## Hamiltonian Zoo

## Nike Dattani\*

Harvard-Smithsonian Center for Astrophysics, McMaster University

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. Born-Oppenheimer Model
  - 2. Watson Model

## B. Fine and Hyperfine Structure

- 1. Stark
- 2. Zeeman

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

 $<sup>^*</sup>$  n.dattani@cfa.harvard.edu

3. Complete magnetic dipole interaction

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

- 4. Frosch-Foley
  - $5. \quad Spin-orbit$
- 6. Orbit-orbit
- 7. Spin-other-orbit (Gaunt)
  - 8. Fermi Contact

## C. Special Relativity

- 1. Dirac
- 2. Klein-Gordon
- 3. Darwin  $(1e^{-})$

$$H_{\text{Darwin-1}} = \alpha_{\text{FS}}^2 \frac{\pi Z}{2} \sum_i \delta(\vec{r}_i)$$
 (4)

4. Darwin (2e<sup>-</sup>)

$$H_{\text{Darwin-2}} = \alpha_{\text{FS}}^2 \pi \sum_{i < j} \delta(\vec{r}_{ij})$$
 (5)

5. Mass Velocity

$$H_{\text{Mass-Velocity}} = -\alpha_{\text{FS}}^2 \frac{1}{8} \sum_{i} \nabla_i^4.$$
 (6)

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

#### D. Quantum Electrodynamics

1. Aracki-Sucher

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

2. One-Loop

$$H_{1-\text{loop}} = \alpha_{\text{FS}}^4 \pi Z^2 \left( \frac{427}{96} - \ln 2 \right) \sum_i \delta\left( \vec{r}_i \right)$$
 (8)

- 3. Schwinger-Dyson
- E. Nuclear Motion

$$H_{\text{Nuc}} = -\frac{\hbar^2}{2} \sum_{i=1}^{N} \sum_{\alpha=1}^{3} \frac{1}{M_i} \frac{\partial^2}{\partial R_{i\alpha}^2} + V(\mathbf{R}_1, \dots, \mathbf{R}_N)$$
(9)

- 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

$$H_{SU(2)} = \sum_{i} \epsilon_i n_i - g \sum_{ij} P_i^+ P_j \tag{11}$$

SO(5), Rank 2 algebra

$$H_{SO(5)} = \sum_{i} \epsilon_i n_i - g \sum_{ijk} P_{ik}^+ P_{jk}$$
(12)

SO(8), Rank 4 algebra

$$H_{SO(8)} = \sum_{i} \epsilon_{i} n_{i} - g_{T} \sum_{ijk} P_{ik}^{+} P_{jk} - g_{S} \sum_{ijk} D_{ik}^{+} D_{jk}$$
(13)

4. t-J model

## J. Models of Superfluidity

1. 2D p-wave Fermi superfluid

$$H_{2DFSF} = \sum_{i} \epsilon_{i} a_{i}^{\dagger} a_{i} + \frac{i\Delta_{i}}{2} \left( a_{i}^{\dagger} a_{-i}^{\dagger} + \text{H.c.} \right)$$
 (14)

## 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

$$H_{\text{Honeycomb}} = -J_x \sum_{x-\text{links}} x_i x_j - J_y \sum_{y-\text{links}} y_i y_j - J_z \sum_{z-\text{links}} z_i z_j$$
 (15)

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

$$z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$
 (16)

$$s_{+} \equiv \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{x + iy}{2} \tag{17}$$

$$s_{-} \equiv \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \frac{x - iy}{2} \tag{18}$$

$$s_{\alpha} \equiv \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \frac{1 + z}{2} \equiv b \tag{19}$$

$$s_{\beta} \equiv \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{\mathbb{1} - z}{2} \tag{20}$$

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

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

$$(21)$$

$$\lambda_{1} \equiv \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_{2} \equiv \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_{3} \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_{4} \equiv \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \tag{22}$$

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

$$(23)$$

$$s_{3+} \equiv \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} = \frac{x_3 + iy_3}{2} \tag{24}$$

$$s_{3-} \equiv \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = \frac{x_3 - iy_3}{2} \tag{25}$$

$$s_{3,1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \frac{11+z}{2} \equiv t \tag{26}$$

$$s_{3,2} \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{27}$$

$$s_{3,3} \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \frac{1 - z}{2} \equiv t \tag{28}$$

$$|1\rangle\langle 2| \equiv \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} = \frac{1}{2} \left( \lambda_6 + i\lambda_7 \right) \tag{29}$$

$$\lambda_7 \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{30}$$

$$\lambda_7 \lambda_5 = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_3 \lambda_7 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_7 \lambda_3 + \lambda_3 \lambda_7 = \lambda_1 \tag{31}$$

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

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

$$(32)$$

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

$$(33)$$

$$s_{4+} \equiv \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix} \equiv \frac{x_{3/2} + iy_{3/2}}{2} \equiv \frac{x_{4\times 4} + iy_{4\times 4}}{2} \tag{34}$$

$$s_{4-} \equiv \begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix} \equiv \frac{x_4 - iy_4}{2} \tag{35}$$

$$\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix} = \frac{1}{2} \left( \mathbb{1} - z_1 + z_1 z_2 + z_2 \right) \tag{40}$$

$$\begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix} = \frac{1}{2} \left( \mathbf{1} - z_2 + z_1 z_2 + z_1 \right) \tag{41}$$

$$|10\rangle\langle01| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} \left( x_1 x_2 - i y_1 x_2 + i x_1 y_2 + y_1 y_2 \right) \tag{42}$$

$$|10\rangle\langle01| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \frac{1}{4} \left( x_1 x_2 - i x_1 y_2 + i y_1 x_2 + y_1 y_2 \right) \tag{43}$$

$$CNOT = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix} = \frac{1}{2} (1 + z_1 + x_2 - z_1 x_2) \tag{44}$$

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

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

$$(46)$$

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

$$(47)$$

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

$$\equiv \begin{pmatrix}
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix} = \frac{1}{4} (z\lambda_1 + \lambda_1 + iz\lambda_2 + i\lambda_2) \tag{61}$$

$$\equiv \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix} = \frac{1}{4} (z\lambda_4 + \lambda_4 - iz\lambda_5 - i\lambda_5) \tag{65}$$

$$\equiv \begin{pmatrix}
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix} = \frac{1}{4} (z\lambda_4 + \lambda_4) \tag{66}$$

## 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- $Jones$		
$Morse/Long ext{-}range$		
Tiemann		
$Morse ext{-}Rosen$		
	D.	Triatomics
Jensen		
Schwenke		
PolyMLR		

E. Torsion Potentials

## Functional Zoo

## **Function Zoo**

## Master Equation Zoo

## Particle Zoo

https://en.wikipedia.org/wiki/Particle\_zoo

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

 $https://complexityzoo.uwaterloo.ca/Complexity\_Zoo$ 

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

 $\rm https://math.nist.gov/quantum/zoo/$