Quantum Theory of Many-Particle Systems, Phys. 540

• Questions about organization
• Second quantization
• Questions about last class and assignments?
• Comments?
IPM for fermions in finite systems

- IPM = independent particle model
- Only consider Pauli principle
- Localized fermions
- Examples
- Hamiltonian many-body problem: $\hat{H} = \hat{T} + \hat{V} = \hat{H}_0 + \hat{H}_1$
  - with $\hat{H}_0 = \hat{T} + \hat{U}$
  - and $\hat{H}_1 = \hat{V} - \hat{U}$
- Suitably chosen auxiliary one-body potential $U$
- Many-body problem can be solved for $\hat{H}_0$ !!
- Also works with fixed external potential $U_{ext}$
  $\hat{H} = \hat{T} + \hat{U}_{ext} + \hat{V} = \hat{H}_0 + \hat{H}_1$
Role of $U$

- Can be chosen to minimize effect of two-body interaction
- Ground state of total Hamiltonian may break a symmetry
  - Spontaneous magnetization
- Can speed up convergence of perturbation expansion in $\hat{H}_1$

- Spherical symmetry: sp problem straightforward but may have to be done numerically
- Assume solved: e.g. 3D-harmonic oscillator in nuclear physics
  \[ H_0 |\lambda\rangle = (T + U) |\lambda\rangle = \varepsilon_{\lambda} |\lambda\rangle \]
- For nuclei \(|\lambda\rangle = |n(\ell \frac{1}{2})jm_j\rangle\)
- For atoms (include Coulomb attraction to nucleus) \(|\lambda\rangle = |n\ell m_{\ell \frac{1}{2}}m_s\rangle\)
Use second quantization

- Consider in the \( \{|\lambda\rangle\} \) basis (discrete sums for simplicity)

\[
\hat{H}_0 = \sum_{\lambda\lambda'} \langle \lambda | (T + U) | \lambda' \rangle a^\dagger_\lambda a_{\lambda'} \\
= \sum_{\lambda\lambda'} \epsilon_{\lambda'} \delta_{\lambda,\lambda'} a^\dagger_\lambda a_{\lambda'} = \sum_{\lambda} \epsilon_{\lambda} a^\dagger_\lambda a_{\lambda}
\]

- All many-body eigenstates of \( \hat{H}_0 \) are of the form

\[
|\Phi^N_n \rangle = |\lambda_1 \lambda_2 ... \lambda_N \rangle = a^\dagger_{\lambda_1} a^\dagger_{\lambda_2} ... a^\dagger_{\lambda_N} |0\rangle
\]

- with eigenvalue

\[
E^N_n = \sum_{i=1}^{N} \epsilon_{\lambda_i}
\]
Explicitly

• Employ

\[
\left[ \hat{H}_0, a^\dagger_{\lambda_i} \right] = \varepsilon_{\lambda_i} a^\dagger_{\lambda_i}
\]

• and therefore

\[
\begin{align*}
\hat{H}_0 |\lambda_1 \lambda_2 \lambda_3 \ldots \lambda_N \rangle &= \hat{H}_0 a^\dagger_{\lambda_1} a^\dagger_{\lambda_2} \ldots a^\dagger_{\lambda_N} |0\rangle \\
&= [\hat{H}_0, a^\dagger_{\lambda_1}] a^\dagger_{\lambda_2} \ldots a^\dagger_{\lambda_N} |0\rangle + a^\dagger_{\lambda_1} \hat{H}_0 a^\dagger_{\lambda_2} \ldots a^\dagger_{\lambda_N} |0\rangle \\
&= [\hat{H}_0, a^\dagger_{\lambda_1}] a^\dagger_{\lambda_2} \ldots a^\dagger_{\lambda_N} |0\rangle + a^\dagger_{\lambda_1} [\hat{H}_0, a^\dagger_{\lambda_2}] \ldots a^\dagger_{\lambda_N} |0\rangle + \ldots + a^\dagger_{\lambda_1} a^\dagger_{\lambda_2} \ldots [\hat{H}_0, a^\dagger_{\lambda_N}] |0\rangle \\
&= \left\{ \sum_{i=1}^{N} \varepsilon_{\lambda_i} \right\} |\lambda_1 \lambda_2 \lambda_3 \ldots \lambda_N \rangle
\end{align*}
\]

• Corresponding many-body problem solved!

• Ground state

\[
|\Phi^N_0 \rangle = \prod_{\lambda_i \leq F} a^\dagger_{\lambda_i} |0\rangle
\]

• Fermi sea \( \Rightarrow F \)
Electrons in atoms

- Atomic units (a.u.) are standard usage
  - electron mass \( m_e \) unit of mass
  - elementary charge \( e \) unit of charge
  - length and time such that numerical values of \( \hbar \) and \( 4\pi\varepsilon_0 \) are unity
  - then atomic unit of length Bohr radius
    \[
    a.u. \text{ (length)} = a_0 = \frac{4\pi\varepsilon_0\hbar^2}{e^2m_e} \approx 5.29177 \times 10^{-11} \text{ m}
    \]
    - and time a.u. (time) = \( a_0 \frac{e^2}{\alpha c} \approx 2.41888 \times 10^{-17} \text{ s} \)
    - where \( \alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} \approx \frac{1}{137.036} \) is the fine structure constant
  - energy unit = Hartree
    \[
    E_H = \frac{\hbar^2}{m_ea_0^2} \approx 27.2114 \text{ eV}
    \]
Hamiltonian in a.u.

- Most of atomic physics can be understood on the basis of

\[ H_N = \sum_{i=1}^{N} \frac{p_i^2}{2} - \sum_{i=1}^{N} \frac{Z}{|r_i|} + \frac{1}{2} \sum_{i \neq j}^{N} \frac{1}{|r_i - r_j|} + V_{mag} \]

- for most applications \( V_{mag} \Rightarrow V_{eff} = \sum_{i} \zeta_i \ell_i \cdot s_i \)

- Relativistic description required for heavier atoms
  - binding sizable fraction of electron rest mass
  - binding of lowest s state generates high-momentum components

- Sensible calculations up to Kr without \( V_{mag} \)

- Shell structure well established
Ionization energy

- Noble gases

- What does it mean?
Shell structure

• Simulate with

\[ H_0^N = \sum_{i=1}^{N} H_0(i) \]

• with

\[ H_0(i) = \frac{p_i^2}{2} - \frac{Z}{r_i} + U(r_i) \]

• even without auxiliary potential \( \Rightarrow \) shells
  - hydrogen-like: \((2\ell + 1) \ast (2s + 1)\) degeneracy
  - but \( \varepsilon_n = -\frac{Z^2}{2n^2} \) does not give correct shell structure (2,10,28...
  - degeneracy must be lifted
  - how?
Other electrons

- Consider effect of electrons in closed shells for neutral Na
- large distances: nuclear charge screened to 1
- close to the nucleus: electron “sees” all 11 protons
- approximately:

  \[ \varepsilon_{2s} < \varepsilon_{2p} \]
  \[ \varepsilon_{3s} < \varepsilon_{3p} < \varepsilon_{3d} \]

- “Far away” orbits: still hydrogen-like!
Ground state Na

- Fill the lowest shells
- Use schematic potential
\[ H_0 |n\ell m_\ell m_s\rangle = \varepsilon_{n\ell} |n\ell m_\ell m_s\rangle \]
- Ground state
\[ |300m_s, 211\frac{1}{2}, 211 -\frac{1}{2}, ..., 100\frac{1}{2}, 100 -\frac{1}{2}\rangle = a_{300m_s}^\dagger a_{211\frac{1}{2}}^\dagger a_{211-\frac{1}{2}}^\dagger ... a_{100\frac{1}{2}}^\dagger a_{100-\frac{1}{2}}^\dagger |0\rangle \]
- Excited states?
Closed-shell atoms

- Neon
- Ground state
  \[ |\Phi_0\rangle = a_{2}^\dagger a_{1/2}^\dagger \cdots a_{100}^\dagger a_{100-1/2}^\dagger |0\rangle, \]
- Excited states
  \[ |n\ell (2p)^{-1}\rangle = a_{n\ell}^\dagger a_{2p} |\Phi_0\rangle \]
- Note the H-like states
- Splitting?
- Basic shell structure of atoms understood \(\Rightarrow\) IPM
Nucleons in nuclei

- Atoms: shell closures at 2, 10, 18, 36, 54, 86
- Similar features observed in nuclei
- Notation:
  - # of neutrons $N$
  - # of protons $Z$
  - # of nucleons $A = N + Z$
- Equivalent of ionization energy: separation energy
  - for protons $S_p(N, Z) = B(N, Z) - B(N, Z - 1)$
  - for neutrons $S_n(N, Z) = B(N, Z) - B(N - 1, Z)$
  - binding energy
    $$M(N, Z) = \frac{E(N, Z)}{c^2} = N m_n + Z m_p - \frac{B(N, Z)}{c^2}$$
Chart of nuclides

- Lots of nuclei and lots to be discovered

- Links to astrophysics
Shell closure at $N=126$

- Odd-even effect: plot only even $Z$

Also at other values $N$ and $Z$

Solid: $N-Z=41$
Dashed: $N-Z=43$
Illustration of odd-even effect

- from Bohr & Mottelson Vol.1 (BM1)

\[ S_n (N,Z) = B(N,Z) - B(N-1,Z) \]
Neutrons

• BM1 figure

\[ S_n(N, Z) = \beta(N, Z) - \beta(N-1, Z) \]

\( \text{N odd} \)

\( \text{Z even} \)
Protons

- BM1 figure
Systematics excitation energies in even-even nuclei

- Ground states $0^+$
- First excited state almost always $2^+$
- Excitation energy in MeV
Heavy nuclei

- Magic numbers for nuclei near stability:
  - $Z=2, 8, 20, 28, 50, 82$
  - $N=2, 8, 20, 28, 50, 82, 126$
Nuclear shell structure

- Ground-state spins and parity of odd nuclei provide further evidence of “magic numbers”
- Character of magic numbers may change far from stability (hot)


- N=20 may disappear and N=16 may appear
Empirical potential

- Analogy to atoms suggests finding a sp potential $\Rightarrow$ shells + IPM
- Difference(s) with atoms?
- Properties of empirical potential
  - overall?
  - size?
  - shape?
- Consider nuclear charge density

Nuclear density distribution

- Central density \((A/Z^* \text{ charge density})\) about the same for nuclei heavier than \(^{16}O\), corresponding to 0.16 nucleons/fm\(^3\)

- Important quantity

- Shape roughly represented by

\[
\rho_{ch}(r) = \frac{\rho_0}{1 + \exp\left(\frac{r-c}{z}\right)}
\]

\[c \approx 1.07A^{\frac{1}{3}} \text{fm}\]

\[z \approx 0.55 \text{fm}\]

- Potential similar shape
Empirical potential

• BM1

\[ U = V f(r) + V_{ls} \left( \frac{\ell \cdot s}{\hbar^2} \right) r_0^2 \frac{1}{r} \frac{d}{dr} f(r) \]

• Central part roughly follows shape of density

\[ f(r) = \left[ 1 + \exp \left( \frac{r - R}{a} \right) \right]^{-1} \]

• Woods-Saxon form

• Depth \( V = \left[ -51 \pm 33 \left( \frac{N - Z}{A} \right) \right] \text{ MeV} \)
  + neutrons
  - protons

• radius \( R = r_0 A^{1/3} \) with \( r_0 = 1.27 \text{ fm} \)

• diffuseness \( a = 0.67 \text{ fm} \)
Analytically solvable alternative

- Woods-Saxon (WS) generates finite number of bound states
- IPM: fill lowest levels $\Rightarrow$ nuclear shells $\Rightarrow$ magic numbers
-reasonably approximated by 3D harmonic oscillator

\[
U_{HO}(r) = \frac{1}{2} m \omega^2 r^2 - V_0
\]

\[
H_0 = \frac{\mathbf{p}^2}{2m} + U_{HO}(r)
\]

- Eigenstates in spherical basis

\[
H_{HO} |n\ell m_\ell m_s\rangle = (\hbar \omega (2n + \ell + \frac{3}{2}) - V_0) |n\ell m_\ell m_s\rangle
\]
Harmonic oscillator

- Filling of oscillator shells
- # of quanta $N = 2n + \ell$

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<th>$n$</th>
<th>$\ell$</th>
<th># of particles</th>
<th>“magic #”</th>
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Need for another type of sp potential

- 1949 Mayer and Jensen suggest the need of a spin-orbit term
- Requires a coupled basis

\[ |n(\ell s)jm_j\rangle = \sum_{m_\ell m_s} |n\ell m_\ell m_s\rangle (\ell \ m_\ell \ s \ m_s | j \ m_j) \]

- Use \( \ell \cdot s = \frac{1}{2}(j^2 - \ell^2 - s^2) \) to show that these are eigenstates

\[ \frac{\ell \cdot s}{\hbar^2} |n(\ell s)jm_j\rangle = \frac{1}{2} \left( j(j + 1) - \ell(\ell + 1) - \frac{1}{2} \left( \frac{1}{2} + 1 \right) \right) |n(\ell s)jm_j\rangle \]

- For \( j = \ell + \frac{1}{2} \) eigenvalue \( \frac{1}{2} \ell \)

- while for \( j = \ell - \frac{1}{2} \) \( -\frac{1}{2} (\ell + 1) \)

- so SO splits these levels! and more so with larger \( \ell \)
Inclusion of SO potential and magic numbers

• Sign of SO?

\[ V_{\ell s} \left( \frac{\ell \cdot s}{\hbar^2} \right) r_0^2 \frac{1}{r} \frac{d}{dr} f(r) \]

\[ V_{\ell s} = -0.44V \]

• Consequence for

- \( 0f_{\frac{7}{2}} \)
- \( 0g_{\frac{9}{2}} \)
- \( 0h_{\frac{11}{2}} \)
- \( 0i_{\frac{13}{2}} \)

• Noticeably shifted

• Correct magic numbers!

\[ N = 6, \pi+ \quad - 0i, 1g, 2d, 3s - \]

\[ N = 5, \pi- \quad - 0h, 1f, 2p - \]

\[ N = 4, \pi+ \quad - 0g, 1d, 2s - \]

\[ N = 3, \pi- \quad - 0f, 1p - \]

\[ N = 2, \pi+ \quad - 0d, 1s - \]

\[ N = 1, \pi- \quad - 0p - \]

\[ N = 0, \pi+ \quad - 0s \]
$^{208}$Pb for example

- Empirical potential & sp energies
  \[ \hat{H}_0 \, a_\alpha^\dagger \, |^{208}\text{Pb}_{g.s.}\rangle = \left[ \varepsilon_\alpha + E(208\text{Pb}_{g.s.}) \right] \, a_\alpha^\dagger \, |^{208}\text{Pb}_{g.s.}\rangle \]

- \( A+1 \): “sp energies” \( E_n^{A+1} - E_0^A \) directly from experiment

- \( A-1 \):
  \[ \hat{H}_0 \, a_\alpha \, |^{208}\text{Pb}_{g.s.}\rangle = \left[ E(208\text{Pb}_{g.s.}) - \varepsilon_\alpha \right] \, a_\alpha \, |^{208}\text{Pb}_{g.s.}\rangle \]

- also directly from \( E_0^A - E_n^{A-1} \)

- Shell filling for nuclei near stability follows empirical potential
Comparison with experiment

• Now how to explain this potential ...
Closed-shells and angular momentum

• Atoms: consider one closed shell (argument the same for more)

\[ |n\ell m_\ell = \ell m_s = \frac{1}{2}, n\ell m_\ell = \ell m_s = -\frac{1}{2}, \ldots n\ell m_\ell = -\ell m_s = \frac{1}{2}, n\ell m_\ell = -\ell m_s = -\frac{1}{2} \rangle \]

• Expect?

• Example: He

\[ |(1s)^2 \rangle = \frac{1}{\sqrt{2}} \left\{ |1s \uparrow 1s \downarrow \rangle - |1s \downarrow 1s \uparrow \rangle \right\} \]

\[ = |(1s)^2 \rangle \; ; \; L = 0 \; S = 0 \rangle \]

• Consider nuclear closed shell

\[ |\Phi_0 \rangle = |n(\ell \frac{1}{2}) j m_j = j, n(\ell \frac{1}{2}) j m_j = j - 1, \ldots, n(\ell \frac{1}{2}) m_j = -j \rangle \]
Angular momentum and second quantization

- **z-component of total angular momentum**
  \[
  \hat{J}_z = \sum_{n\ell jm} \sum_{n'\ell' j'm'} \langle n\ell jm | j_z | n'\ell' j'm' \rangle a_{n\ell jm}^\dagger a_{n'\ell' j'm'} \\
  = \sum_{n\ell jm} \hbar m a_{n\ell jm}^\dagger a_{n\ell jm}
  \]

- **Action on single closed shell**
  \[
  \hat{J}_z |n\ell j; m = -j, -j + 1, ..., j \rangle = \sum_{m} \hbar m a_{n\ell jm}^\dagger a_{n\ell jm} |n\ell j; m = -j, -j + 1, ..., = j \rangle \\
  = \{ \sum_{m=-j}^{j} \hbar m \} |n\ell j; m = -j, -j + 1, ..., j \rangle \\
  = 0 \times |n\ell j; m = -j, -j + 1, ..., = j \rangle
  \]
  
  - Also \( \hat{J}_\pm |n\ell j; m = -j, -j + 1, ..., = j \rangle = 0 \)

- **So total angular momentum** \( J = 0 \)

- **Closed shell atoms**
  \( L = 0 \)
  \( S = 0 \)
Nucleon-nucleon interaction

- Shell structure in nuclei and lots more to be explained on the basis of how nucleons interact with each other in free space

- QCD
- Lattice calculations
- Effective field theory
- Exchange of lowest bosonic states
- Phenomenology

- Realistic NN interactions: describe NN scattering data up to pion production threshold plus deuteron properties
- Note: extra energy scale from confinement of nucleons
Nuclear Matter

- Nuclear masses near stability
  \[ M(N, Z) = \frac{E(N, Z)}{c^2} = N m_n + Z m_p - \frac{B(N, Z)}{c^2} \]

- Data
- Each A most stable N,Z pair
- Where fission?
- Where fusion?
Nuclear Matter

- Smooth curve

\[ B = b_{vol} A - b_{surf} A^{2/3} - \frac{1}{2} b_{sym} \frac{(N - Z)^2}{A} - \frac{3}{5} \frac{Z^2 e^2}{R_c} \]

- volume \( b_{vol} = 15.56 \text{ MeV} \)
- surface \( b_{surf} = 17.23 \text{ MeV} \)
- symmetry \( b_{sym} = 46.57 \text{ MeV} \)
- Coulomb \( R_c = 1.24A^{1/3} \text{ fm} \)

Great interest in limit: \( N=Z; \) no Coulomb; \( A \to \infty \)

Two most important numbers in Nuclear Physics

\[ \frac{B}{A} \approx 16 \text{ MeV} \quad \rho_0 \approx 0.16 \text{ fm}^3 \]
Saturation problem of nuclear matter

Given $V_{NN} \Rightarrow$ predict correct minimum of $E/A$ in nuclear matter as a function of density inside empirical box

Describe the infinite system of neutrons

$\Rightarrow$ properties of neutron stars
Isospin

- Shell closures for N and Z the same!!
- Also \( m_n c^2 \approx m_p c^2 \) \( 939.56 \text{ MeV} \) vs. \( 938.27 \text{ MeV} \)
- So strong interaction Hamiltonian (QCD) invariant for \( p \leftrightarrow n \)
- But weak and electromagnetic interactions are not
- Strong interaction dominates \( \Rightarrow \) consequences

- Notation (for now) \( p_\alpha^\dagger \) adds proton
  \( n_\alpha^\dagger \) adds neutron

- Anticommutation relations
  \( \{ p_\alpha^\dagger, p_\beta \} = \delta_{\alpha,\beta} \)
  \( \{ n_\alpha^\dagger, n_\beta \} = \delta_{\alpha,\beta} \)

- All others 0
Isospin

- Z proton & N neutron state
  \[ |\alpha_1 \alpha_2 \ldots \alpha_Z; \beta_1 \beta_2 \ldots \beta_N \rangle = p^\dagger_{\alpha_1} p^\dagger_{\alpha_2} \ldots p^\dagger_{\alpha_Z} n^\dagger_{\beta_1} n^\dagger_{\beta_2} \ldots n^\dagger_{\beta_N} |0\rangle \]

- Exchange all p with n
  \[ \hat{T}^+ = \sum_{\alpha} p^\dagger_{\alpha} n_{\alpha} \]

- and vice versa
  \[ \hat{T}^- = \sum_{\alpha} n^\dagger_{\alpha} p_{\alpha} \]

- Expect
  \[ [\hat{H}_S, \hat{T}^\pm] = 0 \]

- Consider
  \[ \hat{T}_3 = \frac{1}{2} [\hat{T}^+, \hat{T}^-] = \frac{1}{2} \sum_{\alpha \beta} (p^\dagger_{\alpha} n_{\alpha} n^\dagger_{\beta} p_{\beta} - n^\dagger_{\beta} p_{\beta} p^\dagger_{\alpha} n_{\alpha}) \]
  \[ = \frac{1}{2} \sum_{\alpha \beta} (p^\dagger_{\alpha} p_{\beta} \delta_{\alpha, \beta} - n^\dagger_{\beta} n_{\alpha} \delta_{\alpha, \beta}) = \frac{1}{2} \sum_{\alpha} (p^\dagger_{\alpha} p_{\alpha} - n^\dagger_{\alpha} n_{\alpha}) \]

- will also commute with \( H_S \)
Isospin

• Check \([\hat{T}_3, \hat{T}^\pm] = \pm \hat{T}^\pm\)
• Then operators
  \[
  \hat{T}_1 = \frac{1}{2} (\hat{T}^+ + \hat{T}^-) \\
  \hat{T}_2 = \frac{1}{2i} (\hat{T}^+ - \hat{T}^-) \\
  \hat{T}_3
  \]

obey the same algebra as \(J_x, J_y, J_z\)
so spectrum identical and \(\hat{H}_S, \hat{T}^2, \hat{T}_3\) simultaneously diagonal!

proton \(\mid r m_s \rangle_p = \mid r m_s m_t = \frac{1}{2} \rangle\)
neutron \(\mid r m_s \rangle_n = \mid r m_s m_t = -\frac{1}{2} \rangle\)

For this doublet
\[
\hat{T}_2 \mid r m_s m_t \rangle = \frac{1}{2} (\frac{1}{2} + 1) \mid r m_s m_t \rangle
\]
and
\[
\hat{T}_3 \mid r m_s m_t \rangle = m_t \mid r m_s m_t \rangle
\]
States with total isospin constructed as for angular momentum
Assignment

- Do 3.2 to be discussed on Monday 9/14
- Check out numerical assignment