Evaluating the Spin-Dependence of the Three-Body Fermionic Wavefunction

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Introduction

Similar to the three boson bound state problem in the lectures, we present a bound system of three fermions. To do so, we:

- Consider the coupling of spin s, total angular momentum j, and isospin τ of the particles
- Take into account the spin-dependence of the interaction between the particles

Theory

Schrödinger equation for this system would be

$$\hat{H}\,|\Psi\rangle = (\hat{H}_0 + \hat{V}_{12} + \hat{V}_{23} + \hat{V}_{31} + \hat{V}_{123})\,|\Psi\rangle$$

We neglect the three body force term, and using the definition of the permutation operator ($V_{23} = P_{12}P_{23}V_{12}P_{23}P_{12}$)

$$|\Psi\rangle = \frac{1}{(E - H_0)}(\mathbb{1} + \underbrace{P_{12}P_{23} + P_{13}P_{23}}_{=P})V_{12}\,|\Psi\rangle$$

Theory

For convenience, defining the Faddeev component.

$$|\psi_{12}\rangle = \frac{1}{E - H_0} V_{12} |\Psi\rangle$$

So the Schrödinger equation in terms of the Faddeev component would be written as:

$$|\psi_{12}\rangle = \frac{1}{E - H_0} V_{12}(\mathbb{1} + P) |\psi_{12}\rangle$$

Theory

Using the Lippmann-Schwinger equation,

$$t_{12} = V_{12} + V_{12} \frac{1}{E - H_0} t_{12}$$

we can simplify the Schrödinger equation in the Faddeev component

$$|\psi_{12}\rangle = \frac{1}{E - H_0} t_{12} P |\psi_{12}\rangle$$

This is the Faddeev equation.

Theory (Jacobi Coordinates)

We use Jacobi coordinates because we can describe the entire system in terms of the t_{12}

$$\vec{p}_{12} = \frac{1}{2}(\vec{k}_1 - \vec{k}_2)$$
$$\vec{p}_3 = \frac{2}{3}\vec{k}_3 - \frac{1}{3}(\vec{k}_1 + \vec{k}_2)$$
$$\vec{P} = \vec{k}_1 + \vec{k}_2 + \vec{k}_3$$

These follow:

$$\langle \vec{p}'_{12}\vec{p}'_3 | \vec{p}_{23}\vec{p}_1 \rangle = \delta^{(3)}(\vec{p}_{23} + \frac{1}{2}\vec{p}'_{12} + \frac{3}{4}\vec{p}'_3)\delta^{(3)}(\vec{p}_1 - \vec{p}'_{12} + \frac{1}{2}\vec{p}'_3)$$

Permutation Operator

In terms of the Jacobi coordinates, the representation of the Permutation operator would be:

$$ {}_{(12)3}\langle \vec{p}'_{12}\vec{p}'_3|P_{12}P_{23}|\vec{p}_{12}\vec{p}_3\rangle_{(12)3} = {}_{(12)3}\langle \vec{p}'_{12}\vec{p}'_3|\vec{p}_{12}\vec{p}_3\rangle_{(23)1} $$

Using this,

$$ {}_{(12)3}\langle \vec{p}'_{12}\vec{p}'_3|P|\vec{p}_{12}\vec{p}_3\rangle_{(12)3} = 2\,{}_{(12)3}\langle \vec{p}'_{12}\vec{p}'_3|\vec{p}_{12}\vec{p}_3\rangle_{(23)1} $$

Now, most of the attention goes into evaluating ${}_{(12)3}\langle \vec{p}'_{12}\vec{p}'_3|\vec{p}_{12}\vec{p}_3\rangle_{(23)1}$

Permutation Operator (Partial Wave Representation)

In the partial wave representation, the Permutation operator can be simplified to:

$$
{}_{(12)3}\langle p'_{12} p'_3 \alpha' M' | p_{12} p_3 \alpha M \rangle_{(23)1} =
$$

$$
\int_{-1}^{1} dx \frac{\delta(p_{12} - \pi_{12}(p'_3 p_3 x))}{p_{12}^2} \frac{\delta(p'_{12} - \pi'_{12}(p'_3 p_3 x))}{p'^2_{12}} \times G_{\alpha' \alpha}(p'_3 p_3 x)
$$

Where, $G_{\alpha' \alpha}$ depends upon the definition of the Wigner 9j and 6j symbols.

The Wigner 6j and 9j symbols

When involving the coupling of three or more angular momenta, we would need to use the Wigner 6j and 9j symbols (similar to the Clebsch-Gordan coefficients). One advantage of using these are also because of their symmetry properties.

Wigner-9j: $\langle a(bc),(de)f;im|(ad)g,(be)h;im\rangle =$

$$\sqrt{(2c+1)(2f+1)(2g+1)(2h+1)}\begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{Bmatrix}$$

Wigner-6j: $\langle a,(bc)d;JM|(ab)e,c;JM\rangle =$

$$(-1)^{a+b+c+J}\sqrt{(2d+1)(2e+1)}\begin{Bmatrix} a & b & e \\ c & J & d \end{Bmatrix}$$

Permutation Operator (Partial Wave Representation)

The function $G_{\alpha'\alpha}(p_3' p_3 x)$ is defined as:

$$
\begin{aligned}
G_{\alpha'\alpha} = & \sum_L \sum_S (2S+1)\sqrt{\tilde{j}_{12}\tilde{j}'_{12}\tilde{j}_3\tilde{j}'_3} \\
& \times \begin{Bmatrix} l_{12} & s_{12} & j_{12} \\ l_3 & \frac{1}{2} & j_3 \\ L & S & J \end{Bmatrix} \begin{Bmatrix} l'_{12} & s'_{12} & j'_{12} \\ l'_3 & \frac{1}{2} & j'_3 \\ L & S & J \end{Bmatrix} \\
& \times (-1)^{s_{12}} \sqrt{(2s'_{12}+1)(2s_{12}+1)} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & s'_{12} \\ \frac{1}{2} & S & s_{12} \end{Bmatrix} \\
& \times (-1)^{\tau_{12}} \sqrt{(2\tau'_{12}+1)(2\tau_{12}+1)} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & \tau'_{12} \\ \frac{1}{2} & T & \tau_{12} \end{Bmatrix} \\
& \times 8\pi^2 \sum_M \mathcal{Y}^{*LM}_{l'_{12} l'_3} \mathcal{Y}^{LM}_{l_{12} l_3}
\end{aligned}
$$

Discretization

For a numerical implementation, we need to discretize the integrals in the Lippmann-Schwinger equation and the Faddeev equations. For the Faddeev equation, we have:

$$\psi(i'j'\alpha') = \sum_{ij\alpha} K(i'j'\alpha'; ij\alpha)\psi(ij\alpha)$$

where,

$$K(i'j'\alpha'; ij\alpha) = \frac{1}{E - \frac{{p'_{12}}^2}{m} - \frac{3{p'_3}^2}{4m}} \omega^q_{j'} q^2_{j'} \sum_{\tilde{\alpha}} \delta_{\tilde{\alpha}_3\alpha'_3}$$
$$\times \sum_k \omega^x_k \sum_m S_m(\pi'_{12}(q_{j'}q_j x_k)) \times t_{12}(p_i, \alpha'_{12}; p_m\tilde{\alpha}_m; q_{j'})$$
$$\times G_{\tilde{\alpha}\alpha}(q_{j'}q_j x_k) \times S_i(\pi_{12}(q_{j'}q_j x_k))$$

Discretization

The Lippmann-Schwinger equation is discretized similarly to how it was done in the lecture:

$$\sum_{\alpha''_{12},m} A(p_i, \alpha'_{12}, p_m, \alpha''_{12}) \cdot t_{12}(p_m, \alpha'_{12}; p_m\tilde{\alpha}_m; q_k)$$
$$= V_{12}(p_i, \alpha'_{12}, p_j, \alpha_{12})$$

where the matrix A is defined as such:

$$A(p_i,\alpha'_{12}, p_m, \alpha''_{12}) = \delta_{p_i p_m}\delta_{\alpha'_{12}\alpha''_{12}}$$
$$- \omega_{p_m} p_m^2 V_{12}(p_i, \alpha'_{12}, p_m, \alpha''_{12}) \frac{1}{E - \frac{p_m^2}{m} - \frac{3p_3^2}{4m}}$$

Discretization

The wave function can now be obtained using the fact that

$$|\Psi\rangle = (\mathbb{1} + P)\,|\psi_{12}\rangle$$

So finally, we obtain the discretized equation for the wave function as:

$$\begin{aligned}\Psi(p_i', q_j', \alpha_{12}') = \sum_{p_i, q_j, \alpha_{12}} \sum_k \omega_k^x (\mathbb{1} + \alpha G_{\alpha'\alpha}(p_{i'} q_j x_k)) \\ \times S_i(\pi_{12}(p_{i'} q_{j'} x_k)) S_j(\pi_3(p_{i'} q_{j'} x_k)) \psi(p_i, q_j, \alpha_{12})\end{aligned}$$

The Interaction Potential

We consider two cases:

- Spin independent interaction: One Boson Exchange (OBE)
- Spin dependent interaction: One Pion Exchange (OPE)

The expression for the spin-independent interaction is the same as in the Lecture. The same parameters are used for our analysis.

For the spin-dependent interaction, the Wigner 9j and 6j symbols are used because of the coupling of the spin and orbital angular momenta.

Implementation: Lippmann-Schwinger Equation

Solving the Lippmann-Schwinger Equation for the two-body off-shell t-matrix element t_{12} is done as with the three-boson case:

1. Compute the numerical form of the potential V_{12}
2. Construct the matrix equation $A \cdot t_{12} = V_{12}$
3. Solve for t_{12} using `numpy.linalg.solve`

This is done for each quantum state $\alpha_{12} = (l_{12}, s_{12}, j_{12}, \tau_{12})$.

Implementation: Faddeev Equation

The Faddeev equation is solved as an eigenvalue equation with an eigenvalue of $\eta_{true} = 1$, determined by the bound state energy E that yields such value:

1. Choose two energy values in $K(i'j'\alpha'; ij\alpha)$
2. Determine the discretized permutation operator $G_{\tilde{\alpha}\alpha}$ to construct the matrix $K(i'j'\alpha'; ij\alpha)$
3. Evaluate the Faddeev equation using `numpy.linalg.eig`
4. Repeat using the secant method until convergent eigenvalue is obtained

From our analysis, we obtained an energy value of $E = -5.221\,\mathrm{MeV}$ with an eigenvalue of $|\eta_{true} - \eta| = 2.07 \times 10^{-13}$.

Implementation: Quantum Mechanical Parameters

Maximal quantum numbers were chosen to consider the possible partial wave channels. We used the following maximal quantum numbers for our simulation:

$l_{12_{max}}$	$l_{3_{max}}$	$s_{12_{max}}$	$j_{12_{max}}$	$j_{3_{max}}$	$\tau_{12_{max}}$	$\tau_{3_{max}}$
1	0	1	2	$1/2$	1	$1/2$

Table 1: Maximal values of quantum numbers utilized in the simulation.

This constrains our analysis to total angular momentum states $J = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$.

Implementation: Optimization

Optimization routines performed to reduce runtime for Python for loops:

- `numpy.einsum` used instead of nested for loops for matrix multiplication
- Iterative solver used to determine eigenvalues once correct bound state energy is known
- Quantum states α are contained as one index $\rightarrow$ reduces dimensionality of problem
- Index reduced to one dimension for further reduction of dimensionality (where N_p, N_q are the grid size for p, q respectively):

$$\psi(ij\alpha) \rightarrow \psi(i + jN_p + \alpha N_p N_q)$$

Results: Off-shell t-matrix

Off-shell t-matrix yields more oscillatory modes at higher p, p' with higher angular states:

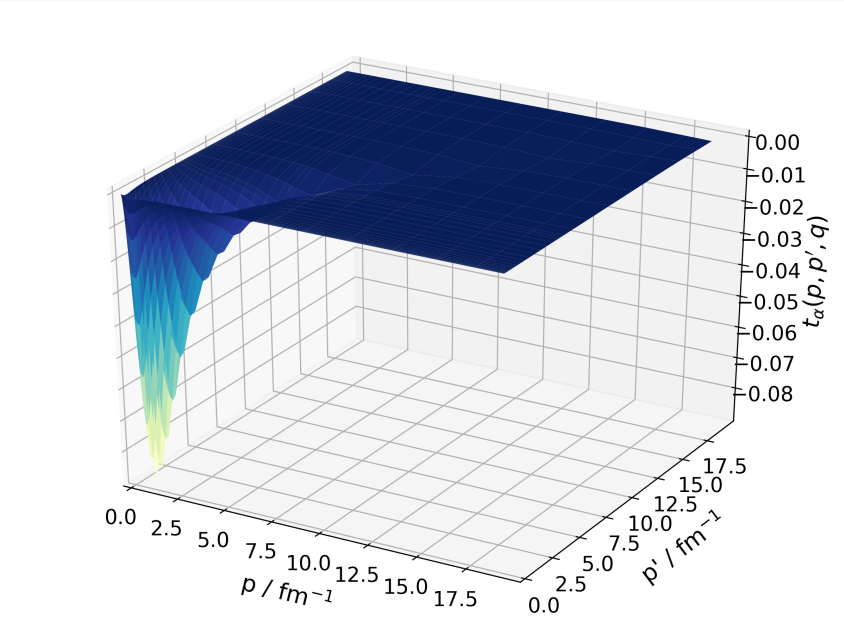


Figure 1: $j_{12} = 1,\ q = 0.00\,\mathrm{fm}^{-1}$

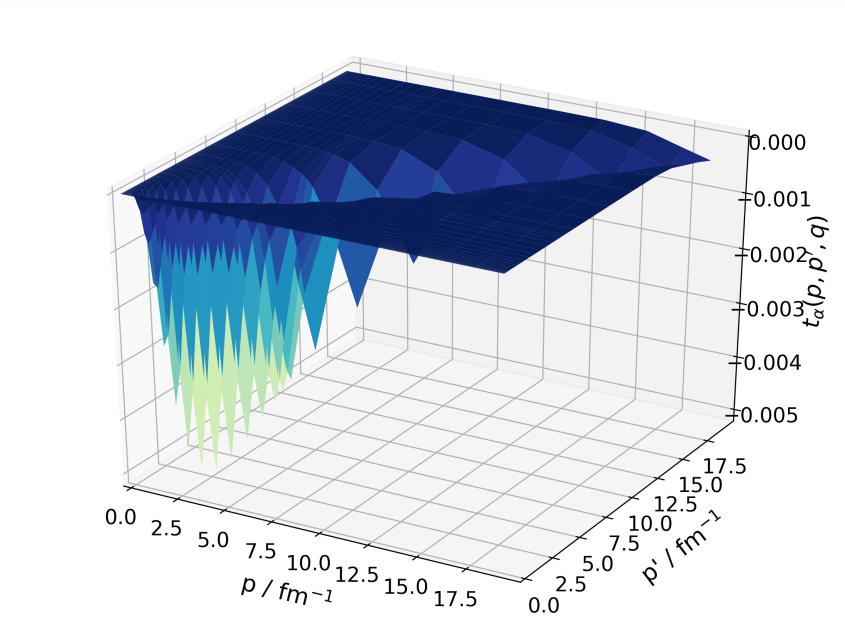


Figure 2: $j_{12} = 5,\ q = 0.00\,\mathrm{fm}^{-1}$

Results: Angular States

Three-Body fermionic wavefunction $|\Psi|$ at different total angular states:

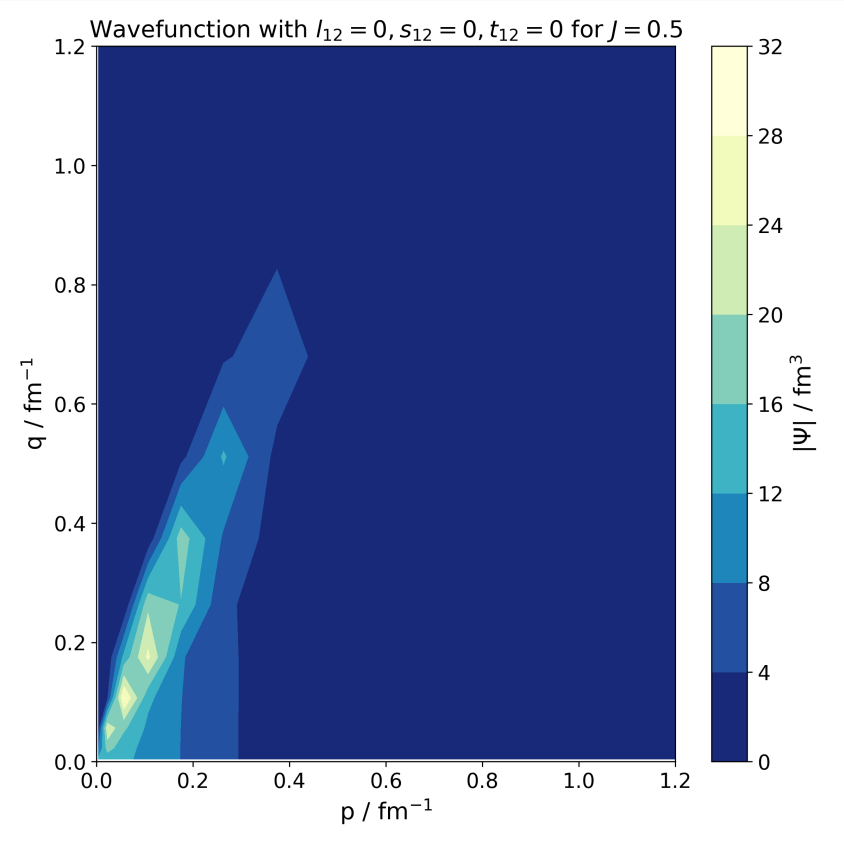


Figure 3: $J = \frac{1}{2}$

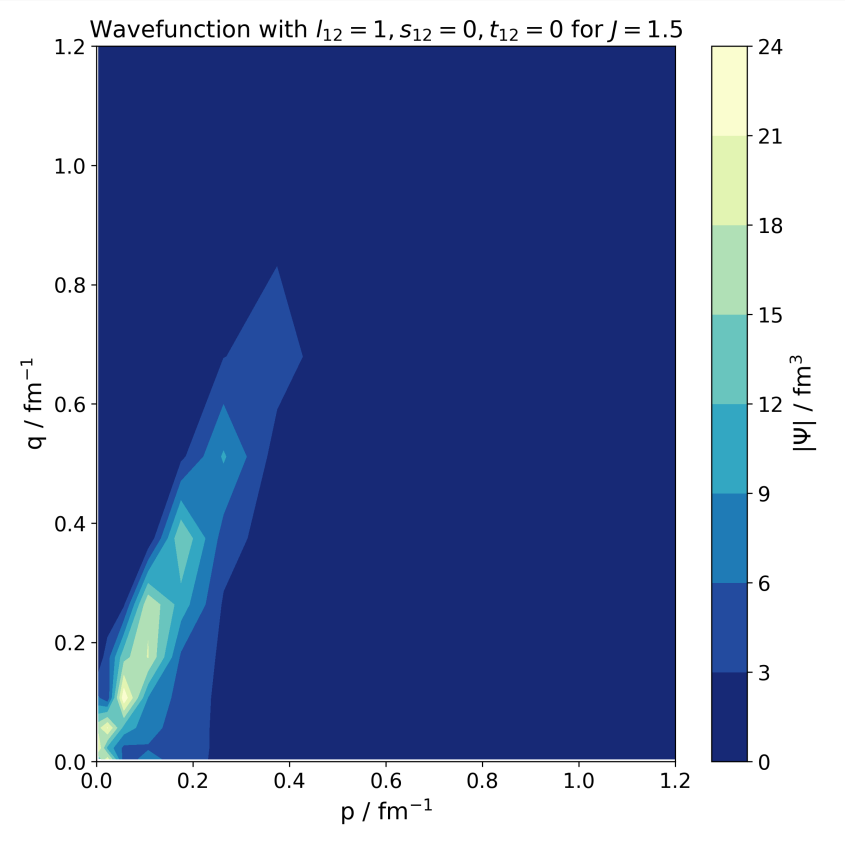


Figure 4: $J = \frac{3}{2}$

Results: Angular States

We project our results for different values of the spectator momentum q.

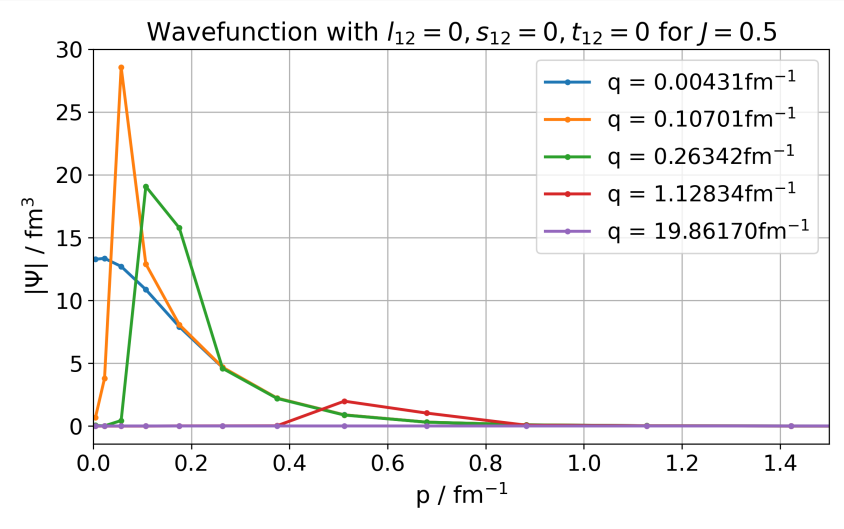


Figure 5: $J = \frac{1}{2}$

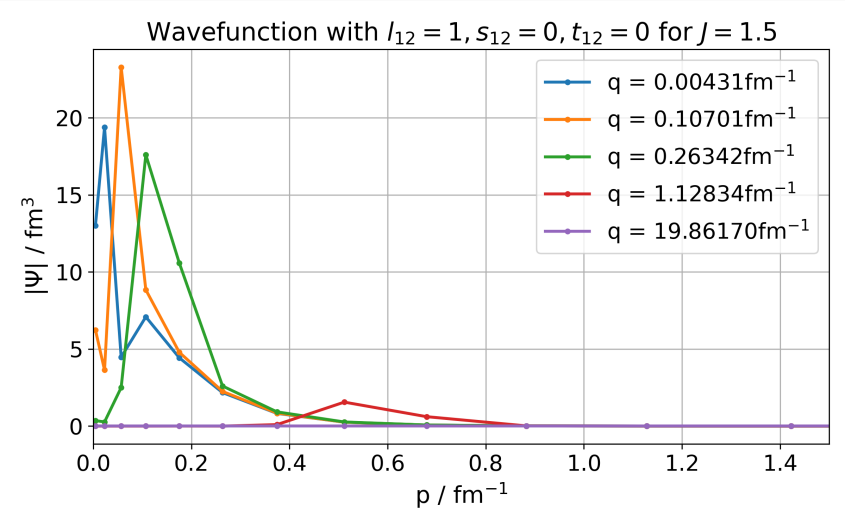
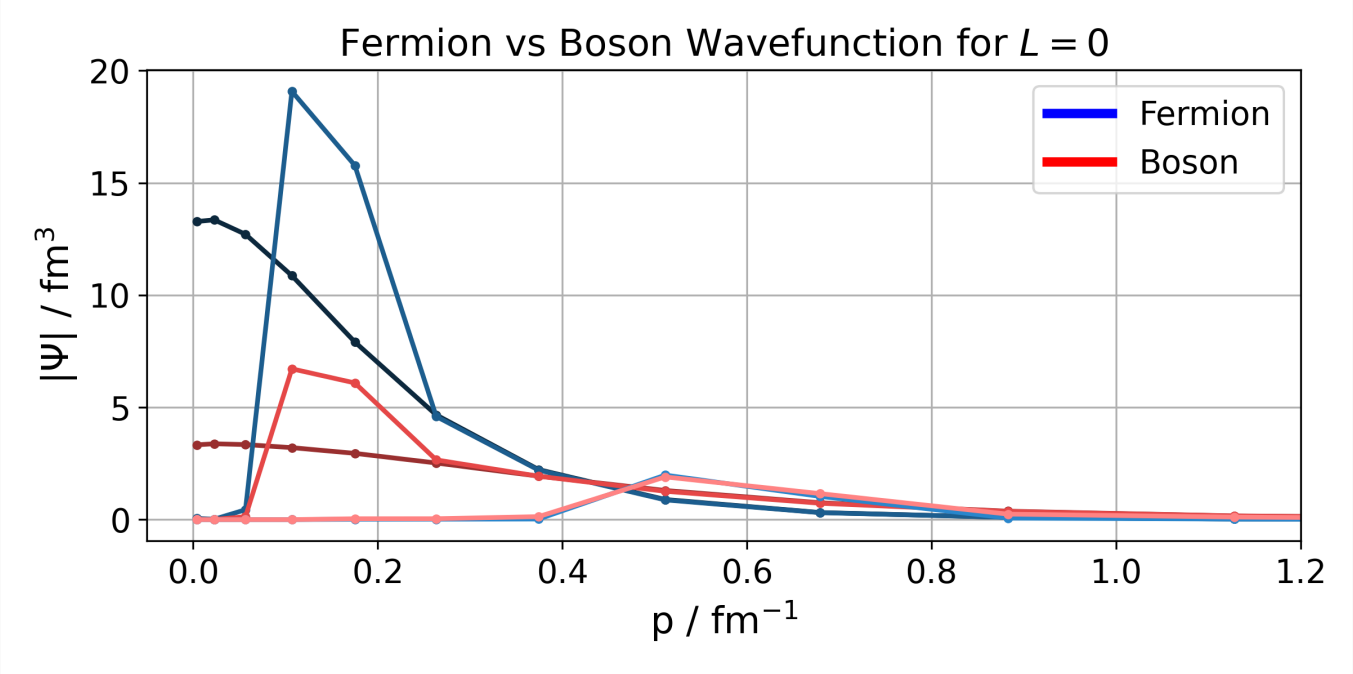


Figure 6: $J = \frac{3}{2}$

Both solutions decay at higher q, but the $J = \frac{1}{2}$ state has a smoother structure overall.

Results: Fermion vs Boson

We compare our results with the three-body bosonic wavefunction from the lectures:



The amplitude for the fermion wavefunction is much larger than the boson case!

Results: Kinetic Energy

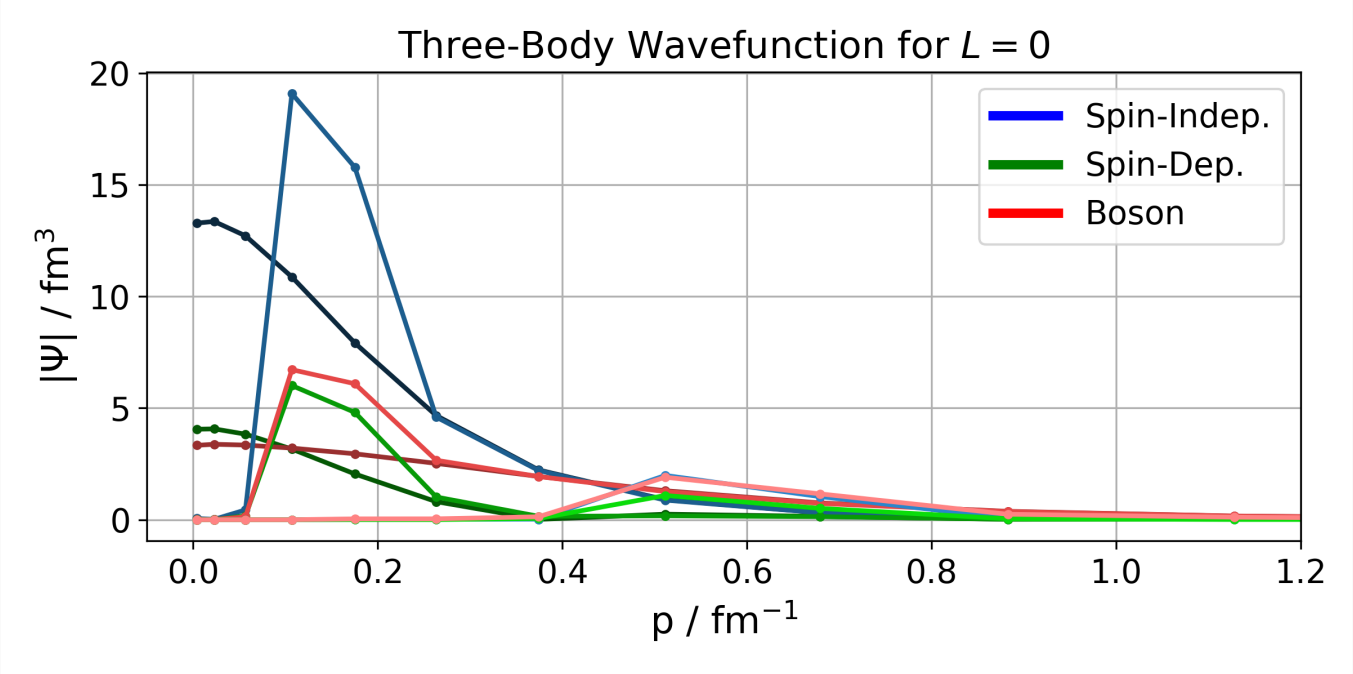
We evaluate the kinetic energy $\langle H_0 \rangle = \langle \Psi | H_0 | \Psi \rangle$ for three different quantum states:

J	$\langle H_0 \rangle$ / MeV
0	57.46
$^1/_2$	15.02
$^3/_2$	3.46

Table 2: Expectation value of the kinetic energy H_0 of the three-body system with different total angular momenta.

Results: Spin-Dependent Potential

We compare with the wavefunction obtained from the spin-dependent potential:



This yields a more realistic form of the fermionic wavefunction with comparable amplitudes to the bosonic case.

Conclusion & Outlook

- Solved the three-body fermionic wavefunction by considering s, j, τ quantum states from the bosonic case.
  - Modified Faddeev and Lippmann-Schwinger equation to include such states
  - Included spin-dependence into OBE potential
- Determined wavefunction for $J = \frac{1}{2}, \frac{3}{2}$ states
  - Lower angular states leads to smoother wavefunctions
  - Higher amplitudes than three-boson case
  - Spin-dependent potential makes wavefunction comparable to boson case
- Extension of project by including three-body force V_{123} and considering the four-body problem

Acknowledgments

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