hat{r}\right) - \vec{I} \cdot \vec{S} \right) + \frac{g_{s}}{3S_{z}} \sum_{i} \hat{s}_{zi} \delta^{3}\left(\vec{r}_{i}\right) \vec{I} \cdot \vec{S} \right)$$

$$(4)$$

4. Frosch-Foley

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

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

where

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

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

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

- 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 $(1e^-)$

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

4. Darwin (2e⁻)

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

5. Mass Velocity

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

- 6. Breit-Pauli
- 7. Dirac-Coulomb-Breit

D. Quantum Electrodynamics

1. Aracki-Sucher

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

2. One-Loop

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

- 3. Schwinger-Dyson
- E. Nuclear Motion

$$H_{\text{Nuc}} = -\frac{\hbar^2}{2} \sum_{i=1}^{N} \sum_{\alpha=1}^{3} \frac{1}{M_i} \frac{\partial^2}{\partial R_{i\alpha}^2} + V(\mathbf{R}_1, \dots, \mathbf{R}_N)$$
(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. Bose-Hubbard (Boson Hubbard)
- 2. Fermi-Hubbard (Fermi Hubbard)
 - 3. Jaynes-Cummings-Hubbard
 - 4. Tavis-Cummings-Hubbard

H. Open Quantum Systems

- 1. Rabi model
- 2. Spin-Boson
- 3. Feynman-Vernon
- 4. Leggett-Caldeira

2. Richardson-Gaudin

3. Exactly solvable pairing Hamiltonians

SU(2), Rank 1 algebra

$$H_{SU(2)} = \sum_{i} \epsilon_i n_i - g \sum_{ij} P_i^+ P_j \tag{18}$$

SO(5), Rank 2 algebra

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

$$\tag{19}$$

SO(8), Rank 4 algebra

$$H_{SO(8)} = \sum_{i} \epsilon_{i} n_{i} - g_{T} \sum_{ijk} P_{ik}^{+} P_{jk} - g_{S} \sum_{ijk} D_{ik}^{+} D_{jk}$$
 (20)

4. t-J model

J. Models of Superfluidity

1. 2D p-wave Fermi superfluid

$$H_{2DFSF} = \sum_{i} \epsilon_{i} a_{i}^{\dagger} a_{i} + \frac{i\Delta_{i}}{2} \left(a_{i}^{\dagger} a_{-i}^{\dagger} + \text{H.c.} \right)$$
 (21)

K. Spin models

- 1. Ising
- 2. Transverse Ising
 - 3. XY
 - 4. XYZ
- L. Heisenberg
- M. J1-J2 Model
- N. Majumdar-Ghosh
 - O. AKLT Model
 - P. Kitaev Models
 - 1. Toric Code
 - 2. Ocko-Yoshida
 - 3. Honeycomb Model

$$H_{\text{Honeycomb}} = -J_x \sum_{x-\text{links}} x_i x_j - J_y \sum_{y-\text{links}} y_i y_j - J_z \sum_{z-\text{links}} z_i z_j$$
 (22)

Matrix Zoo

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

$$z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$
 (23)

$$s_{+} \equiv \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{x + iy}{2} \tag{24}$$

$$s_{-} \equiv \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \frac{x - iy}{2} \tag{25}$$

$$s_{\alpha} \equiv \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1 + z}{2} \equiv b \tag{26}$$

$$s_{\beta} \equiv \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1 - z}{2} \tag{27}$$

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

$$z_{3} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, x = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, y = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

$$(28)$$

$$\lambda_{1} \equiv \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_{2} \equiv \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_{3} \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_{4} \equiv \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \tag{29}$$

$$\lambda_{5} \equiv \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \lambda_{6} \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \lambda_{7} \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \lambda_{8} \equiv \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

$$(30)$$

$$s_{3+} \equiv \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} = \frac{x_3 + iy_3}{2} \tag{31}$$

$$s_{3-} \equiv \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = \frac{x_3 - iy_3}{2} \tag{32}$$

$$s_{3,1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \frac{11 + z}{2} \equiv t \tag{33}$$

$$s_{3,2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{34}$$

$$s_{3,3} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \frac{1 - z}{2} \equiv t \tag{35}$$

$$|1\rangle\langle 2| \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} = \frac{1}{2} \left(\lambda_6 + i\lambda_7\right) \tag{36}$$

$$\lambda_7 \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{37}$$

$$\lambda_7 \lambda_5 = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_3 \lambda_7 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_7 \lambda_3 + \lambda_3 \lambda_7 = \lambda_1 \tag{38}$$

$$\lambda_7 \lambda_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} = -\lambda_6 \lambda_1, \lambda_2 \lambda_7 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = -\lambda_1 \lambda_6, \lambda_7 \lambda_2 + \lambda_2 \lambda_7 = -\lambda_4, \lambda_6 \lambda_1 + \lambda_1 \lambda_6 = \lambda_4$$
(39)

$$\lambda_5^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = |\lambda_1| \tag{40}$$

$$\lambda_5 \lambda_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \lambda_2 \lambda_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_3 \lambda_2 + \lambda_2 \lambda_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = \lambda_6 \tag{41}$$

$$\lambda_2^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} = |\lambda_3| \tag{42}$$

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

$$z_{4} = \begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}, x_{4} = \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}, y_{4} = \begin{pmatrix} 0 & -\sqrt{3}i & 0 & 0 \\ \sqrt{3}i & 0 & 2 & 0 \\ 0 & 2 & 0 & -\sqrt{3}i \\ 0 & 0 & \sqrt{3}i & 0 \end{pmatrix}$$

$$(43)$$

$$\gamma^{0} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \gamma^{1} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & -1 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \gamma^{2} = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix}, \gamma^{3} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \gamma^{5} = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

$$(44)$$

$$s_{4+} \equiv \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix} \equiv \frac{x_{3/2} + iy_{3/2}}{2} \equiv \frac{x_{4\times 4} + iy_{4\times 4}}{2} \tag{45}$$

$$s_{4-} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix} \equiv \frac{x_4 - iy_4}{2} \tag{46}$$

$$\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix} = \frac{1}{2} \left(\mathbb{1} - z_1 + z_1 z_2 + z_2 \right) \tag{51}$$

$$\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix} = \frac{1}{2} \left(\mathbf{1} - z_2 + z_1 z_2 + z_1 \right) \tag{52}$$

$$|10\rangle\langle01| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} \left(x_1 x_2 - i y_1 x_2 + i x_1 y_2 + y_1 y_2 \right)$$

$$(53)$$

$$|10\rangle\langle01| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} \left(x_1 x_2 - i x_1 y_2 + i y_1 x_2 + y_1 y_2 \right)$$

$$(54)$$

$$CNOT = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix} = \frac{1}{2} (1 + z_1 + x_2 - z_1 x_2) \tag{55}$$

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

$$s_{5+} \equiv \begin{pmatrix} 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{6} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{6} & 0 \\ 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \equiv \frac{x_{5\times5} + iy_{5\times5}}{2} \equiv \frac{x_{(5)} + iy_{(5)}}{2}$$

$$(57)$$

$$s_{5-} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{6} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{6} & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \end{pmatrix} \equiv \frac{x_{5\times5} + iy_{5\times5}}{2} \equiv \frac{x_{(5)} + iy_{(5)}}{2}$$

$$(58)$$

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

$$\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix} = \frac{1}{4} (z\lambda_1 + \lambda_1 - iz\lambda_2 - i\lambda_2) \tag{71}$$

$$\begin{bmatrix}
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix} = \frac{1}{4} (z\lambda_1 + \lambda_1 + iz\lambda_2 + i\lambda_2) \tag{72}$$

$$\equiv \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix} = \frac{1}{4} (z\lambda_4 + \lambda_4 - iz\lambda_5 - i\lambda_5) \tag{76}$$

$$\equiv \begin{pmatrix}
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix} = \frac{1}{4} (z\lambda_4 + \lambda_4) \tag{77}$$

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 Morse $Lenard ext{-}Jones$ Morse/Long-range TiemannMorse-Rosen D. **Triatomics** Jensen SchwenkePolyMLR

Torsion Potentials

Functional Zoo

Function Zoo

Master Equation Zoo

Particle Zoo

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

$Complexity \ Zoo \ \ ({\rm founded} \ {\rm by} \ {\rm Scott} \ {\rm Aarsonson} \ {\rm of} \ {\rm UWaterloo})$

 $https://complexityzoo.uwaterloo.ca/Complexity_Zoo$

$Algorithms \ Zoo \ \ ({\rm founded} \ {\rm by} \ {\rm Stephen} \ {\rm Jordan} \ {\rm of} \ {\rm NIST})$

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