Quantum Simulations of Physical Systems

Julie Butler

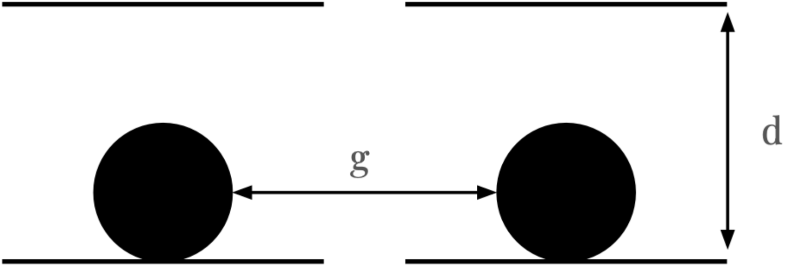
The No-Broken Pairs Pairing Model

Introduction to the Pairing Model

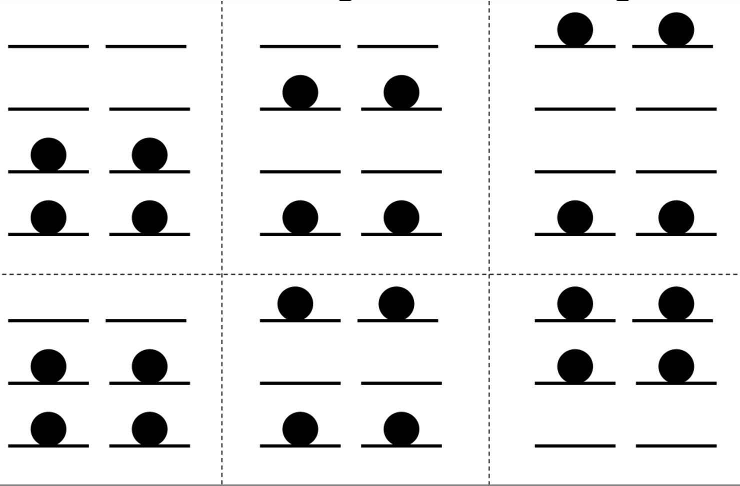
- Consider a system with x particles and 2x single particle states (x is even)
  - Each energy level is doubly degenerate $\longrightarrow$ there are two single particle states per energy level
- Energy levels are separated by a set constant t
- Particles interact with a strength of g
- Particles which start next to each other must stay next to each other (pairs cannot be broken)
- Note: this is a *toy model*

Two-Particle Two-Hole Pairing Model

- **Ground State**



Two-Particle Two-Hole Pairing Model All Configurations

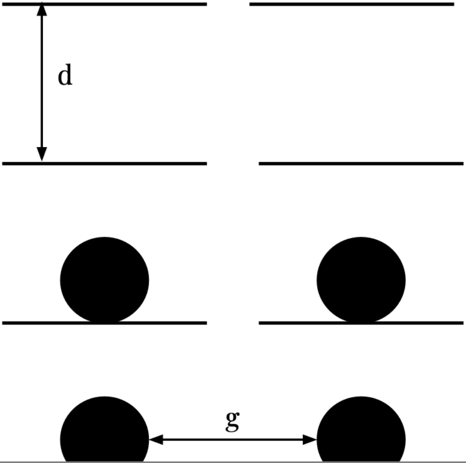


Two-Particle Two-Hole Pairing Model Hamiltonian

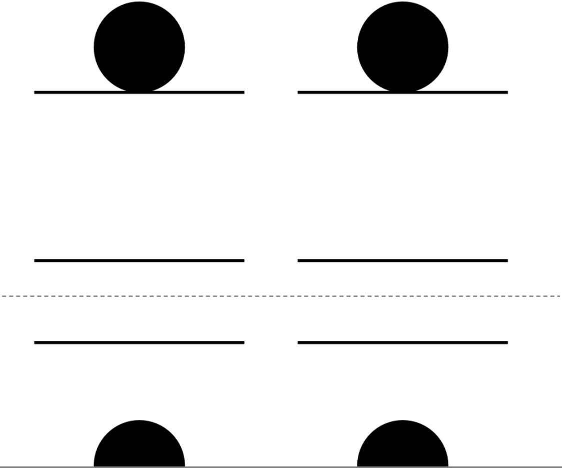
- Hamiltonian

$$H_{2p2h} = \begin{bmatrix} 0d - \frac{g}{2} & 0 \\ 0 & 2d - \frac{g}{2} \end{bmatrix} = \begin{bmatrix} \frac{-g}{2} & 0 \\ 0 & 2d - \frac{g}{2} \end{bmatrix}$$

Four-Particle Four-Hole Pairing Model



Four-Particle Four-Hole Pairing All Configurations



Four-Particle Four-Hole Pairing Model Hamiltonian

$$H_{4p4h} = \begin{bmatrix} 2d-g & \frac{-g}{2} & \frac{-g}{2} & \frac{-g}{2} & \frac{-g}{2} & 0 \\ \frac{-g}{2} & 4d-g & \frac{-g}{2} & \frac{-g}{2} & 0 & \frac{-g}{2} \\ \frac{-g}{2} & \frac{-g}{2} & 6d-g & 0 & \frac{-g}{2} & \frac{-g}{2} \\ \frac{-g}{2} & \frac{-g}{2} & 0 & 6d-g & \frac{-g}{2} & \frac{-g}{2} \\ \frac{-g}{2} & 0 & \frac{-g}{2} & \frac{-g}{2} & 8d-g & \frac{-g}{2} \\ 0 & \frac{-g}{2} & \frac{-g}{2} & \frac{-g}{2} & \frac{-g}{2} & 10d-g \end{bmatrix}$$

Determining Energy (A Review)

Hamiltonian $\longrightarrow$ Energy

- Eigenvalues of the Hamiltonian matrix are the energies of the system

$$H_{2p2h} = \begin{bmatrix} \frac{-g}{2} & 0 \\ 0 & 2d - \frac{g}{2} \end{bmatrix}$$

- Eigenvalues are $\frac{-g}{2}$ and $2d - \frac{g}{2}$
  - $\frac{-g}{2}$ is the smallest energy, it is the **ground state energy**

Finding Energy of Realistic Systems

- For the simple quantum systems we study in class, using a simple eigenvalue solver is enough to find the ground state energy (we could even do some of them by hand)
- However, the size of a quantum system grows quickly, especially as we attempt to model realistic systems
- 2p2h $\longrightarrow$ 2 energies, 4p4h $\longrightarrow$ 6 energies, 6p6h $\longrightarrow$ 20 energies, 8p8h $\longrightarrow$ 70 energies, 10p10h $\longrightarrow$ 252 energies, ... and this is where I crashed my Mac

Finding Energy of Realistic Systems (Continued)

- Hamiltonians for realistic systems can easily be thousands of elements by thousands of elements $\longrightarrow$ we cannot simply create a matrix for the Hamiltonian and find with eigenvalues and eigenvectors with traditional solvers
- **Computational Many-Body Physics**: If you cannot find the energies of a system with its eigenvalues then you have to use approximation methods
  - Many-Body Perturbation Theory
  - Coupled-Cluster Theory
  - Density Functional Theory
  - Mean-Field Theory (Hartree-Fock Theory)
  - Variational Principle

Variational Method for Finding Energy

Introduction to the Variational Method

- Given a system which can be described by the Hamiltonian H, we can approximate the energy as:

$$E = \frac{\langle \Psi_{trial}(a) | H | \Psi_{trial}(a) \rangle}{\langle \Psi_{trial}(a) | \Psi_{trial}(a) \rangle}$$

- Denominator ensures normalization
- $|\Psi_(trial)(a)\rangle$ is known as the trial wavefunction
  - Constructed using knowledge of the system (size, symmetries, properties)
- a is a optimization parameter, once E is found once it is minimized with respect to a.
- The variational principle says that no matter what $E \leq E_0$, where E_0 is the true energy.

Example: Two-Particle Two-Hole Pairing Model

$$H_{2p2h} = \begin{bmatrix} \frac{-g}{2} & 0 \\ 0 & 2d - \frac{g}{2} \end{bmatrix}$$

* What do we know about the wavefunction? * Find the initial value for E * Optimization