**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 \( U_{ext} \)
  \[ \hat{H} = \hat{T} + \hat{U}_{ext} + \hat{V} = \hat{H}_0 + \hat{H}_1 \]
Use second quantization

• Solve \( H_0 |\lambda\rangle = \varepsilon_\lambda |\lambda\rangle \)

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

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

• 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

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

• Employ
  \[ \left[ \hat{H}_0, a_{\lambda_i}^\dagger \right] = \varepsilon_{\lambda_i} a_{\lambda_i}^\dagger \]

• and therefore

\[
\hat{H}_0 |\lambda_1 \lambda_2 \lambda_3 ... \lambda_N\rangle = \hat{H}_0 a_{\lambda_1}^\dagger a_{\lambda_2}^\dagger ... a_{\lambda_N}^\dagger |0\rangle
\]
\[
= \left[ \hat{H}_0, a_{\lambda_1}^\dagger \right] a_{\lambda_2}^\dagger ... a_{\lambda_N}^\dagger |0\rangle + a_{\lambda_1}^\dagger \hat{H}_0 a_{\lambda_2}^\dagger ... a_{\lambda_N}^\dagger |0\rangle
\]
\[
= \left[ \hat{H}_0, a_{\lambda_1}^\dagger \right] a_{\lambda_2}^\dagger ... a_{\lambda_N}^\dagger |0\rangle + a_{\lambda_1}^\dagger \left[ \hat{H}_0, a_{\lambda_2}^\dagger \right] ... a_{\lambda_N}^\dagger |0\rangle + ... + a_{\lambda_1}^\dagger a_{\lambda_2}^\dagger ... \left[ \hat{H}_0, a_{\lambda_N}^\dagger \right] |0\rangle
\]
\[
= \left\{ \sum_{i=1}^{N} \varepsilon_{\lambda_i} \right\} |\lambda_1 \lambda_2 \lambda_3 ... \lambda_N\rangle
\]

• Corresponding many-body problem solved!

• Ground state
  \[ |\Phi_0^N\rangle = \prod_{\lambda_i \leq F} a_{\lambda_i}^\dagger |0\rangle \]

• 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

\[
a_{\text{u. (length)}} = a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{e^2 m_e} \approx 5.29177 \times 10^{-11} \text{ m}
\]

- and time \( a_{\text{u. (time)}} = \frac{a_0}{\alpha c} \approx 2.41888 \times 10^{-17} \text{ s} \)

- where \( \alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c} \approx \frac{1}{137.036} \) is the fine structure constant

- energy unit = Hartree

\[
E_H = \frac{\hbar^2}{m_e a_0^2} \approx 27.2114 \text{ eV}
\]
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 \( V_{mag} \Rightarrow V_{so}^{eff} = \sum_i \zeta_i \ell_i \cdot s_i \)

• 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: \((2\ell + 1) \times (2s + 1)\) degeneracy
  - but \( \varepsilon_n = -\frac{Z^2}{2n^2} \) does not give correct shell structure \((2,10,28,...)\)
  - degeneracy must be lifted
  - how?
Wave functions

- Shells
- Orthogonality
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:

\[ \frac{1}{r} \]

- lifts H-like degeneracy: \( \varepsilon_{2s} < \varepsilon_{2p} \)

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

- “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?
Wave functions

- Ne wave functions (solid lines)
- compared with hydrogenic wave functions (dashed lines)
Closed-shell atoms

- Neon

- Ground state

\[ |\Phi_0\rangle = a_{211}^{\dagger} \frac{1}{2} a_{211}^{\dagger} \frac{1}{2} \ldots a_{100}^{\dagger} \frac{1}{2} a_{100}^{\dagger} \frac{1}{2} |0\rangle \]

- 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 ⇒ IPM
Level sequence (approximately)
H Ground state

• Ground state wave function of Hydrogen in momentum space

\[ \phi_{10} = 4 \sqrt{\frac{2}{\pi}} \left( \frac{\hbar}{a_0} \right)^{5/2} \frac{1}{\left( p^2 + \frac{\hbar^2}{a_0^2} \right)^2} \]
Direct knockout reactions

- Atoms: \((e,2e)\) reaction
- Nuclei: \((e,e'p)\) reaction [and others like \((p,2p), (d,^3He), (p,d),\) etc.]
- Physics: transfer large amount of momentum and energy to a bound particle; detect ejected particle together with scattered projectile \(\rightarrow\) construct spectral function
- Impulse approximation: struck particle is ejected
- Other assumption: final state \(\sim\) plane wave on top of N-1 particle eigenstate (more serious in practical experiments) but good approximation if ejectile momentum large enough
- If relative momentum large enough, final state interaction can be neglected as well
- \(\rightarrow\) PWIA = plane wave impulse approximation
- Cross section proportional to spectral function
(e,2e) data for atoms

- Start with Hydrogen
- Ground state wave function \( \phi_{1s}(p) = \frac{2^{3/2}}{\pi} \frac{1}{(1 + p^2)^2} \)
- (e,2e) removal amplitude

\[
\langle 0 | a_p | n = 1, \ell = 0 \rangle = \langle p | n = 1, \ell = 0 \rangle = \phi_{1s}(p)
\]

Hydrogen 1s wave function "seen" experimentally
Helium

- IPM description is very successful
- Closed-shell configuration $1s^2$
- Reaction more complicated than for Hydrogen
- DWIA (distorted wave impulse approximation)

\[ S = \int dp \left| \langle \Psi_{n-1}^N | a_p | \Psi_0^N \rangle \right|^2 \]

agreement with IPM! → 1

Other closed-shell atoms

- Spectroscopic factor becomes less than 1
- Neon $2p$ removal: $S = 0.92$ with two fragments each 0.04
- IPM not the whole story: fragmentation of sp strength
- Summed strength: like IPM
- IPM wave functions still excellent
- Example: Argon $3p$ $S = 0.95$
- Rest in 3 small fragments
Fragmentation in atoms

• All the strength remains below (above) the Fermi energy in closed-shell atoms

• Fragmentation can be interpreted in terms of mixing between

\[ a_\alpha |\Phi_0^N \rangle \]

and

\[ a_\beta a_\gamma a_\delta^\dagger |\Phi_0^N \rangle \]

• with the same “global” quantum numbers

• Example: Argon ground state

\[ |\Phi_0^N \rangle = |(3s)^2 (3p)^6 (2s)^2 (2p)^6 (1s)^2 \rangle \]

• \( \text{Ar}^+ \) ground state

\[ |(3p)^{-1} \rangle = a_{3p} |\Phi_0^N \rangle = |(3s)^2 (3p)^5 (2s)^2 (2p)^6 (1s)^2 \rangle \]

• excited state

\[ |(3s)^{-1} \rangle = a_{3s} |\Phi_0^N \rangle = |(3s)^1 (3p)^6 (2s)^2 (2p)^6 (1s)^2 \rangle \]

• also

\[ |(3p)^{-2} 4s \rangle = a_{3p} a_{3p} a_{4s}^\dagger |\Phi_0^N \rangle = |(4s)^1 (3s)^2 (3p)^4 (2s)^2 (2p)^6 (1s)^2 \rangle \]

• and

\[ |(3p)^{-2} nd \rangle = a_{3p} a_{3p} a_{nd}^\dagger |\Phi_0^N \rangle = |(nd)^1 (3s)^2 (3p)^4 (2s)^2 (2p)^6 (1s)^2 \rangle \]
Argon spectroscopic factors

- s strength also in the continuum: Ar$^{2+}$ + e
- note vertical scale
- red bars: 3s fragments exhibit substantial fragmentation