

Baryon spectrum analysis using Dirac's covariant constraint dynamics

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We present a relativistic quark model for the baryons that combines three related relativistic formalisms. The three-body constraint formalism of Sazdjian is used to recast three relativistic two-body equations for the three pairs of interacting quarks into a single relativistically covariant three-body equation for the bound state energies, having a Schrodinger-like structure. The two-body equations are the two-body Dirac equations of constraint dynamics derived by Crater and Van Alstine for combined world vector and scalar interactions providing the necessary spin dependent and spin independent interaction terms. The minimal quasipotential formalism of Todorov is used to provide an invariant framework for the vector and scalar dynamics used in the two-body Dirac equations into which is inserted a local simplified version of the Richardson potential. The spectral results are analyzed and compared to experiment using a best fit method and several different algorithms, including a gradient approach, and a Monte Carlo method.

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I. INTRODUCTION

Recent quark model calculations done by Crater *et al.* [1–3] using covariant two-body Dirac equations (TBDE) in a relativistic constraint dynamics formalism have given a good description of the meson masses for both light and heavy quarks. The good quality of the fit has been attributed to the exact two-body kinematics merged with a QCD interaction potential based on vector and scalar potentials that uses a minimal number of variable parameters. The vector potential, in turn, has a structure originally derived from the classical electrodynamics of Wheeler and Feynman [4]. This structure can also be obtained from quantum electrodynamics by using a covariant three-dimensional truncation of the Bethe-Salpeter equation [5] based on the Todorov quasipotential approach [6], which is then compared to the TBDE. [7] The comparison is done in order to identify the appropriate invariant potential functions that will be used in the potential model. These nonperturbative (numerical) results hold up well when compared to other methods for meson spectroscopy.

In this paper, we extend the Hamiltonian constraint dynamics formalism for the two-body system to the three-body quark problem for baryon spectroscopy [8]. In taking the two-body equations to a three-body system we still regard the system as the naive quark model in that the interactions are between each pair of quarks and there is no overarching three-body interaction to be considered and no consideration of the effects of baryon decays on their masses, but the system now has three sets of interactions instead of just one. Thus, all of our interactions are still two-body interactions, but for three sets of quarks.

The Hamiltonian constraint dynamics formalism [9] allows for a relativistic method of accounting for two-body effects. In addition, constraint dynamics as developed by Crater and Van Alstine [10] provides not only the usual spin interaction dependence seen in the Dirac equation but also

additional terms needed to make the approach mathematically consistent. It is useful in both a classical and a quantum mechanical formalism as well as correctly accounting for fine and hyperfine structures in positronium and muonium systems [7,11]. We review the two-body formalism with an eye toward its adaptation to the three-body system using Sazdjian's approach to relativistic N -body problem [12].

In our adaptation of the two-body formalism to the numerical solution of three quark bound states, the variational principle is used together with a new type of Gaussian basis wave functions of total JM to solve our eigenvalue equation. We show how this new Gaussian basis is used in conjunction with a variational approach in obtaining the appropriate eigenvalues with the matrix being truncated after a reasonable limit is reached (in theory an infinitely large variational matrix would give the exact reflection of the states of the model). Since the effective potentials are dependent on the center of momentum (c.m.) total energy eigenvalue $w = m_1 + m_2 + m_3 + E$, the standard approach to using the variational principle must be modified to include a recursion algorithm with an embedded E dependence in the matrix elements of the effective Hamiltonian \mathcal{H} . This E will change as we approach convergence. The program then is designed to iteratively solve these equations until a desired level of convergence is reached. The matrix elements of our Hamiltonian can be determined exactly for the kinematics but including the interacting potentials requires, of course, a numerical treatment. Also as in the two-body case, the interacting potentials we used [2] depend only on three parameters characterizing just two invariant functions, embodying the world vector and scalar potentials appearing in the TBDE. The numerical fitting routine uses a chi-squared minimization Monte Carlo routine combined with a simplified gradient approach to acquire a best fit for the spectrum of known baryons. We have compared our

numerical results to both experimental data and to other theories, most notably the approach of Capstick and Isgur [13], while also comparing the quark masses and potential parameters we obtained in our fit with those found in the meson spectral results of [2].

II. REVIEW OF RELATIVISTIC TWO-BODY CONSTRAINT APPROACH

In this and in the following subsections we present a review of the constraint formalism in preparation for its implementation in the three-body problem.¹ The relativistic two-body bound state problem has a natural origin from quantum field theory in the form of the Bethe-Salpeter equation [5]. However, this equation is not usually applied in its full four-dimensional form due to the difficulty of treating the relative time coordinate [14]. Numerous three-dimensional truncations of the Bethe-Salpeter equation have been proposed for the relativistic two-body problem [6,15]. Some of these types of approximate methods have previously been applied with considerable success to the $q\bar{q}$ meson spectrum [16–22],[1] and [23–28].

The TBDE of constraint dynamics provide a manifestly covariant three-dimensional truncation of the Bethe-Salpeter equation that more efficiently distills two-body bound state and elastic scattering results. Sazdjian [29] has shown that the Bethe-Salpeter equation can be algebraically transformed into two independent equations. The first yields a covariant three-dimensional eigenvalue equation which for spinless particles takes the form

$$(\mathcal{H}_{10} + \mathcal{H}_{20} + 2\Phi)\Psi(x_1, x_2) = 0, \quad (2.1)$$

where $\mathcal{H}_{i0} = p_i^2 + m_i^2$. He finds that the quasipotential² Φ is a modified geometric series in the Bethe-Salpeter kernel K such that in lowest order in K

$$\Phi = \pi i w \delta(P \cdot p) K, \quad (2.2)$$

where $P = p_1 + p_2$ is the total momentum, $p = \eta_2 p_1 - \eta_1 p_2$ is the relative momentum, w is the invariant total center of momentum (c.m.) energy with $P^2 = -w^2$. The η_i must be chosen so that the relative coordinate $x = x_1 - x_2$ and p are canonically conjugate, i.e. $\eta_1 + \eta_2 = 1$. The second independent equation overcomes the difficulty of treating the relative time in the c.m. system by setting an invariant condition on the relative momentum p ,

$$(\mathcal{H}_{10} - \mathcal{H}_{20})\Psi(x_1, x_2) = 0 = 2P \cdot p \Psi(x_1, x_2). \quad (2.3)$$

¹This section follows closely the corresponding review section given in [1].

²An earlier description of the connection of the constraint approach to the quasipotential approach involving Lippmann-Schwinger type of equations is given by Todorov [30] and Crater *et al.* [7] (see also [23]).

Note that this implies $p^\mu \Psi = p_\perp^\mu \Psi \equiv (\eta^{\mu\nu} + \hat{P}^\mu \hat{P}^\nu) p_\nu \Psi$ in which $\hat{P}^\mu = P^\mu/w$ is a timelike unit vector ($\hat{P}^2 = -1$) in the direction of the total momentum.

One can further combine the sum and the difference of Eqs. (2.1) and (2.3) to obtain a set of two relativistic equations one for each particle with each equation specifying two generalized mass-shell constraints

$$\mathcal{H}_i \Psi(x_1, x_2) = (p_i^2 + m_i^2 + \Phi) \Psi(x_1, x_2) = 0, \quad i = 1, 2, \quad (2.4)$$

including the interaction with the other particle by way of the quasipotential Φ . These constraint equations were originally derived using Dirac's Hamiltonian constraint dynamics [9,31]. Dirac's constraint dynamics stipulate that these two constraints must satisfy the compatibility condition, $[\mathcal{H}_1, \mathcal{H}_2]\Psi = 0$, that is, they must be first class.³ With no external potentials, the coordinate dependence of the quasipotential Φ would be through x and the compatibility condition becomes $[p_1^2 - p_2^2, \Phi]\Psi = P^\mu \partial \Phi / \partial x^\mu = 0$. In order for this to be true in general, Φ must depend on the relative coordinate x only through its component, x_\perp , perpendicular to P ,

$$x_\perp^\mu = (\eta^{\mu\nu} + \hat{P}^\mu \hat{P}^\nu)(x_1 - x_2)_\nu. \quad (2.5)$$

Since the total momentum is conserved, the single component wave function Ψ in coordinate space is a product of a plane wave eigenstate of P and an internal part ψ [32], depending on this x_\perp .⁴

We find a plausible structure for the two-body quasipotential Φ by examining how scalar and vector interactions are introduced in the one-body Klein-Gordon equation $(p^2 + m^2)\psi = (\mathbf{p}^2 - \epsilon^2 + m^2)\psi = 0$. This takes the form $(\mathbf{p}^2 - \epsilon^2 + m^2 + 2mS + S^2 + 2\epsilon A - A^2)\psi = 0$ when one introduces a scalar interaction and timelike vector interaction via $m \rightarrow m + S$ and $\epsilon \rightarrow \epsilon - A$. In the two-body case, separate classical [33] and quantum field theory [34] arguments show that when one includes world scalar and vector interactions between the two particles, then Φ depends on two underlying but unspecified invariant functions $S(r)$ and $A(r)$ through the two-body

³These constraint equations were originally proposed in the form of classical generalized mass shell first class constraints $\mathcal{H}_i = (p_i^2 + m_i^2 + \Phi_i) \approx 0$, and their quantization $\mathcal{H}_i \Psi = 0$ without reference to a quantum field theory. For the classical \mathcal{H}_i to be compatible, their Poisson bracket with one another must either vanish strongly or depend on the constraints themselves, $\{\mathcal{H}_1, \mathcal{H}_2\} \approx 0$. The simplest solution of this equation is $\Phi_1 = \Phi_2$, a kind of relativistic third law condition, together with their common transverse coordinate dependence $\Phi_w(x_\perp)$, just as with its quantum version.

⁴We use the same symbol P for the eigenvalue so that the w dependence in Eq. (2.6) is regarded as an eigenvalue dependence. The wave function Ψ can be viewed as a relativistic 2-body wave function.

Klein-Gordon-like potential form with the same general structure, that is

$$\Phi = 2m_w S + S^2 + 2\varepsilon_w A - A^2. \quad (2.6)$$

Those field theory based arguments point to the following c.m. energy dependent forms

$$m_w = m_1 m_2 / w, \quad (2.7)$$

and

$$\varepsilon_w = (w^2 - m_1^2 - m_2^2) / 2w. \quad (2.8)$$

They were first introduced by Todorov [35] as the relativistic reduced mass and effective particle energy for the two-body system. Similar to what happens in the nonrelativistic two-body problem, in the relativistic case we have the motion of this effective particle taking place as if it were in an external field (here generated by S and A). The two kinematical variables (2.7) and (2.8) are related to one another by the Einstein condition

$$\varepsilon_w^2 - m_w^2 = b^2(w), \quad (2.9)$$

where the invariant

$$b^2(w) \equiv (w^4 - 2w^2(m_1^2 + m_2^2) + (m_1^2 - m_2^2)^2) / 4w^2, \quad (2.10)$$

is the c.m. value of the square of the relative momentum expressed as a function of w . One also has

$$b^2(w) = \varepsilon_1^2 - m_1^2 = \varepsilon_2^2 - m_2^2, \quad (2.11)$$

in which ε_1 and ε_2 are the invariant c.m. energies of the individual particles satisfying

$$\varepsilon_1 + \varepsilon_2 = w, \quad \varepsilon_1 - \varepsilon_2 = (m_1^2 - m_2^2) / w. \quad (2.12)$$

In terms of these invariants, the relative momentum appearing in Eqs. (2.2) and (2.3) is given by

$$p^\mu = (\varepsilon_2 p_1^\mu - \varepsilon_1 p_2^\mu) / w, \quad (2.13)$$

so that $\eta_1 + \eta_2 = (\varepsilon_1 + \varepsilon_2) / w = 1$. In [36] the forms for these two-body and effective particle variables are given sound justifications based solely on relativistic kinematics, supplementing the dynamical arguments of [33] and [34]. In summary, the wave function $\Psi(x_1, x_2)$ for spinless two body systems satisfies

$$P \cdot p \Psi(x_1, x_2) = 0,$$

$$(p^2 + \Phi) \Psi(x_1, x_2) = b^2 \Psi(x_1, x_2). \quad (2.14)$$

Originally, the two-body Dirac equations of constraint dynamics arose from a supersymmetric treatment of two pseudoclassical constraints (with Grassmann variables in place of gamma matrices) which were then quantized [10]. Sazdjian later derived [29] different forms of these same equations, just as with their spinless counterparts above, as a covariant three-dimensional truncation of the Bethe-Salpeter equation. The forms of the equations are varied but the one that is the most familiar is the “external potential” form similar in structure to the ordinary Dirac equation.⁵ For two particles interacting through world scalar and vector interactions they are

$$\begin{aligned} \mathcal{S}_1 \Psi &\equiv \gamma_{51} (\gamma_1 \cdot (p_1 - \tilde{A}_1) + m_1 + \tilde{S}_1) \Psi = 0, \\ \mathcal{S}_2 \Psi &\equiv \gamma_{52} (\gamma_2 \cdot (p_2 - \tilde{A}_2) + m_2 + \tilde{S}_2) \Psi = 0. \end{aligned} \quad (2.15)$$

Here Ψ is a 16 component wave function consisting of an external plane wave part that is an eigenstate of P and an internal part $\psi = \psi(x_\perp)$. The vector potential \tilde{A}_i^μ is taken to be an electromagnetic-like four-vector potential with the time and spacelike portions both arising from a single invariant function A .⁶ The tilde on these four-vector potentials as well as on the scalar ones \tilde{S}_i indicate that these are not only position dependent but also spin dependent by way of the gamma matrices. The operators \mathcal{S}_1 and \mathcal{S}_2 must commute or at the very least $[\mathcal{S}_1, \mathcal{S}_2] \Psi = 0$ since they operate on the same wave function.⁷ This compatibility condition gives restrictions on the spin dependence which the vector and scalar potentials

$$\begin{aligned} \tilde{A}_i^\mu &= \tilde{A}_i^\mu(A(r), p_\perp, \hat{P}, w, \gamma_1, \gamma_2), \\ \tilde{S}_i &= \tilde{S}_i(S(r), A(r), p_\perp, \hat{P}, w, \gamma_1, \gamma_2) \end{aligned} \quad (2.16)$$

are allowed to have⁸ in addition to requiring that they depend on the invariant separation $r \equiv \sqrt{x_\perp^2}$ through the

⁵So-called hyperbolic forms of the two-body Dirac equations display more directly the connection between the source of the interactions and the matrix structure of the three point vertex interactions of quantum field theory. See [37] and [38].

⁶In a perturbative context, i.e. for weak potentials, that would mean that this aspect of \tilde{A}_i^μ is regarded as arising from a Feynman gauge vertex coupling of a form proportional to $\gamma_1^\mu \gamma_{2\mu} A$.

⁷The γ_5 matrices for each of the two particles are designated by γ_{5i} $i = 1, 2$. The reason for putting these matrices out front of the whole expression is that including them facilitates the proof of the compatibility condition, see [10].

⁸The dependence of the scalar potentials \tilde{S}_i on the invariant $A(r)$ responsible for the electromagneticlike potential is seen in [32] and [34] to result from the way the scalar and vector fields combine. That combination leads to a two-body Klein-Gordon-like potential portion of Φ_w to be of the form given in Eq. (2.6).

invariants $A(r)$ and $S(r)$. The covariant constraint (2.3) can also be shown to follow from Eq. (2.15). We give the explicit connections between \tilde{A}_i^μ , \tilde{S}_i and the invariants $A(r)$, and $S(r)$ in Appendix A of [39]. The Pauli reduction of these coupled Dirac equations lead to a covariant Schrödinger-like equation for the relative motion with an explicit spin-dependent potential Φ ,

$$(p_\perp^2 + \Phi(A(r), S(r), p_\perp, \hat{P}, w, \sigma_1, \sigma_2))\psi_+ = b^2(w)\psi_+, \quad (2.17)$$

with $b^2(w)$ playing the role of the eigenvalue.⁹ This eigenvalue equation can then be solved for the four-component effective particle spinor wave function ψ_+ related to the 16 component spinor $\psi(x_\perp)$ (See Appendix A of [1]). In Ref. [1] a number of important and desirable features of the set of Eq. (2.15) and the equivalent Schrödinger-like equation (2.17) are discussed.

In [22] we presented details of the application of this formalism to meson spectroscopy using a covariant version of the Adler-Piran static quark potential. Note especially that the equations used there displayed a *single* $\Phi(A(r), S(r), p_\perp, \hat{P}, w, \sigma_1, \sigma_2)$ in Eq. (2.17). It depends on the quark masses through factors such as those that appear in Eq. (2.6). However its dependence is the same for all quark mass ratios—hence a single structure for all the $Q\bar{Q}$, $q\bar{q}$, and $q\bar{q}$ mesons in a single overall fit. We found that the fit provided by the TBDE for the entire meson spectrum (from the pion to the excited bottomonium states) competes with the best fits to partial spectra provided by other approaches and does so with the smallest number of interaction functions [just $A(r)$ and $S(r)$] without additional cutoff parameters necessary to make those approaches numerically tractable. We also found that the pion bound state displays some characteristics of a Goldstone boson. That is, as the quark mass tends to zero, the pion mass (unlike the ρ and the excited π) vanishes, in contrast to almost every other relativistic potential model.

In Appendix A of [1] we outline the steps needed to obtain the explicit c.m. form of Eq. (2.17). That form is [22,40,41],

$$\begin{aligned} & \{\mathbf{p}^2 + \Phi(r, m_1, m_2, w, \sigma_1, \sigma_2)\}\psi_+ \\ &= \{\mathbf{p}^2 + 2m_w S + S^2 + 2\varepsilon_w A - A^2 + \Phi_D \\ &+ \mathbf{L} \cdot (\sigma_1 + \sigma_2)\Phi_{SO} + \sigma_1 \cdot \hat{\mathbf{r}}\sigma_2 \cdot \hat{\mathbf{r}}\mathbf{L} \cdot (\sigma_1 + \sigma_2)\Phi_{SOT} \\ &+ \sigma_1 \cdot \sigma_2\Phi_{SS} + (3\sigma_1 \cdot \hat{\mathbf{r}}\sigma_2 \cdot \hat{\mathbf{r}} - \sigma_1 \cdot \sigma_2)\Phi_T \\ &+ \mathbf{L} \cdot (\sigma_1 - \sigma_2)\Phi_{SOD} + i\mathbf{L} \cdot \sigma_1 \times \sigma_2\Phi_{SOX}\}\psi_+ \\ &= b^2\psi_+. \end{aligned} \quad (2.18)$$

⁹Due to the dependence of Φ_w on w , this is a nonlinear eigenvalue equation.

Thus is derived a relativistic two-body Schrödinger-like equation for world scalar and vector interactions. The minimal $2m_w S + S^2 + 2\varepsilon_w A - A^2$ portion is the classical interaction potential part (which also appears in the spinless Klein-Gordon equations), the $\mathbf{L} \cdot (\sigma_1 \pm \sigma_2)$ terms represent magnetic dipole moment interactions with an effective magnetic field and Thomas precession, and $\sigma_1 \cdot \hat{\mathbf{r}}\sigma_2 \cdot \hat{\mathbf{r}}\sigma_1 \cdot \sigma_2$ terms arise from dipole-dipole interactions and their relativistic corrections. A main focus of this work will be to derive a similar equation to Eq. (2.18) for the three-body baryon system as a whole. The detailed forms of the separate quasipotentials Φ are given in Appendix A of [1]. The subscripts of most of the quasipotentials are self-explanatory¹⁰. After the eigenvalue b^2 of (2.18) is obtained, the invariant mass of the composite two-body system w can then be obtained by inverting Eq. (2.10). It is given explicitly by

$$w = \sqrt{b^2 + m_1^2} + \sqrt{b^2 + m_2^2}. \quad (2.19)$$

The structure of the linear and quadratic terms in Eq. (2.18) as well as the Darwin and spin-orbit terms, are plausible in light of the discussion given above Eq. (2.6) and in light of the static limit Dirac structures that come about from the Pauli reduction of the Dirac equation. Their appearance as well as that of the remaining spin structures are direct outcomes of the Pauli reductions of the simultaneous TBDE Eq. (2.15).

This is the framework for the two-body system in a fully relativistic formalism, so from here we go to larger systems. Sazdjian [12] has done considerable work on the N -body system, which will be reviewed shortly. Although he does not deal with spin dependence with as much detail as done here, he does provide a very useful framework for the N -body problem in a constraint formalism.

A. Two-body Dirac equations: Explicit forms of the potentials

Since the forms of the potentials in the three-body case are similar to those in the two-body case, it is of use to briefly describe the two-body interacting potentials and how they affect the wave function. This section then contains a review of how the operators of the tensor, spin-spin, spin-orbit, spin-orbit difference, and spin-orbit exchange work on a $\langle jlsn \rangle$ state coupling, where n is the

¹⁰The subscript on quasipotential Φ_D refers to Darwin. It consists of what are called Darwin terms, those that are the two-body analogue of terms that accompany the spin-orbit term in the one-body Pauli reduction of the ordinary one-body Dirac equation, and ones related by canonical transformations to Darwin interactions [33,42], momentum dependent terms arising from retardation effects. The subscripts on the other quasipotentials refer respectively to SO (spin-orbit), SOD (spin-orbit difference), SOX (spin-orbit cross terms), SS (spin-spin), T (tensor), SOT (spin-orbit-tensor).

radial quantum number. In the three-body case there will be two n 's, one for each relative coordinate, but here there is just one.

First, our quasipotential (energy-dependent effective potential) is defined by

$$\begin{aligned}\Phi &= \Phi_{SI} + \Phi_D + \mathbf{L} \cdot (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \Phi_{SO} \\ &+ \boldsymbol{\sigma}_1 \cdot \hat{\mathbf{r}} \boldsymbol{\sigma}_2 \cdot \hat{\mathbf{r}} \mathbf{L} \cdot (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \Phi_{SOT} + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \Phi_{SS} \\ &+ (3\boldsymbol{\sigma}_1 \cdot \hat{\mathbf{r}} \boldsymbol{\sigma}_2 \cdot \hat{\mathbf{r}} - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) \Phi_T + \mathbf{L} \cdot (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \Phi_{SOD} \\ &+ i\mathbf{L} \cdot \boldsymbol{\sigma}_1 \times \boldsymbol{\sigma}_2 \Phi_{SOX}, \\ \Phi_{SI} &= 2m_w S + S^2 + 2\varepsilon_w A - A^2,\end{aligned}\quad (2.20)$$

where the potential terms Φ_D , Φ_{SO} , Φ_{SOT} , Φ_{SS} , Φ_T , Φ_{SOD} , Φ_{SOX} described earlier are all collections of two-body terms depending on the masses, distances between the two particles, invariant c.m. energies of the two particles, and the invariant energy of the total two-body system. The explicit forms of these are therefore not important to the current discussion of the operators and so will be left in this form for simplicity's sake. The spin-independent and Darwin terms have no spin operators and so when used on a $\langle jlsn|$ state they just give

$$\begin{aligned}\langle jlsn|\Phi_{SI}|j'l's'n'\rangle &= \delta_{ll'}\delta_{ss'}\langle n|\Phi_{SI}|n'\rangle, \\ \langle jlsn|\Phi_D|j'l's'n'\rangle &= \delta_{ll'}\delta_{ss'}\langle n|\Phi_{SI}|n'\rangle.\end{aligned}\quad (2.21)$$

The spin-orbit gives

$$\begin{aligned}\langle jlsn|\mathbf{L} \cdot (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)\Phi_{SO}|j'l's'n'\rangle \\ = [j(j+1) - l(l+1) - 2]\delta_{ll'}\delta_{ss'}\delta_{s1}\langle n|\Phi_{SO}|n'\rangle.\end{aligned}\quad (2.22)$$

As we will show later, while in the two-body case this l , j , and s are for the entire system, in the three-body problem it is just for each pair of particles and so this spin-orbit function requires additional (and extensive) manipulation in order to reach a completely coupled $|JLS\rangle$ state *for each set of particles*. The emphasis here is important as this is the main difficulty in going from the two-body formalism to a three-body one, in this work as well as others.

The tensor and spin-orbit tensor terms allow for coupling of different l states as well as identical l states, as shown in [7], while the spin-orbit difference and spin-orbit exchange *only* allow couplings between different spin states. The exact derivations of these potential terms are done in [1–3]. Since one of the goals of this work is to compare essentially the same methods that worked well for the meson spectrum to the baryon spectrum, we use these same potential terms in mostly the same form as they appear in the pure two-body case. The two-body operators are therefore defined and described in preparation for their adaptation to the three-body potential. Now we will give definitions for the

scalar and vector potentials used in our model and from that define the two-body potentials Φ_D , Φ_{SO} , Φ_{SOT} , Φ_{SS} , Φ_T , Φ_{SOD} , and Φ_{SOX} .

B. Explicit forms of the QCD model potentials

The authors of [22] have used a sophisticated form of the static quark potential developed by Adler and Piran [43], one that has ties at all length scales to field theoretic data and from this obtained good agreement with the quarkonium spectrum from experimental data. However, it is much more common in nonrelativistic treatments to use the static quark Cornell potential [44] for potential model studies,

$$V(r) = -\frac{\alpha_c}{r} + br, \quad (2.23)$$

as in [45,46]. Although not displaying asymptotic freedom, it does give the dominant Coulomb-like behavior as well as the linear quark confinement. Early on a model was proposed by Richardson for a static potential which both depends only a single scale size Λ and interpolates in a simple way between asymptotic freedom and linear confinement [47]. Richardson's model for the static interquark potential in momentum space is

$$\tilde{V}(\mathbf{q}) = -\frac{16\pi}{27} \frac{1}{\mathbf{q}^2 \ln(1 + \mathbf{q}^2/\Lambda^2)}, \quad (2.24)$$

arising from the assumption that

$$\tilde{V}(\mathbf{q}) = -\frac{4\alpha_s(\mathbf{q}^2)}{3\mathbf{q}^2}, \quad (2.25)$$

(including the color factor $-4/3$). It is important to note that this is for a $q\bar{q}$ color singlet state for the meson spectrum. In order to properly account for asymptotic freedom, we must have $\mathbf{q}^2/\Lambda^2 \gg 1$, which gives

$$\alpha_s(\mathbf{q}^2) \rightarrow \frac{8\pi}{27} \frac{1}{\ln(\mathbf{q}^2/\Lambda^2)}. \quad (2.26)$$

On the other hand, the property of linear confinement requires that for $\Lambda r \gg 1$, $V(r) \propto r$ or equivalently that for $\mathbf{q}^2/\Lambda^2 \ll 1$ one must impose $\alpha_s(\mathbf{q}^2) \sim \mathbf{q}^{-2}$. The interpolation of Eq. (2.24) is not tied at all in the intermediate region and only roughly tied in the large r region to any field theoretic data. Nevertheless it provides a convenient one-parameter form for the static quark potential. In coordinate space it has the form

$$V(r) = \frac{8\pi\Lambda^2 r}{27} - \frac{8\pi f(\Lambda r)}{27r}, \quad (2.27)$$

where $f(\Lambda r)$ is given by a complicated integral transform¹¹ that displays the asymptotic freedom behavior for $r \rightarrow 0$ of

$$f(\Lambda r) \rightarrow -\frac{1}{\ln \Lambda r}, \quad (2.28)$$

while for $r \rightarrow \infty$,

$$f(\Lambda r) \rightarrow 1. \quad (2.29)$$

A simpler model for the potential function $f(r)$, which we use in this paper and one which displays the same large and small r behavior is¹²

$$V(r) = \frac{8\pi\Lambda^2 r}{27} - \frac{16\pi}{27r \ln(e^2 + 1/(\Lambda r)^2)}. \quad (2.30)$$

It amounts to replacing Richardson's $f(\Lambda r)$ by $2/\ln(e^2 + 1/(\Lambda r)^2)$, having the same limits ($e = \exp(1)$). The slightly modified forms of the scalar and vector invariant potentials, including the electromagnetic part

$$S = \frac{8\pi\Lambda^2 r}{27}, \quad A = -\frac{16\pi}{27r \log\left(Ke^2 + \frac{B}{(\Lambda r)^2}\right)} + \frac{e_1 e_2}{4\pi r} \quad (2.31)$$

are used to construct all of the individual Φ terms. Their explicit forms, derived from the above A and S are given in Appendix A of [39]. In the case of the baryons these are slightly changed due to a different color factor [48] ($-4\alpha_s/3$ becomes $-2\alpha_s/3$ due to this being quark-quark and not quark-antiquark interactions as with mesons) to

$$S = \frac{4\pi\Lambda^2 r}{27}, \quad A = -\frac{8\pi}{27r \log\left(Ke^2 + \frac{B}{(\Lambda r)^2}\right)} + \frac{e_1 e_2}{4\pi r} \quad (2.32)$$

and also of course there is no longer just one interaction but three, so r becomes r_{12} , r_{13} , or r_{23} , depending on which potential we are currently discussing. The scalar confining interaction, unlike the vector one, is not regarded as coming from fundamental vertices or potentials involving current quarks. If it were treated as fundamental then the scalar interaction would be repulsive within baryons if it is attractive within mesons. Instead we treat the confining interaction as arising from effective potentials between constituent quarks and use this freedom to allow us, for

¹¹In addition to the spin independent nonrelativistic model presented in [47] see also a relativistic extension of it given in [49].

¹²An earlier coordinate space form that displays asymptotic freedom as well as linear quark confinement proposed in [50] is $V = (8\pi/27)(1 - \lambda r)^2/(r \ln \lambda r)$.

phenomenological reasons, to choose the sign of the qq scalar potential to be the same sign as the $q\bar{q}$ scalar potential¹³.

The technique that Crater *et al.* used in the two body problem [7] for finding the eigenvalues is called the inverse power method and its application depends on the variables being separable. Unlike the two-body problem, the variables are not separable in the three-body problem. This requires the use of the variational principle, which in turn requires a basis which we will describe in a later section. We turn now to a discussion of the three-body problem.

III. THE THREE-BODY PROBLEM

Now that we have completed our review of constraint dynamics and associated potentials for the relativistic two-body problem, we move on to the relativistic three-body one. The approach to the N -body problem that we use are those developed H. Sazdjian [12]. They are not directly solvable for more than $N = 2$, except for confined systems in which the problems of cluster decomposition do not need to be addressed. In this paper we adapt our two-body constraint formalism to his formalism for $N = 3$ and from there we obtain to a Schrödinger-like form for the three-body system, as we did in the two-body problem.

A. Sazdjian's N body formalism and the three-body problem

This section will focus on reviewing Sazdjian's work on the two-body and N -body systems [12]. We describe his derivations for the N -body problem and distill them down to a three-body formalism that we can then use for bound states of quarks in baryons. Sazdjian begins by applying the covariant formalism with N constraints for the N -particle case of the form

$$\mathcal{H}_a \psi = (p_a^2 + m_a^2 + \Phi_a) \psi = 0. \quad (3.1)$$

The compatibility condition is then

$$[\mathcal{H}_a, \mathcal{H}_b] \Psi = 0 \quad (a, b = 1, \dots, N), \quad (3.2)$$

which are $N(N-1)/2$ in number and give conditions on the interaction potentials (Φ_a). However, these equations, unlike the two-body ones (where Φ is a function of x_\perp) have no closed form solutions. Furthermore, the two body

¹³The problem with vector confining interactions is that (i) they will generate long distance spin-spin interactions and (ii) in the context of Dirac-like equations produce anticonfining ($-A^2$) terms. See [48] for a more detailed discussion of this problem. See also [51] where it is shown that the Dirac structure of confinement for mesons could be of a timelike-vector nature in the heavy quark limit of QCD. This would alleviate the problem of (i). Further, they find that nonperturbative mixing between ordinary and hybrid $Q\bar{Q}$ states seems to allow spin orbit effects as if arising from confining scalar interactions.

potentials would become nonlocal operators, due to the two-body momentum operators $P_{ab} = p_a + p_b$ no longer representing the total momentum of the system; since they would not be constants of the motion they would not possess corresponding eigenvalues. On the other hand, the total momentum in the two-body case is a number (an eigenvalue). Sazdjian abandons this approach and instead takes a simpler one that works only for confined systems where questions of correct cluster decompositions do not have to be addressed.

Sazdjian begins by working with the free N -body system where one can be guided by the simplifying features of the two-body system. Since the system must reduce to that of the free case in the absence of interactions, he found it useful to begin with the N -body system without any interacting potentials. A review of the details of his approach is given in Appendix B of [39], but the end result is a single N -body wave equation for the system as a whole and set of N equations for the individual invariant c.m. particle energies ε_a . This latter equation is

$$N\varepsilon_a - \sum_b \frac{(m_a^2 - m_b^2)}{(\varepsilon_a + \varepsilon_b)} = w, \quad (a = 1, \dots, N), \quad (3.3)$$

where w is the total invariant c.m. energy

$$w = \sum_b \varepsilon_b. \quad (3.4)$$

These equations cannot be solved exactly for the ε_b simply except in the two-body case, which reduce down to Eq. (2.12)

$$\varepsilon_1 - \varepsilon_2 = \frac{m_1^2 - m_2^2}{w}, \quad (3.5)$$

as expected. He shows it is possible, however, to find an approximate solution for the ε_b by using successive iterations in the general case given by

$$\varepsilon_a = \frac{w}{N} + \frac{1}{N} \sum_{b \neq 1}^N \frac{(m_a - m_b)}{[1 + (w - M)/2m_a m_b \sum_{c=1}^N 1/2m_c]}; \quad (3.6)$$

$a = 1, \dots, N.$

The full N -body equation which utilizes these c.m. energy eigenvalues is

$$\sum_{a=1}^N \left[-\varepsilon_a^2 + N \frac{p_{a\perp}^2 / (2\varepsilon_a)}{\sum_{b=1}^N 1/2\varepsilon_b} + m_a^2 \right] \Psi = 0. \quad (3.7)$$

This equation (3.7) determines the total c.m. energy w in terms of the masses and the transverse momenta. For

$N = 2$, this becomes the free form of the two-body system earlier given in Eq. (2.14)

$$(p_{\perp}^2 - b^2)\Psi = 0, b^2 = \varepsilon_1^2 - m_1^2 = \varepsilon_2^2 - m_2^2 \quad (3.8)$$

Finally, he also gives the system of N Klein-Gordon equations

$$\left\{ -\varepsilon_a^2 + \left[\sum_{b=1}^N \frac{p_{b\perp}^2}{(2\varepsilon_b)} \right] / \left(\sum_{c=1}^N \frac{1}{2\varepsilon_c} \right) + m_a^2 \right\} \Psi = 0$$

$(a = 1, \dots, N).$ (3.9)

Sazdjian finds that in the interacting case, the structure of these N nonindependent wave equations as well as Eq. (3.7) are kinematic in nature and should not be modified by the interactions. For example, particle a “feels” an interaction potential Φ_a that enters additively into its kinetic energy term by the relation

$$p_{\perp a}^2 \rightarrow p_{\perp a}^2 + \Phi_a. \quad (3.10)$$

Equation (3.7) then becomes

$$\sum_a \left[-\varepsilon_a^2 + N \frac{(p_{a\perp}^2 + \Phi_a) / (2\varepsilon_a)}{\sum_b 1/2\varepsilon_b} + m_a^2 \right] \Psi = 0, \quad (3.11)$$

which in the two-body case is

$$2 \left[\frac{p_{1\perp}^2 + \Phi_1}{w} \varepsilon_2 \right] + 2 \left[\frac{p_{2\perp}^2 + \Phi_2}{w} \varepsilon_1 \right] \Psi = (\varepsilon_1^2 - m_1^2 + \varepsilon_2^2 - m_2^2) \Psi. \quad (3.12)$$

Since $p_{1\perp}^2 = p_{2\perp}^2$ and $\Phi_1 = \Phi_2$ this reduces to Eq. (2.14). In the general N -body case, the individual wave equations (3.9) become

$$\left\{ -\varepsilon_a^2 + \left[\sum_{b=1}^N \frac{(p_{b\perp}^2 + \Phi_b)}{(2\varepsilon_b)} \right] / \left(\sum_c \frac{1}{2\varepsilon_c} \right) + m_a^2 \right\} \Psi = 0$$

$(a = 1, \dots, N).$ (3.13)

A sufficient condition for compatibility of these wave equations is to take

$$\Phi_a = \sum_{b \neq a}^N \Phi_{ab}(x_{ab\perp}),$$

$$x_{ab\perp}^\mu = (x_a^\mu - x_b^\mu) - P^\mu \hat{P} \cdot (x_a^\mu - x_b^\mu), \quad (3.14)$$

where again, P is the *total* momentum¹⁴

$$P = \sum_{a=1}^N p_a. \quad (3.15)$$

We choose the Φ_{ab} in this equation [Eq. (3.14)] to have the same functional dependence on S and A as in Eq. (2.20) our two-body Dirac approach. Sazdjian does not deal directly with the explicit form of the potential. Our choice in this work is to use the potential from the TBDE in the Sazdjian three-body equations. In this paper we do not include three body forces.

1. Our adaptation of Sazdjian's three-body generalization

In order to apply the work done by Sazdjian to our problem, we have to specialize his N -body equations to the three-body system and derive the appropriate effective Hamiltonian, eventually ending up with an equation that looks very much like a nonrelativistic three body Schrödinger equation, reducing to it in the nonrelativistic limit. We obtain the following approximation for the three-body eigenvalue equation, which comes from specializing the expanded three-body version of Eq. (3.11) as follows:

$$\begin{aligned} 0 = & \left[\varepsilon_1^2 - m_1^2 - 3 \frac{p_{1\perp}^2 + \Phi_1}{\varepsilon_1(1/\varepsilon_1 + 1/\varepsilon_2 + 1/\varepsilon_3)} + \varepsilon_2^2 - m_2^2 \right. \\ & - 3 \frac{p_{2\perp}^2 + \Phi_2}{\varepsilon_2(1/\varepsilon_1 + 1/\varepsilon_2 + 1/\varepsilon_3)} + \varepsilon_3^2 - m_3^2 \\ & \left. - 3 \frac{p_{3\perp}^2 + \Phi_3}{\varepsilon_3(1/\varepsilon_1 + 1/\varepsilon_2 + 1/\varepsilon_3)} \right] \psi(x_{12\perp}, x_{23\perp}, x_{31\perp}), \end{aligned} \quad (3.16)$$

in which the epsilons, representing the c.m. energy of each quark, are given to a good approximation by Eq. (3.6). The potentials Φ_i are linear combinations of the two-body interacting potentials

$$\begin{aligned} \Phi_1 &= \Phi_{12}(x_{12\perp}, \varepsilon_1, \varepsilon_2) + \Phi_{23}(x_{23\perp}, \varepsilon_2, \varepsilon_3), \\ \Phi_2 &= \Phi_{23}(x_{23\perp}, \varepsilon_2, \varepsilon_3) + \Phi_{31}(x_{31\perp}, \varepsilon_3, \varepsilon_1), \\ \Phi_3 &= \Phi_{31}(x_{31\perp}, \varepsilon_3, \varepsilon_1) + \Phi_{12}(x_{12\perp}, \varepsilon_1, \varepsilon_2). \end{aligned} \quad (3.17)$$

This Eq. (3.16) is essentially the three-body version of the two-body equation:

¹⁴Note that this dependence of the potential on the part of the potential that depends on component of the relative coordinates perpendicular to the momentum of the total system, is allowed as long as the issue of cluster decomposition need not be addressed. In that event, where one could separate out a part of the system from the remaining part, it is not meaningful to require the potentials to depend on the total momentum of the total system instead of that of its pairs of subconstituents.

$$\mathcal{H} = \frac{(p_1^2 + m_1^2 + \Phi)}{2\varepsilon_1} + \frac{(p_2^2 + m_2^2 + \Phi)}{2\varepsilon_2}, \quad (3.18)$$

as long as one restricts oneself to confining interactions. In the above Eq. (3.16)

$$\begin{aligned} p_{i\perp} &= p_i + p_i \cdot \hat{P} \hat{P}, \\ x_{ij\perp} &= x_{ij} + x_{ij} \cdot \hat{P} \hat{P}, \\ \hat{P} &= \frac{P}{\sqrt{-P^2}}, \\ P &= p_1 + p_2 + p_3. \end{aligned} \quad (3.19)$$

We define

$$E = w - M \equiv \varepsilon_1 + \varepsilon_2 + \varepsilon_3 - m_1 - m_2 - m_3, \quad (3.20)$$

in order to bring (3.16) into a more usable and familiar (Schrödinger-like) form. This form is given by

$$\begin{aligned} H\psi &\equiv \frac{1}{F} \left(\frac{p_{1\perp}^2 + \Phi_{12} + \Phi_{13}}{2\varepsilon_1(E, m_1, m_2, m_3)} + \frac{p_{2\perp}^2 + \Phi_{23} + \Phi_{12}}{2\varepsilon_2(E, m_1, m_2, m_3)} \right. \\ &\quad \left. + \frac{p_{3\perp}^2 + \Phi_{31} + \Phi_{23}}{2\varepsilon_3(E, m_1, m_2, m_3)} \right) \psi \\ &= E\psi, \end{aligned} \quad (3.21)$$

where the function $F = F(w, m_1, m_2, m_3)$, an invariant function of the total energy of the system and the masses of the particles [52], is the result of an algebraic manipulation (details and explicit form given in Appendix C of [39]). The functional forms of the ε_i are given in Eq. (3.6). The effects of spin are included by choosing for the Φ_{ij} given in Eq. (2.20). Equation (3.21) serves as our basic three-body bound state equation for quarks in the baryon. Even though the structure of the equation is nonrelativistic it is Lorentz invariant as it is composed of invariant portions. They are of two sorts, the square of spacelike and timelike vectors represented, respectively, by $p_{i\perp}^2$ and $x_{ij\perp}^2$ one the one hand, and $P^2 = -w^2$ on the other. In the c.m. frame the former become the squares \mathbf{p}_i^2 and \mathbf{x}_{ij}^2 of three vectors. In the nonrelativistic limit when $|E| \ll m_i$, then the invariant $F \rightarrow 1$, $\varepsilon_i \rightarrow m_i$ and the operator \mathcal{H} in Eq. (3.21) becomes an ordinary nonrelativistic Hamiltonian.

So now, we have gone from Sazdjian's N -body formalism to a condensed three-body one that is easy to work with in the constraint dynamics approach, as the Hamiltonian is now in a familiar form. This equation has the distinct advantage that it is like (for the purposes of solving it anyway) a nonrelativistic Schrödinger equation. It is, of course, still relativistic, but it is now in a form that is much more easily recognizable and usable than Eq. (3.13). It is important to note the recursive nature of this equation as

this becomes highly relevant in the numerical studies. The Φ 's are dependent on the e 's and w and so we must begin with an initial guess and solve the equation iteratively until an acceptable level of convergence of w is met.

IV. THE RELATIVISTIC THREE-BODY PROBLEM FOR BARYONS

It should be noted that models such as our two body and its three-body relativistic generalizations are often referred to as “naive quark models” in that they do not account for the swarm of gluons and sea quark-antiquark pair interactions directly. Rather, the model has all of the interacting forces existing only between each quark-quark pair.

The process of going from a two-body system to a three-body one is not as straightforward as one might expect. Since the interacting potentials are limited to each quark-quark pair, there are now three times as many terms. Additionally, there are three sets of coordinates ($\mathbf{r}_1 - \mathbf{r}_2$, $\mathbf{r}_2 - \mathbf{r}_3$, $\mathbf{r}_1 - \mathbf{r}_3$) instead of just one distance between the quarks as in the two-body case. This is best treated with a relative coordinate substitution that reduces the number of relative coordinates from three to two. The coordinate transform used in this work is similar to and uses the same notation as Capstick and Isgur's ([13]) work, but is not an identical transformation due to treating the more general case of all three quarks as possibly having different masses, in particular not choosing the u and d quarks to be identical in mass. It also uses invariant c.m. energies ε_a in place of masses.

The sections that follow describe the methods used in going from a two-body system to a three-body one, mostly dealing with the potentials and coordinate transforms. We also describe our Gaussian basis functions and the reasoning behind them. Referring to Eq. (2.20), the Φ_{SI} and Darwin (Φ_D) terms now expand simply from one term to three (to account for all three two-body interactions) and their matrix elements are no more complicated in principle than what occurs in the two body problem. However, matrix elements for the spin-spin (Φ_{SS}), spin-orbit (Φ_{SO} , Φ_{SOT} , Φ_{SOX}), and tensor (Φ_T) terms require manipulations related to total J , total L , and total S and are considerably more complex than what appears in the that the two-body system.

A. Spin-flavor-space states

Here we list all of the spin-flavor states for all the baryons in our fit. They are composed of products of spin wave functions, denoted χ , and flavor wave functions, denoted as φ [48]. The flavor wave functions are not listed for charmed or bottom baryons as those are the same wave functions with a b or c quark in place of a u , d , or s , depending on the baryon. The spin wave functions are, explicitly

$$\begin{aligned}\chi^s\left(S_z = \frac{3}{2}\right) &= \uparrow\uparrow\uparrow, \\ \chi'\left(S_z = \frac{1}{2}\right) &= \frac{1}{\sqrt{2}}(\uparrow\downarrow\uparrow - \downarrow\uparrow\uparrow), \\ \chi''\left(S_z = \frac{1}{2}\right) &= \frac{1}{\sqrt{6}}(2\uparrow\uparrow\downarrow - \uparrow\downarrow\uparrow - \downarrow\uparrow\uparrow). \quad (4.1)\end{aligned}$$

There are four different flavor wave functions, denoted as φ' , φ'' , φ^s , φ^a , corresponding here to the ground state octet and decimet baryons and their extensions to include charm and bottom quarks (see Table I). Note that φ^s is a symmetric linear combination of the listed quarks (e.g. $uud = \frac{1}{\sqrt{3}}[uud + udu + duu]$) and the singlet state

$$\varphi^a = \frac{1}{\sqrt{6}}(uds + dsu + sud - dus - usd - sdu) \quad (4.2)$$

φ and φ' combinations are chosen so that for the overall state [not including the antisymmetric color state] is totally symmetric. There are eleven possible combinations of these spin and flavor states for (most of) the known baryons with FSS standing for flavor, spin, and space and N referring to the SU(3) representation (see Table II). The wave function ψ_0 is a total $L = l_\rho = l_\lambda = 0$ wave function and ψ' and ψ'' are total $L = 1$ and $l_\rho = 1$ or $l_\lambda = 1$ wave functions, respectively ($L = 1$ states have parity of -1 , so l_ρ and l_λ cannot both be 1). In addition, φ' , φ'' , φ^s , and φ^a are all purely flavor wave functions and χ' , χ'' , χ^s are all purely spin wave functions, having total $S = 1/2$, $1/2$, and $3/2$, respectively. These merely contain all possible combinations of flavor or spin so that the product of the two gives all possible spin-flavor couplings so that, (not counting color) the total wave function is symmetric. All of these wave functions are orthogonal to the others in the set (that is, χ' is orthogonal to χ'' and χ^s , etc.).

These wave functions then define a grouping of baryons and the individual baryons themselves are defined by the flavor state from there, as given below in Table III. Before discussing the orbital and radial parts of the wave function we introduce the coordinate system including relative coordinates for our three-body problem.

B. Coordinate system transforms

This section provides a description of how the coordinate system is set up for the relativistic three-body problem. One of the simplest and most common ways to begin handling a three-body system is to redefine the coordinate system so that there are only two relative coordinates instead of three. In the following section we describe the way the coordinate system is defined for the three-body system and then reduced to two relative coordinates, plus a “center of mass.” We then address how those are further simplified with additional coordinate transforms in order to

TABLE I. Baryon flavor wave functions.

	φ^s	φ'	φ''
p		$\frac{1}{\sqrt{2}}(udu - duu)$	$\frac{1}{\sqrt{6}}(2uud - duu - udu)$
n		$\frac{1}{\sqrt{2}}(udd - dud)$	$\frac{1}{\sqrt{6}}(dud - udd - 2ddu)$
Λ		$\frac{1}{2\sqrt{3}}(usd + sdu - sud - dsu - 2dus + 2uds)$	$\frac{1}{2}(sud + usd - sdu - dsu)$
Δ^{++}	uuu		
Δ^+	uud		
Δ^0	udd		
Δ^-	ddd		
Σ^+	uus	$\frac{1}{\sqrt{2}}(suu - usu)$	$\frac{1}{\sqrt{6}}(suu - usu - 2uus)$
Σ^0	uds	$\frac{1}{2}(sud + sdu - usd - dsu)$	$\frac{1}{2\sqrt{3}}(usd + sdu + sud + dsu - 2dus - 2uds)$
Σ^-	dds	$\frac{1}{\sqrt{2}}(sdd - dsd)$	$\frac{1}{\sqrt{6}}(sdd - dsd - 2dds)$
Ξ^0	uss	$\frac{1}{\sqrt{2}}(sus - uss)$	$\frac{1}{\sqrt{6}}(2ssu - sus - uss)$
Ξ^-	dss	$\frac{1}{\sqrt{2}}(sds - dss)$	$\frac{1}{\sqrt{6}}(2ssd - sds - dds)$
Ω^-	sss		
Σ_c	uuc	$\frac{1}{\sqrt{2}}(cuu - ucu)$	$\frac{1}{\sqrt{6}}(cuu - ucu - 2uuc)$
Σ_b	uub	$\frac{1}{\sqrt{2}}(buu - ubu)$	$\frac{1}{\sqrt{6}}(buu - ubu - 2uub)$
Λ_c		$\frac{1}{2\sqrt{3}}(ucd + cdu - cud - dcu - 2duc + 2udc)$	$\frac{1}{2}(cud + ucd - cdu - dcu)$
Λ_b		$\frac{1}{2\sqrt{3}}(ubd + bdu - bud - dbu - 2dub + 2udb)$	$\frac{1}{2}(bud + ubd - bdu - dbu)$
Ξ_c	usc	$\frac{1}{\sqrt{2}}(suc - usc)$	$\frac{1}{\sqrt{6}}(2scu - suc - usc)$
Ξ_b	usb	$\frac{1}{\sqrt{2}}(sub - usb)$	$\frac{1}{\sqrt{6}}(2sbu - sub - usb)$
Ω_c	ssb	$\frac{1}{\sqrt{2}}(ssc - scs)$	$\frac{1}{\sqrt{6}}(css - scs - 2ssc)$

analytically solve as much of the problem as possible before going to numerical methods.

Let us return to Eq. (3.21). Our goal is to create a coordinate system in which the kinetic terms can be evaluated analytically and the variational principle will be used to solve for the energy eigenvalues. The general form of each Φ_{ij} is

$$\begin{aligned}
\Phi_{ij} = & \Phi_{Slij} + \Phi_{Dij} + \mathbf{L} \cdot (\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_j) \Phi_{SOij} \\
& + \boldsymbol{\sigma}_i \cdot \hat{\mathbf{r}}_{ij} \boldsymbol{\sigma}_j \cdot \hat{\mathbf{r}}_{ij} \mathbf{L} \cdot (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \Phi_{SOTij} \\
& + \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j \Phi_{SSij} + (3\boldsymbol{\sigma}_i \cdot \hat{\mathbf{r}}_{ij} \boldsymbol{\sigma}_j \cdot \hat{\mathbf{r}}_{ij} - \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_j) \Phi_{Tij} \\
& + \mathbf{L} \cdot (\boldsymbol{\sigma}_i - \boldsymbol{\sigma}_j) \Phi_{SODij},
\end{aligned} \tag{4.3}$$

and the various Φ terms are all functions of S_{ij} , A_{ij}

$$\begin{aligned}
S_{ij} &= \frac{4\pi\Lambda^2 r_{ij}}{27}, \\
A_{ij} &= -\frac{8\pi}{27r_{ij} \ln\left(Ke^2 + \frac{B}{(\Lambda r_{ij})^2}\right)} + \frac{e_1 e_2}{4\pi r_{ij}},
\end{aligned} \tag{4.4}$$

and their derivatives (explicit forms given in Appendix A of [39]). Note here how they still account for the asymptotic freedom and linear confinement mentioned earlier. The scalar term goes to infinity as r goes to an infinite value,

providing confinement, while the logarithm in the vector term becomes large at short distance, giving asymptotic freedom (this causes the vector term to behave like $\sim \alpha/r \ln r$).

We now define a coordinate system such that in place of the three coordinates r_{ij} we have two relative coordinates that can be written in terms of the original r_{ij} distances between each quark pair. The notation used is the same as from [13], with the actual transformation having individual particle masses m_i replaced by their corresponding c.m. energies ε_i given in Eq. (3.6). A total center of energy system, $\varepsilon_1 \mathbf{r}_1 + \varepsilon_2 \mathbf{r}_2 + \varepsilon_3 \mathbf{r}_3 = w \mathbf{R} = 0$, has been used to eliminate one of the coordinates, which is why \mathbf{r}_1 does not appear in the equations below for ρ and λ .

$$\begin{aligned}
\rho &= \mathbf{r}_2 - \mathbf{r}_3, \\
\lambda &= \frac{w\varepsilon_2}{(\varepsilon_2 + \varepsilon_3)\varepsilon_1} \mathbf{r}_2 + \frac{w\varepsilon_3}{(\varepsilon_2 + \varepsilon_3)\varepsilon_1} \mathbf{r}_3, \\
\mathbf{r}_1 - \mathbf{r}_2 &= -\frac{\varepsilon_3}{\varepsilon_2 + \varepsilon_3} \rho - \lambda, \\
\mathbf{r}_1 - \mathbf{r}_3 &= -\frac{\varepsilon_2}{\varepsilon_2 + \varepsilon_3} \rho + \lambda, \\
\mathbf{r}_2 - \mathbf{r}_3 &= \rho, \\
\varepsilon_\rho &= \frac{\varepsilon_1(\varepsilon_2 + \varepsilon_3)}{w}, \quad \varepsilon_\lambda = \frac{\varepsilon_2 \varepsilon_3}{\varepsilon_2 + \varepsilon_3}.
\end{aligned} \tag{4.5}$$

Again, w is the total baryon energy eigenvalue and the epsilons are the individual c.m. energies of each quark, such that

$$w = \varepsilon_1 + \varepsilon_2 + \varepsilon_3, \quad (4.6)$$

and the ε_ρ , and ε_λ can be regarded as reduced energy terms (similar to reduced mass, but using c.m. energies instead of masses). The corresponding conjugate momenta are given by

$$\mathbf{p}_\rho = \frac{\varepsilon_3 \mathbf{p}_2 - \varepsilon_2 \mathbf{p}_3}{\varepsilon_2 + \varepsilon_3}, \quad \mathbf{p}_\lambda = \frac{\varepsilon_1}{w} (\mathbf{p}_2 + \mathbf{p}_3). \quad (4.7)$$

In this new system of relative coordinates, the original Hamiltonian of Eq. (3.21) now becomes

$$\begin{aligned} \mathcal{H} = & \frac{1}{F} \left(\frac{p_\rho^2}{2\varepsilon_\rho(E, m_1, m_2, m_3)} + \frac{p_\lambda^2}{2\varepsilon_\lambda(E, m_1, m_2, m_3)} \right. \\ & + \frac{\Phi_{12} + \Phi_{13}}{2\varepsilon_1(E, m_1, m_2, m_3)} + \frac{\Phi_{23} + \Phi_{12}}{2\varepsilon_2(E, m_1, m_2, m_3)} \\ & \left. + \frac{\Phi_{31} + \Phi_{23}}{2\varepsilon_3(E, m_1, m_2, m_3)} \right). \end{aligned} \quad (4.8)$$

C. Variational principle and the Gaussian-like basis functions

Here we will briefly detail how our wave functions are used to construct the basis for use with the variational theorem. In order to expand Eq. (3.21) into a general matrix eigenvalue equation, we define

$$\begin{aligned} |\Psi\rangle &= \sum_n c_n |\Psi_n\rangle, \\ \langle \Psi | \mathcal{H} | \Psi \rangle &= \sum_{n,m} c_n c_m^* \langle \Psi_m | \mathcal{H} | \Psi_n \rangle = \sum_{n,m} c_n c_m^* \mathcal{H}_{mn}, \\ \langle \Psi | \Psi \rangle &= \sum_{n,m} c_n c_m^* \langle \Psi_m | \Psi_n \rangle \equiv \sum_{n,m} c_n c_m^* B_{mn}. \end{aligned} \quad (4.9)$$

Since the basis we will choose for the baryons is not orthogonal, B is not the usual Kronecker delta. Using the method of Lagrange multipliers we arrive at the eigenvalue equation in matrix form (where \mathbb{H} and \mathbb{B} are matrices, \mathbf{c} is a vector, and E our scalar eigenvalue)

$$\mathbb{H}\mathbf{c} = E\mathbb{B}\mathbf{c}. \quad (4.10)$$

As for the radial wave functions themselves, we use a Gaussian-like basis detailed in the appendix and given by

$$\begin{aligned} & \frac{u_{l_\rho}(\rho)}{\rho} \frac{u_{l_\lambda}(\lambda)}{\lambda}; \\ \frac{u_{l_\rho}(\rho)}{\rho} &= \rho^{l_\rho} \sum_{n=1}^{2N-1} e_n \sqrt{a^3 \sqrt{\frac{f_n^3}{\pi^3}}} \exp\left(-\frac{f_n a^2 \rho^2}{2}\right), \\ \frac{u_{l_\lambda}(\lambda)}{\lambda} &= \rho^{l_\lambda} \sum_{n=1}^{2N-1} e_n \sqrt{a^3 \sqrt{\frac{f_n^3}{\pi^3}}} \exp\left(-\frac{f_n a^2 \lambda^2}{2}\right), \\ f_n &= \frac{1}{n}; \quad 1 \leq n \leq N. \\ f_n &= n+1-N; \quad N+1 \leq n \leq 2N-1. \end{aligned} \quad (4.11)$$

These display an advantage over the usual Gaussian basis in that for a given choice of the inverse length scale factor a they span both large and small distances, important when relativistic potentials are included, having broadly different length scales. Allowing n_ρ and n_λ to stand for f_n the total angular and radial portions for the combined typical wave function are given by

$$\begin{aligned} \psi_{n_\rho n_\lambda l_\rho l_\lambda L M_L} &= \sum_{m_\rho m_\lambda} \langle l_\rho l_\lambda m_\rho m_\lambda | L M_L \rangle \\ &\times \mathcal{N} \rho^{l_\rho} \lambda^{l_\lambda} e^{-n_\rho \alpha_\rho^2 \rho^2 / 2 - n_\lambda \alpha_\lambda^2 \lambda^2 / 2} Y_{l_\rho}^{m_\rho} Y_{l_\lambda}^{m_\lambda}, \end{aligned} \quad (4.12)$$

where \mathcal{N} is a normalization constant. The general state $|\Psi\rangle$ and the sum given in Eq. (4.9) [as well as (4.14) below] would include the above wave function attached to the appropriate flavor, color, and spin portions with the index in the summation and coefficients given in that equation including the summations and e_n coefficients given in Eq. (4.11).

In the two-body problem with tensor coupling as appears in Φ_{ij} above, the states $l = j-1$ and $l = j+1$ are mixed, so we need a mixed wave function

$$\begin{aligned} |\Psi\rangle &= \sum_n c_n^+ |\Psi_{n+}\rangle + \sum_n c_n^- |\Psi_{n-}\rangle, \\ &\rightarrow l = j-1, \\ &+ \rightarrow l = j+1. \end{aligned} \quad (4.13)$$

Using this Ψ in Eq. (4.9) gives

$$\begin{aligned} \langle \Psi | \mathcal{H} | \Psi \rangle &= \sum_{n,m} (c_m^{*+} c_n^+ \mathcal{H}_{mn}^{++} + c_m^{*-} c_n^+ \mathcal{H}_{mn}^{-+} \\ &+ c_m^{*+} c_n^- \mathcal{H}_{mn}^{+-} + c_m^{*-} c_n^- \mathcal{H}_{mn}^{--}), \\ \langle \Psi | \Psi \rangle &\equiv \sum_{n,m} (c_m^{*+} c_n^+ B_{mn}^{++} + c_m^{*-} c_n^+ B_{mn}^{-+} \\ &+ c_m^{*+} c_n^- B_{mn}^{+-} + c_m^{*-} c_n^- B_{mn}^{--}) \end{aligned} \quad (4.14)$$

in which

$$\begin{aligned}
B_{mn}^{++} &= \langle \Psi_{m+} | \Psi_{n+} \rangle, & B_{mn}^{--} &= \langle \Psi_{m-} | \Psi_{n-} \rangle, & \langle \Psi_n | \mathcal{H} | \Psi_m \rangle &= \langle JL(l_\rho l_\lambda) S(S_1 S_2 S_3) \\
\mathcal{H}_{mn}^{++} &= \langle \Psi_{m+} | \mathcal{H} | \Psi_{n+} \rangle, & \mathcal{H}_{mn}^{--} &= \langle \Psi_{m-} | \mathcal{H} | \Psi_{n-} \rangle, & & \times Mn_\rho n_\lambda | \mathcal{H} | JL(l'_\rho l'_\lambda) S'(S'_1 S'_2 S'_3) Mn'_\rho n'_\lambda \rangle. \\
\mathcal{H}_{mn}^{+-} &= \langle \Psi_{m+} | \mathcal{H} | \Psi_{n-} \rangle, & \mathcal{H}_{mn}^{-+} &= \langle \Psi_{m-} | \mathcal{H} | \Psi_{n+} \rangle, & &
\end{aligned} \tag{4.15}$$

and similar to before, this leads to the eigenvalue equation with the matrix structure

$$\begin{pmatrix} \mathbb{H}^{++} & \mathbb{H}^{+-} \\ \mathbb{H}^{-+} & \mathbb{H}^{--} \end{pmatrix} \begin{pmatrix} \mathbf{c}^+ \\ \mathbf{c}^- \end{pmatrix} = E \begin{pmatrix} \mathbb{B}^{++} & 0 \\ 0 & \mathbb{B}^{--} \end{pmatrix} \begin{pmatrix} \mathbf{c}^+ \\ \mathbf{c}^- \end{pmatrix}. \tag{4.16}$$

As outlined above, we use the variational principle

$$\langle \Psi | \mathcal{H} | \Psi \rangle = E \langle \Psi | \Psi \rangle, \tag{4.17}$$

to find the eigenvalues of our Hamiltonian, with the wave function of total J , L and S as

$$|JL(l_\rho l_\lambda) S(S_1 S_2 S_3) Mn_\rho n_\lambda \rangle \equiv |\Psi_n \rangle. \tag{4.18}$$

where total L is composed of the angular momenta associated with the ρ and λ coordinates and total S is composed of the individual spins of each of the three quarks, with S_1 , S_2 , and S_3 corresponding to the spins of quarks 1, 2, and 3, respectively. Therefore a typical matrix element of the Hamiltonian would be

One major advantage of this particular choice of coordinates is that the kinetic terms can be analytically evaluated. The matrix elements for the kinetic term

$$\begin{aligned}
\langle \psi_{n_\rho n_\lambda} | T | \psi_{n'_\rho n'_\lambda} \rangle &= \langle \psi_{n_\rho n_\lambda} | \frac{1}{F} \left(\frac{p_\rho^2}{2\varepsilon_\rho(E, m_1, m_2, m_3)} \right. \\
&\quad \left. + \frac{p_\lambda^2}{2\varepsilon_\lambda(E, m_1, m_2, m_3)} \right) | \psi_{n'_\rho n'_\lambda} \rangle \tag{4.20}
\end{aligned}$$

are functions of l_ρ , l_λ , n_ρ , n_λ and the Gaussian parameters α_ρ and α_λ (see Appendix E of [39]).

The matrix elements for the potentials, however, must be evaluated numerically. For simplicity, here we just show the matrix elements for the spin-independent components of the potential (this leaves out the Clebsch-Gordon coefficients and spherical harmonics since they norm to 1). With the current substitution, the r_{23} term is relatively simple since $r_{23} = \rho$. The matrix elements for the spin-independent $\Phi_{23}(r_{23})$ quasipotentials ($\Phi_{S123}(r_{23})$) and $\Phi_{D23}(r_{23})$ reduce down to a single radial integral

$$\begin{aligned}
\langle \psi_{n_\rho n_\lambda} | \Phi_{23}(\rho) | \psi_{n'_\rho n'_\lambda} \rangle &= \int \Phi_{23}(\rho) \sqrt{\frac{(n_\rho \alpha_\rho^2)^{(2l_\rho+3)/2} (n_\lambda \alpha_\lambda^2)^{(2l_\lambda+3)/2}}{\Gamma[(2l_\rho+3)/2] \Gamma[(2l_\lambda+3)/2]}} \sqrt{\frac{(n'_\rho \alpha_\rho^2)^{(2l'_\rho+3)/2} (n'_\lambda \alpha_\lambda^2)^{(2l'_\lambda+3)/2}}{\Gamma[(2l'_\rho+3)/2] \Gamma[(2l'_\lambda+3)/2]}} \\
&\quad \times \frac{\Gamma[(l_\lambda + l'_\lambda + 3)/2]}{2[(n_\lambda + n'_\lambda) \alpha_\lambda^2]^{(l_\lambda + l'_\lambda + 3)/2}} \times \rho^{(l_\rho + l'_\rho + 2)} e^{-(n_\rho + n'_\rho) \alpha_\rho^2 \rho^2 / 2} d\rho.
\end{aligned}$$

Thus we are left with a function of one variable that can easily be numerically integrated regardless of what $\Phi_{23}(\rho)$ happens to be. However, this is not the case for the other two terms.

The matrix elements of the r_{12} and r_{13} spin-independent interactions are, respectively

$$\begin{aligned}
\langle \psi_{n_\rho n_\lambda} | \Phi_{12}(r_{12}) | \psi_{n'_\rho n'_\lambda} \rangle &= \int \Phi_{12}(\rho, \lambda) \sqrt{\frac{(n_\rho \alpha_\rho^2)^{(2l_\rho+3)/2} (n_\lambda \alpha_\lambda^2)^{(2l_\lambda+3)/2}}{\Gamma[(2l_\rho+3)/2] \Gamma[(2l_\lambda+3)/2]}} \sqrt{\frac{(n'_\rho \alpha_\rho^2)^{(2l'_\rho+3)/2} (n'_\lambda \alpha_\lambda^2)^{(2l'_\lambda+3)/2}}{\Gamma[(2l'_\rho+3)/2] \Gamma[(2l'_\lambda+3)/2]}} \\
&\quad \times \rho^{(l_\rho + l'_\rho)} \lambda^{(l_\lambda + l'_\lambda)} e^{-(n_\rho + n'_\rho) \alpha_\rho^2 \rho^2 / 2 - (n_\lambda + n'_\lambda) \alpha_\lambda^2 \lambda^2 / 2} d^3 \rho d^3 \lambda, \tag{4.21}
\end{aligned}$$

with a similar expression for $\langle \psi_{n_\rho n_\lambda} | \Phi_{13}(r_{13}) | \psi_{n'_\rho n'_\lambda} \rangle$ and so as the potentials are now in terms of two variables, it is much more difficult and time-consuming to numerically evaluate this integral. We therefore wish to make another variable change in the r_{12} and r_{13} systems in order to rewrite them in terms of a single variable as well.

What now follows is a brief description of the variable change simplification using the simplest nontrivial case of $l = 1$; more explicit and general details can be found in Appendix E of [39]. The variable change used is based on properties of the spherical harmonics and how they relate to spherical tensors and similarly for the other spherical harmonics. We specialize our discussion to $l = 1$ and use

$$Y_1^0 r = \frac{1}{2} \sqrt{\frac{3}{\pi}} z, \quad Y_1^{\pm 1} r = \mp \frac{1}{2} \sqrt{\frac{3}{2\pi}} (x \pm iy). \quad (4.22)$$

Therefore, since part of our wave function is a spherical harmonic (which is a trigonometric function) and a coordinate, the wave function can be rewritten in spherical tensor form as

$$\begin{aligned} \Psi_n &= \frac{4}{3\sqrt{\pi}} n_\rho^{5/4} \alpha_\rho^{5/2} n_\lambda^{5/4} \alpha_\lambda^{5/2} \rho \lambda e^{-n_\rho \alpha_\rho^2 \rho^2 / 2 - n_\lambda \alpha_\lambda^2 \lambda^2 / 2} \\ &\times \sum_{m_\rho m_\lambda} \langle 11 m_\rho m_\lambda | 00 \rangle Y_1^{m_\rho} Y_1^{m_\lambda} \\ &= \frac{4}{3\sqrt{\pi}} n_\rho^{5/4} \alpha_\rho^{5/2} n_\lambda^{5/4} \alpha_\lambda^{5/2} e^{-n_\rho \alpha_\rho^2 \rho^2 / 2 - n_\lambda \alpha_\lambda^2 \lambda^2 / 2} \\ &\times \sum_{m_\rho m_\lambda} \langle 11 m_\rho m_\lambda | 00 \rangle \rho_{m_\rho} \lambda_{m_\lambda}, \end{aligned} \quad (4.23)$$

where

$$\rho_{m_\rho} = \rho Y_1^{m_\rho}(\hat{\rho}) \lambda_{m_\lambda} = \lambda Y_1^{m_\lambda}(\hat{\lambda}). \quad (4.24)$$

Additional manipulations are still needed in order to work out the expectation values explicitly. For the r_{12} integration, a new set of variables is defined as

$$\begin{aligned} \rho' &= \mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2, \\ \lambda' &= \frac{w\varepsilon_1}{\varepsilon_3(\varepsilon_1 + \varepsilon_2)} \mathbf{r}_1 + \frac{w\varepsilon_2}{\varepsilon_3(\varepsilon_1 + \varepsilon_2)} \mathbf{r}_2, \end{aligned} \quad (4.25)$$

and then are rewritten in terms of new primed variables and as tensors, using the same tensor substitution done above

$$\begin{aligned} \rho &= \frac{\varepsilon_1}{\varepsilon_1 + \varepsilon_2} \rho' + \lambda', \quad \rho_{m_\rho} = \frac{\varepsilon_1}{\varepsilon_1 + \varepsilon_2} \rho'_{m_\rho} + \lambda'_{m_\rho}, \quad (4.26) \\ \lambda &= \frac{w\varepsilon_2}{(\varepsilon_2 + \varepsilon_3)(\varepsilon_1 + \varepsilon_2)} \rho' - \frac{\varepsilon_3}{\varepsilon_2 + \varepsilon_3} \lambda', \\ \lambda_{m_\lambda} &= \frac{w\varepsilon_2}{(\varepsilon_2 + \varepsilon_3)(\varepsilon_1 + \varepsilon_2)} \rho'_{m_\lambda} - \frac{\varepsilon_3}{\varepsilon_2 + \varepsilon_3} \lambda'_{m_\lambda}. \end{aligned} \quad (4.27)$$

Note that this is not a new coordinate system but rather a change of integration variables. This means that, while we are currently working out the new integral for the r_{12} system, we can use a similar substitution for the r_{13} system and acquire a nearly identical equation with only a few constants changed (constants in terms of the integration variable, not overall constants for the full calculation). Before the new substitution of the primed coordinates, the expectation value of the potential $\Phi_{12}(\rho' = \mathbf{r}_{12})$ is

$$\begin{aligned} \langle \psi_{n_\rho n_\lambda} | \Phi_{12}(\mathbf{r}_{12}) | \psi_{n'_\rho n'_\lambda} \rangle &= \langle \psi_{n_\rho n_\lambda} | \Phi_{12}(\rho') | \psi_{n'_\rho n'_\lambda} \rangle \\ &= \frac{16}{9\pi} \alpha_\rho^5 \alpha_\lambda^5 (n_{\rho 1}^{5/4} n_{\lambda 1}^{5/4} n_{\rho 2}^{5/4} n_{\lambda 2}^{5/4}) \int \Phi_{12}(\rho') \sum_{m_{\rho 1} m_{\lambda 1}} \langle 11 m_{\rho 1} m_{\lambda 1} | 00 \rangle \rho_{m_{\rho 1}}'^* \lambda_{m_{\lambda 1}}'^* \\ &\times \sum_{m_{\rho 2} m_{\lambda 2}} \langle 11 m_{\rho 2} m_{\lambda 2} | 00 \rangle \rho_{m_{\rho 2}}' \lambda_{m_{\lambda 2}}', e^{-(n_{\rho 1} + n_{\rho 2}) \alpha_\rho^2 \rho'^2 - (n_{\lambda 1} + n_{\lambda 2}) \alpha_\lambda^2 \lambda'^2} d^3 \rho' d^3 \lambda'. \end{aligned} \quad (4.28)$$

We use the derived relationships between the primed and unprimed coordinates ρ and λ Eq. (4.25) and one final coordinate change to eliminate $\lambda' \cdot \rho'$ cross terms in the Gaussian. The explicit details can be found in Appendix E of [39]. The end result is that $\langle \psi_{n_\rho n_\lambda} | \Phi_{12}(\mathbf{r}_{12}) | \psi_{n'_\rho n'_\lambda} \rangle$ involves a single radial integral which can be numerically evaluated easily. Similarly the matrix element $\langle \psi_{n_\rho n_\lambda} | \Phi_{13}(\mathbf{r}_{13}) | \psi_{n'_\rho n'_\lambda} \rangle$ can be evaluated. Again, details are listed in Appendix E of [39]. The potential is now in terms of just one variable, so regardless of what potential is used, the numerical calculations will be fairly straightforward. Thus, the coordinate system has been defined and

transformed in such a way as to make a good deal of the problem analytic while keeping what is not analytic still easy to evaluate numerically. With the matrix elements defined for a general potential and for analytic kinetic terms, we now need to explicitly define our potential model.

V. THREE-BODY SPIN-DEPENDENT POTENTIALS

Conceptually speaking, the approach one would take to go from a two-body system with the formalism we have described to a three-body one is straightforward. The

TABLE II. Total spin-flavor-space wave functions.

N	J	L	S	Total State (FSS)	Ψ
8	$\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{1}{\sqrt{2}}(\varphi'\chi' + \varphi''\chi'')\psi_0$	Ψ_1
10	$\frac{3}{2}$	0	$\frac{3}{2}$	$\varphi^s\chi^s\psi_0$	Ψ_2
8	$\frac{1}{2}, \frac{3}{2}$	1	$\frac{1}{2}, \frac{3}{2}$	$\frac{1}{2}[(\varphi'\chi'' + \varphi''\chi')\psi' + (\varphi'\chi' - \varphi''\chi'')\psi'']$	$\Psi_3(J=\frac{1}{2}), \Psi_4(J=\frac{3}{2})$
8	$\frac{1}{2}, \frac{3}{2}, \frac{5}{2}$	1	$\frac{3}{2}, \frac{5}{2}$	$\frac{1}{\sqrt{2}}[\varphi'\chi^s\psi' + \varphi''\chi^s\psi'']$	$\Psi_5(J=\frac{1}{2}), \Psi_6(J=\frac{3}{2}), \Psi_7(J=\frac{5}{2})$
10	$\frac{1}{2}, \frac{3}{2}$	1	$\frac{1}{2}, \frac{3}{2}$	$\frac{1}{\sqrt{2}}[\varphi^s\chi'\psi' + \varphi^s\chi''\psi'']$	$\Psi_8(J=\frac{1}{2}), \Psi_9(J=\frac{3}{2})$
1	$\frac{1}{2}, \frac{3}{2}$	1	$\frac{1}{2}, \frac{3}{2}$	$\frac{1}{\sqrt{2}}[\varphi^a\chi''\psi' - \varphi^a\chi'\psi'']$	$\Psi_{10}(J=\frac{1}{2}), \Psi_{11}(J=\frac{3}{2})$

TABLE III. Baryons and their corresponding spin-flavor wave functions.

$\Psi_1 \rightarrow p, n, \Lambda, \Sigma^+, \Sigma^0, \Xi^0, \Xi^-, N(1440), \Lambda(1600), \Sigma(1660), \Xi(1690), \Sigma_c^+(2455), \Sigma_b^+, \Sigma_b^0, \Lambda_c^+, \Lambda_c^0(2595), \Lambda_b^0$
$\Psi_2 \rightarrow \Delta^{++}, \Delta^+, \Delta^0, \Delta^-, \Sigma^+(1385), \Sigma^0(1388), \Sigma^-(1390), \Xi^0(1530), \Xi^-(1535), \Omega^-, \Delta(1600), \Sigma(1690)$
$\Psi_3 \rightarrow N(1535), \Lambda(1670), \Sigma(1750), \Sigma(1880)$
$\Psi_4 \rightarrow N(1520), \Lambda(1690), \Sigma(1670), \Xi(1820)$
$\Psi_5 \rightarrow N(1650), \Lambda(1800), \Sigma(1750)$
$\Psi_6 \rightarrow N(1700), \Sigma(1940)$
$\Psi_7 \rightarrow N(1675), \Lambda(1830), \Sigma(1775), \Xi(1950)$
$\Psi_8 \rightarrow \Delta(1620)$
$\Psi_9 \rightarrow \Delta(1700)$
$\Psi_{10} \rightarrow \Lambda(1405)$
$\Psi_{11} \rightarrow \Lambda(1520)$

problem is now treated as three two-body problems, with the overall form of the potentials given in Eq. (4.3). The three-body potential is of similar form and essentially just triples the number of terms, with pairwise interactions for all three quarks. For the relatively simple vector (A), scalar (S), and Darwin (Φ_D) terms this is almost trivial, as there are no direct spin-dependent operators; however, the spin-spin, tensor, and spin-orbit terms require extensive reworking, which are outlined in the following sections with details in Appendix F of [39].

A. State couplings and operator methods

We will now describe how we set up our three-body states when using the spin-dependent potential operators. In order to simplify our numerical calculations, it is helpful to note that the potential terms are products of a term involving the coupled angular momentum operators and coordinate dependent terms that have trivial operator dependence, save for the Clebsch-Gordon coefficients and spherical harmonics not norming to 1 in the cases where we have orbital dependence in the operator. Even in this case though, the results of the preceding section still can be applied directly with the added component. This allows us to use the operator angular momentum on a specified state and just get a number back that depends on the angular components of the state itself and not any radial components, so that the numerical integral itself does not involve any angular momentum operators. Thus, our potential terms separated into operator and nonoperator

pieces are given in Table IV and the explicit forms of the Φ terms are given in Appendix A of [39] and the results of all these operators on the possible baryon configurations are given in Appendix F of [39]. The above operators do not affect the radial part of the wave function and so the problem is broken into a radial integral part (as done in the previous section) and an operator component for each interaction term.

For the baryons we have considered, there are a total of eleven different wave functions, which represent all possible spin-flavor couplings for the various particles. The form of these is given in Table II where it has been split into three components: spin, flavor, and space (represented by χ , φ , ψ , respectively), explicitly defined in Appendix F of [39]. As there are six interactions to consider and three couplings per interaction (we are using two-body operators,

TABLE IV. Potential terms, operators and nonoperator components.

Potential Term	Angular Momenta Operator components	Nonoperator component
Spin-Spin	$\sigma_i \cdot \sigma_j$	$\Phi_{SS}(\mathbf{r}_{ij})$
Spin-Orbit	$\mathbf{L}_{ij} \cdot (\sigma_i + \sigma_j)$	$\Phi_{SO}(\mathbf{r}_{ij})$
Spin-Orbit Difference	$\mathbf{L}_{ij} \cdot (\sigma_i - \sigma_j)$	$\Phi_{SOD}(\mathbf{r}_{ij})$
Tensor	$3\sigma_i \cdot \hat{\mathbf{r}}_{ij}\sigma_j \cdot \hat{\mathbf{r}}_{ij} - \sigma_i \cdot \sigma_j$	$\Phi_T(\mathbf{r}_{ij})$
Spin-Orbit Cross	$i\mathbf{L}_{ij} \cdot \sigma_i \times \sigma_j$	$\Phi_{SOX}(\mathbf{r}_{ij})$
Spin-Orbit Tensor	$\sigma_i \cdot \hat{\mathbf{r}}_{ij}\sigma_j \cdot \hat{\mathbf{r}}_{ij}\mathbf{L}_{ij} \cdot (\sigma_i + \sigma_j)$	$\Phi_{SOT}(\mathbf{r}_{ij})$

so there is a 1–2, 1–3, and 2–3 term for each operator), there are a total of 198 possible interactions to consider. Fortunately, many of these are similar or trivial and so the number that must actually be worked out explicitly drops considerably, but there still are quite a large number that are nontrivial. The eleven wave functions are given in Table II. Explicit forms of these terms are given in Appendix F of [39]. The quark flavor combination of the φ terms is different for each baryon, but since the operators we use do not affect the flavor, it does not matter what they are for the purposes of calculating the effects of each operator.

There are two methods we use to determine the effect of each of these operators on the angular momentum states. One is a simple ladder operator approach and the other involves use of the Wigner 6j and 9j recoupling coefficients, the details of which are given in Appendix F of [39]. Both methods are always valid, but not necessarily always useful due to how the operator form affects each individual wave function for the ladder operators. It is worth noting that having two methods be viable also allows for a good check. The ladder operator method works out simply for all operators (except the spin-orbit cross term due to the matrix elements being independent of total M). For the states Ψ_1 , Ψ_2 , Ψ_4 , Ψ_7 , Ψ_9 , and Ψ_{11} , we can set $M = J$ and force $M_s = S$. This means that any operator that changes total M_s will be orthogonal to the original wave function and thus we can eliminate any term that does change total M_s . All of the methods for determining these states are relegated to Appendix F of [39], this includes the ladder operators, 6j and 9j details. Due to having matrix elements for the two-body problem already defined by [7], the difficult part of this problem is recoupling the state into one which can use these matrix elements. To summarize this section, we have written the three-body potentials in terms of two relative coordinates and shown how they can be transformed for each interacting pair. This allows a description of the methods used to adapt the ([1–3]) two-body potential operators of Crater *et al.* derived for the meson spectrum to the three-body problem.

VI. NUMERICAL RESULTS AND COMMENTS

The expectation value of the Hamiltonian in Eq. (3.21) cannot be evaluated analytically, so it falls to numerical studies to acquire an explicit number. We use a Monte Carlo approach combined with a simple gradient method to obtain a best-fit χ^2 for the spectrum as a whole, as compared to current experimental data. It is important to note that a normal χ^2 routine would include in each individual baryon's contribution to the by the inverse square of the experimental error. But this would give particles such as the proton a much higher weight than desired in the overall fit. Therefore, we instead divided each by the greater of their respective experimental errors or 1 MeV, thus preventing very well-known particles from dominating our imperfect fit. The following sections

describe the numerical methods used and give the results after using said methods.

A. Methods and parameter values

The numerical best fits were done using a Monte Carlo approach followed by a gradient method to obtain a least square fit for the spectrum as a whole. We originally attempted to use a more simplified gradient approach but it quickly became apparent that the functions are far too sensitive to changes and thus would get “stuck” in a local minimum much too easily without some other approach. So, we adopted a Monte Carlo routine that would trigger whenever the gradient approach found a new best fit in order to ensure we were reaching the best results for our theory. The integrations were done numerically using Gaussian quadrature and the parameters α_ρ and α_λ were minimized by the Nelder-Mead simplex method, though it is worth noting that the α parameters do not generally vary much from the analytic result if one were to use a harmonic oscillator model. Also note that as the size of our matrix increases, the actual value of these parameters do not affect the fit as much, becoming irrelevant at an infinitely large matrix. As one might expect, benefits from increasing the size of the matrix are subject to diminishing returns and thus our results are given for a point of reasonable convergence (in other words, once increasing the size of the matrix no longer significantly affected results).

Our model has a total of 8 parameters, with u , d , s , c , and b in the Table V corresponding to the masses of the up, down, strange, charm, and bottom quarks, respectively, and Λ , K , and B are coupling constants in our model. These are the same 8 parameters as in [2]. It is worth noting that our model has significantly fewer parameters than most models, with only 8 total and 5 of those being universal to any model (the quark masses themselves)¹⁵. The model of course, is still expected to be accurate regardless of the number of parameters, but it is worth noting in this work. In addition, there are only two parametric functions that define our potential model, the vector and scalar potentials $A(r)$ and $S(r)$ given by Eq. (2.32).

B. Results and comparison to experiment

The complete results of our model are given in Tables V–VIII. As the purpose of this work is to test if the model used in the two-body case works well for the three-body, we are only using those baryons which have a three or four star rating by the Particle Data Group, meaning that they are fairly well known.

The lowest lying baryons are generally slightly high energy-wise for the first 8 and this is most likely to allow the following 10 to be fit relatively accurately (see Table VI). This is not a surprising result of our model

¹⁵Reference [13], for example, has 14 parameters listed.

TABLE V. Parameter values.

This work		Reference 2	
u	157.2 (MeV)	u	55.7(MeV)
d	158.3 (MeV)	d	55.3 (MeV)
s	337.5 (MeV)	s	249.9 (MeV)
Λ	285.8 (MeV)	Λ	421.8 (MeV)
c	2050.3 (MeV)	c	1.476 (GeV)
b	5302.5 (MeV)	b	4.844 (GeV)
K	18.1	K	4.198
B	100.6	B	0.05081

due to the fact that since we are using no purely 3-body potentials, the only difference between these sets of baryons is the spin-spin interaction. The fitting routine used the average value for the experimental masses given in Table VII since these have a wide range, and this value is also used in calculating the difference between our model and experimental data. In this table the first 6 listed baryons are radial excitations of ones in the previous table.

The higher order baryons fall within an acceptable range on the whole, though there are a few outliers. Of important note is that our model does fit very well the often troublesome $\Lambda(1405)$ particle. The other Λ particles however are, as before, missing some sort of interaction that will aid in differentiating among them [the $\Lambda(1520)$, $\Lambda(1670)$, $\Lambda(1690)$ and $\Lambda(1800)$ all fit to around the same value].

In addition, we fit the well-known charmed and bottom baryons, given in Table VIII. The orbital and spin angular momenta are the same as the noncharmed/bottom baryons that correspond to each charmed or bottom

baryon here. These agree relatively well with experimental data.

C. Conclusion and future work

The model has shown that with the use of three-body equation of Sazdjian, it is possible to use the purely two-body approach based on Dirac's constraint dynamics for spin-one-half particle bound states for a good fit of the baryon spectrum. As for future work, one may try to see the effects of higher order eigenvalue equations for the three-body system, as referred to in Appendix B of [39] and as discussed in more detail in [12]. It may be also be possible as in [13] to introduce three-body forces in addition to the two-body ones and to use a fully three-body approach for a coordinate system and JLS couplings. Total JLS couplings for a three-body system are usually done in a mathematically rigorous fashion by coupling two particles together and then coupling their Clebsch-Gordon coupled two-body system to a third particle for a complete three-body system. A fully three-body approach ([53]) to angular momentum couplings may at the very least yield a more elegant formalism and perhaps better overall results. A system derived purely for a three-body problem and including three-body JLS couplings may include additional interactions not seen in a two-body model. We believe this may solve the issue of the same family of particles (i.e. Σ , Λ , N) lacking in enough differentiation as one goes from one J to another, since the angular momentum dependent interactions are the only things that accounts for the difference in mass among different sets of baryons with the same quark configuration. In contrast to many other models ([54]) which tend to fit the lower mass baryons very well

TABLE VI. Low lying baryon states.

Baryon	J	L	S	Theoretical Mass (MeV)	Experimental Mass (MeV)	Exp-Theory (MeV)
p	1/2	0	1/2	947	938	-9
n	1/2	0	1/2	948	939	-9
Σ^+	1/2	0	1/2	1250	1189	-61
Σ^0	1/2	0	1/2	1261	1192	-68
Σ^-	1/2	0	1/2	1271	1197	-73
Ξ^0	1/2	0	1/2	1373	1314	-58
Ξ^-	1/2	0	1/2	1378	1321	-57
Λ^0	1/2	0	1/2	1082	1125	43
Δ^{++}	3/2	0	3/2	1249	1232	-17
Δ^+	3/2	0	3/2	1250	1232	-18
Δ^0	3/2	0	3/2	1251	1232	-19
Δ^-	3/2	0	3/2	1252	1232	-20
$\Sigma^+(1390)$	3/2	0	3/2	1384	1383	-1
$\Sigma^0(1390)$	3/2	0	3/2	1385	1384	-1
$\Sigma^-(1390)$	3/2	0	3/2	1387	1387	0
$\Xi^0(1530)$	3/2	0	3/2	1501	1531	30
$\Xi^-(1530)$	3/2	0	3/2	1507	1535	28
Ω^-	3/2	0	3/2	1609	1672	63

TABLE VII. Orbital and radially excited baryons states.

Baryon	J	L	S	Theoretical Mass (MeV)	Experimental Mass (MeV)	Exp-Theory (MeV)
$N(1440)$	1/2	0	1/2	1557	1420–1470	–117
$\Lambda(1600)$	1/2	0	1/2	1677	1560–1700	–77
$\Sigma(1660)$	1/2	0	1/2	1672	1630–1690	12
$\Xi(1690)$	1/2	0	1/2	1784	1680–1700	–94
$\Delta(1600)$	3/2	0	3/2	1521	1550–1700	78
$\Sigma(1670)$	3/2	1	1/2	1679	1665–1685	–4
$N(1535)$	1/2	1	1/2	1549	1525–1545	–14
$\Lambda(1670)$	1/2	1	1/2	1671	1660–1680	–1
$\Sigma(1750)$	1/2	1	3/2	1644	1730–1800	121
$\Sigma(1775)$	5/2	1	3/2	1661	1770–1780	114
$N(1520)$	3/2	1	1/2	1551	1515–1525	–31
$\Lambda(1690)$	3/2	1	1/2	1670	1685–1695	20
$\Xi(1820)$	3/2	1	1/2	1777	1818–1828	43
$N(1650)$	1/2	1	3/2	1566	1645–1670	84
$\Lambda(1800)$	1/2	1	3/2	1658	1720–1850	142
$\Sigma(1880)$	1/2	0	1/2	1709	1800–1960	171
$N(1700)$	3/2	1	3/2	1568	1650–1750	132
$N(1675)$	5/2	1	3/2	1615	1670–1680	59
$\Lambda(1830)$	5/2	1	3/2	1641	1810–1830	189
$\Xi(1950)$	5/2	1	3/2	1757	1935–1965	192
$\Delta(1620)$	1/2	1	1/2	1542	1600–1660	78
$\Delta(1700)$	3/2	1	1/2	1546	1670–1750	154
$\Lambda(1405)$	1/2	1	1/2	1410	1402–1410	–4
$\Lambda(1520)$	3/2	1	1/2	1680	1518–1521	–160

and the higher order much more poorly, our work tends to maintain the same quality of fit regardless of baryon mass. This lends credence to the theory as a whole being fundamentally sound, but merely incomplete. This missing piece is likely a higher order implementation of Sazdjian's three-body scheme and/or the fully three-body interactions that were not considered in this work; three-body

interactions referring to those in which an interaction between two of the particles can influence the third (as done in [13]), rather than being entirely based on two-body interactions. As can be seen from the fit data, there are many lower than experiment and many higher as well, though this is spread out among all the baryons with the low-lying baryons being larger than experiment while the

TABLE VIII. Charmed and bottom baryons.

Baryon	J	L	S	Theoretical Mass (MeV)	Experimental Mass (MeV)	Exp-Theory (MeV)
$\Sigma_c^{++}(2455)$	1/2	0	1/2	2385	2454	68
$\Sigma_c^{++}(2520)$	3/2	0	3/2	2551	2520	–31
$\Lambda_c^+(2286)$	1/2	0	1/2	2382	2286	–96
$\Lambda_c^+(2595)$	1/2	1	1/2	2415	2595	180
$\Xi_c^+(2467)$	1/2	0	1/2	2561	2467	–94
$\Xi_c^0(2470)$	1/2	0	1/2	2562	2470	–92
$\Xi_c^+(2645)$	3/2	0	3/2	2598	2645	46
$\Xi_c^+(2790)$	1/2	1	3/2	2661	2790	129
$\Xi_c^+(2815)$	3/2	1	3/2	2707	2815	108
$\Omega_c^0(2695)$	1/2	0	1/2	2732	2695	–37
$\Omega_c^0(2770)$	3/2	0	3/2	2745	2770	25
$\Sigma_b^+(5829)$	3/2	0	3/2	5800	5829	29
$\Sigma_b^-(5836)$	3/2	0	3/2	5851	5836	–15
$\Xi_b^0(5790)$	1/2	0	1/2	5854	5790	–64
$\Omega_b^-(6071)$	1/2	0	1/2	6032	6071	39

higher order and charmed/bottom baryons are lower. This prevents one from improving the fits to the low-lying baryons by simply lowering the u , d , s masses since simultaneously this would worsen in the fits on the already low charmed/bottom baryons (both sets of baryons have similar experimental errors).

On the whole though, the fit is nearly as accurate as others, most notably the work of Capstick and Isgur ([13]), which is generally regarded as one of the more valuable references for theoretical baryon spectroscopy. The only marked difference of the results of our model versus other models is that the quality of the fit remains relatively constant regardless of which baryons we are considering (ground state, higher order, heavy, etc.). However, as was discussed, this may actually reinforce that the fundamental approach is sound and it can be upgraded to a more accurate model by considering additional interactions and a more refined treatment of Sazdjian's approach to the 3-body problem of bound systems.

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APPENDIX: GAUSSIAN WAVE FUNCTIONS AND INFINITE INTERVAL DISCRETIZATION

This section describes how our wave functions come about for our basis. The potentials in Eq. (3.21) have both short distance and long distance effects, so we need a basis wave function that can accurately account for that. We define a wave function in terms of some parameter α that determines the effect of the Gaussian wave function for short and long distance interactions. We then split the wave function into those two parts (short and long) and discretize it to a certain N value, from which we get our basis. The wave function is originally defined in an infinite vector space, so we must truncate it in order to work with it.

Boris Kupershmidt, a mathematician, [55] has suggested a Laplace transform/Gaussian basis

$$\psi(\mathbf{x}) = \int_0^\infty d\alpha q(\alpha) \sqrt{\frac{1}{a^3} \sqrt{\frac{\alpha^3}{\pi^3}}} \exp\left(-\frac{\alpha \mathbf{x}^2}{2a^2}\right) \quad (\text{A1})$$

where ψ is essentially the Fourier transform of some function $q(\alpha)$. In order to work with this function, we split the integral into two pieces, one with boundaries from zero to one and the other with boundaries from one to infinity, so that

$$\begin{aligned} \psi(\mathbf{x}) = & \int_0^1 d\alpha q(\alpha) \sqrt{\frac{1}{a^3} \sqrt{\frac{\alpha^3}{\pi^3}}} \exp\left(-\frac{\alpha \mathbf{x}^2}{2a^2}\right) \\ & + \int_1^\infty d\alpha q(\alpha) \sqrt{\frac{1}{a^3} \sqrt{\frac{\alpha^3}{\pi^3}}} \exp\left(-\frac{\alpha \mathbf{x}^2}{2a^2}\right). \end{aligned} \quad (\text{A2})$$

By replacing α with $1/\beta$ in the first half of the equation (so that the integral from 0 to 1 now becomes 1 to infinity) we get

$$\begin{aligned} \psi(\mathbf{x}) = & \int_1^\infty d\beta q(1/\beta) \sqrt{\frac{1}{a^3} \sqrt{\frac{1}{\beta^3 \pi^3}}} \exp\left(-\frac{\mathbf{x}^2}{2\beta a^2}\right) \\ & + \int_1^\infty d\alpha q(\alpha) \sqrt{\frac{1}{a^3} \sqrt{\frac{\alpha^3}{\pi^3}}} \exp\left(-\frac{\alpha \mathbf{x}^2}{2a^2}\right), \end{aligned} \quad (\text{A3})$$

and from there, replacing integrals with sums over arbitrarily large N , this discretizes to

$$\begin{aligned} \psi(\mathbf{x}) = & \sum_{n=1}^N c_n \sqrt{\frac{1}{a^3} \sqrt{\frac{1}{n^3 \pi^3}}} \exp\left(-\frac{\mathbf{x}^2}{2na^2}\right) \\ & + \sum_{n=1}^N d_n \sqrt{\frac{1}{a^3} \sqrt{\frac{n^3}{\pi^3}}} \exp\left(-\frac{n\mathbf{x}^2}{2a^2}\right) \\ = & e_1 \sqrt{\frac{1}{a^3} \sqrt{\frac{1}{\pi^3}}} \exp\left(-\frac{\mathbf{x}^2}{2a^2}\right) \\ & + \sum_{n=2}^N c_n \sqrt{\frac{1}{a^3} \sqrt{\frac{1}{n^3 \pi^3}}} \exp\left(-\frac{\mathbf{x}^2}{2na^2}\right) \\ & + \sum_{n=2}^N d_n \sqrt{\frac{1}{a^3} \sqrt{\frac{n^3}{\pi^3}}} \exp\left(-\frac{n\mathbf{x}^2}{2a^2}\right). \end{aligned} \quad (\text{A4})$$

So, for $N = 1$ we have

$$\psi(\mathbf{x}) = e_1 \sqrt{\frac{1}{a^3} \sqrt{\frac{1}{\pi^3}}} \exp\left(-\frac{\mathbf{x}^2}{2a^2}\right). \quad (\text{A5})$$

For $N = 2$ we have

$$\begin{aligned} \psi(\mathbf{x}) = & e_1 \sqrt{\frac{1}{a^3} \sqrt{\frac{1}{\pi^3}}} \exp\left(-\frac{\mathbf{x}^2}{2a^2}\right) \\ & + c_2 \sqrt{\frac{1}{a^3} \sqrt{\frac{1}{8\pi^3}}} \exp\left(-\frac{\mathbf{x}^2}{4a^2}\right) \\ & + d_2 \sqrt{\frac{1}{a^3} \sqrt{\frac{8}{\pi^3}}} \exp\left(-\frac{\mathbf{x}^2}{a^2}\right). \end{aligned} \quad (\text{A6})$$

Note that the original wave function from $N = 1$ remains as the first term. This is true for all N .

For $N \geq 3$

$$\begin{aligned} \psi(\mathbf{x}) = & e_1 \sqrt{\frac{1}{a^3}} \sqrt{\frac{1}{\pi^3}} \exp\left(-\frac{\mathbf{x}^2}{2a^2}\right) \\ & + \sum_{n=2}^N c_n \sqrt{\frac{1}{a^3}} \sqrt{\frac{1}{n^3 \pi^3}} \exp\left(-\frac{\mathbf{x}^2}{2na^2}\right) \\ & + \sum_{n=2}^N d_n \sqrt{\frac{1}{a^3}} \sqrt{\frac{n^3}{\pi^3}} \exp\left(-\frac{n\mathbf{x}^2}{2a^2}\right) \end{aligned} \quad (\text{A7})$$

or more symmetrically

$$\begin{aligned} \psi(\mathbf{x}) = & \sum_{n=1}^{2N-1} e_n \sqrt{\frac{1}{a^3}} \sqrt{\frac{f_n^3}{\pi^3}} \exp\left(-\frac{f_n \mathbf{x}^2}{2a^2}\right), \\ f_n = & \frac{1}{n}; \quad 1 \leq n \leq N; \\ f_n = & n + 1 - N; \quad N + 1 \leq n \leq 2N - 1. \end{aligned} \quad (\text{A8})$$

As we can see from the $N = 2$ case, the order of the matrix increases as $2N - 1$. Each matrix element of the Hamiltonian matrix is constructed from the expectation value of the Hamiltonian with two of these wave functions. For example, for the $N = 2$ case, our general wave function $|\psi_n(f_n)\rangle$ is

$$\begin{aligned} n = 1 & \rightarrow |\psi_1(1)\rangle, \\ n = 2 & \rightarrow \left| \psi_2\left(\frac{1}{2}\right) \right\rangle, \\ n = 3 & \rightarrow |\psi_3(2)\rangle, \end{aligned} \quad (\text{A9})$$

and thus we have the 3×3 matrix

$$\begin{pmatrix} \langle \psi_1 | \mathcal{H} | \psi_1 \rangle & \langle \psi_1 | \mathcal{H} | \psi_2 \rangle & \langle \psi_1 | \mathcal{H} | \psi_3 \rangle \\ \langle \psi_2 | \mathcal{H} | \psi_1 \rangle & \langle \psi_2 | \mathcal{H} | \psi_2 \rangle & \langle \psi_2 | \mathcal{H} | \psi_3 \rangle \\ \langle \psi_3 | \mathcal{H} | \psi_1 \rangle & \langle \psi_3 | \mathcal{H} | \psi_2 \rangle & \langle \psi_3 | \mathcal{H} | \psi_3 \rangle \end{pmatrix}. \quad (\text{A10})$$

As can be inferred from the values of f_n for $n > 1$, this basis allows the wave function to account for both the long-range and short-range interactions of the Hamiltonian. Smaller f_n values—such as for $n = 2$ in the above example—allow for long-range interactions while larger f_n values (like the $n = 3$ wave function) account for the short-range interactions.

In a similar manner, we can now also write our B matrix from Eq. (4.10) as

$$\begin{aligned} \psi(\mathbf{x}) &= \sum_{n=1}^{2N-1} e_n \psi_n(x); \\ B_{nm} &= \int d^3x \psi_n^*(x) \psi_m(x) \\ &= \sqrt{\frac{1}{a^6}} \sqrt{\frac{f_n^3 f_m^3}{\pi^6}} \int d^3x \exp\left(-\frac{(f_n + f_m) \mathbf{x}^2}{2a^2}\right) \\ &= \sqrt{f_n^{3/2} f_m^{3/2}} \frac{\sqrt{8}}{(f_n + f_m)^{3/2}} \\ &= \sqrt{\frac{8 f_n^{3/2} f_m^{3/2}}{(f_n + f_m)^3}}. \end{aligned} \quad (\text{A11})$$

Thus we get an analytical form for the B matrix that remains the same regardless of coordinate transformations. Note also that this becomes one in the case of $f_n = f_m = 1$, which is expected. This completes our review of the two-body formalism. Since we are attempting to reach a convergence point with as few Gaussians as possible, we do not necessarily include as many wave functions as is possible. So for $N = 2$, we only begin with two wave functions for each coordinate (giving a 4×4 matrix) and then go to three wave functions (going to 9×9). Similarly, $N = 3$ can have up to 5 wave functions per coordinate, but we only add one at a time in order to more quickly converge the energy eigenvalues.

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