Parallel Numerical Solutions of the QCD Bethe-Salpeter Equation

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CMPT 851 Preliminary Presentation

Quantum Bound States

- The study of quantum bound states is important because they are often what is actually observed.
- Simple atomic bound states can be studied with the Schrödinger equation:

$$H\Psi = E\Psi.$$

- More complicated problems require the use of approximation schemes, such as perturbation theory:

$$H = H_0 + \lambda H_1.$$

- For perturbation theory to be valid, the expansion parameter λ must be small.

Beyond Perturbation Theory

- In the theory of the strong nuclear force (quantum chromodynamics or QCD) the coupling can become large, making perturbation theory unsuitable.
- Non-perturbative bound states can be described by an integral equation (IE) called the Bethe-Salpeter equation:

$$\Gamma(p;P) = \int \frac{d^4q}{(2\pi)^4} K(q,p;P)\, S\left(q^+\right) \Gamma(q;P)\, S\left(q^-\right).$$

- $\Gamma(p;P)$ is the Bethe-Salpeter amplitude, and can be thought of as a wavefunction for the bound state.
- $S(q)$ is a quantum propagator for a bound particle.
- The kernel $K(q,p;P)$ represents all possible interactions between the bound particles. It is generally approximated.
- Since these are relativistic quantum objects (spin is important) they are all 4x4 matrices.

Lorentz Decomposition

- Particle physics relies on invariance under Lorentz transformations.
- $\Gamma(p; P)$ can be decomposed into Lorentz basis elements:

$$\Gamma(p; P) = \sum_{i=1}^{N} F_i(p; P)\,\widehat{\tau}_i(p; P).$$

- The matrix structure of these $\widehat{\tau}_i(p; P)$ allows them to be orthogonal under a trace operation:

$$Tr\left[\widehat{\tau}_i(p; P)\,\widehat{\tau}_j(p; P)\right] = \delta_{ij}.$$

- Expanding Γ on both sides and taking the trace of the equation uses the orthogonality to transform the 4x4 IE to N coupled 1x1 IEs.

Chebyshev Decomposition

- 4-dimensional quadrature is ineffiecient, so further simplifications are desired.
- The integral can be transformed into 4-d spherical coordinates:

$$(q_0, q_1, q_2, q_3) \longrightarrow (|q|, \phi_1, \phi_2, \theta).$$

- Due to the rotational symmetry of the problem, the angular dependence can be factored out through a decomposition into orthogonal Chebyshev polynomials (with $u = \cos(\phi_1)$):

$$F_i(p, P) = \sum_{j=0}^{M} U_j(u)\, \tilde{F}_{ij}(p^2, P^2).$$

- Again expanding the F_i on both sides of the system and integrating over the angular variables removes any angular dependence from the solution. The kernel becomes more complicated, however.

Discretization

- There is now a set of $N \times M$ coupled 1-dimensional IEs.
- Written as a vector equation, this looks like:

$$\begin{bmatrix} \tilde{F}_{ij}\left(p^2, P^2\right) \\ \vdots \end{bmatrix} = \left[\mathscr{K}_{ij,kl}\left(p^2, q^2, P^2\right)\right] \begin{bmatrix} \tilde{F}_{kl}\left(p^2, P^2\right) \\ \vdots \end{bmatrix}.$$

- Now the equation is discretized in its p^2 and q^2 dependecies on a grid of size r:

$$\begin{bmatrix} \left[\tilde{F}_{ij}\right] \\ \vdots \end{bmatrix} = \begin{bmatrix} \left[\mathscr{K}_{ij,kl}\left(P^2\right)\right] & \cdots \\ \vdots & \ddots \end{bmatrix} \begin{bmatrix} \left[\tilde{F}_{kl}\right] \\ \vdots \end{bmatrix}.$$

- The result is a $r \times N \times M$ dimensional linear system.

Eigenvalue Problem

- The system still has a free parameter P, which needs to be fixed.
- An artifical eigenvalue depending on P is inserted into the equation, turning it into a proper eigenvalue problem:

$$\lambda\left(P^2\right)\left[\tilde{F}_{ij}\right]=\left[\mathscr{K}\left(P^2\right)\right]\left[\tilde{F}_{kl}\right].$$

- To solve the equation with $\lambda\left(P^2\right)=1$, the eigenvalue problem needs to be solved for many different values of P. The value of P that gives an eigenvalue of 1 is the correct value.
- Physically, P is the mass of the bound state and the solution $\left[\tilde{F}_{ij}\right]$ gives the components of the bound state wavefunction.
- Solving this eigenvalue problem is then equivalent to solving the IE.

Summary and Parallelization

- There are three separate computational problems which might benefit from parallelization.
- First is the computation of the matrix $\left[\mathscr{K}\left(P^2\right)\right]$, which involves tens of millions of double quadratures.
- Second is the eigenvalue computation, which is relatively cheap.
- Finally, the above two steps must be repeated for a range of P values until $\lambda\left(P^2\right) = 1$ is found.