Lattice Quantum Chromodynamics Spectroscopy

Monte Carlo Searches For Exotic Charmonium Meson States

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4th April 2012

- *Quantum Chromodynamics* (QCD)– The theory of the *Strong Nuclear Force*
- An $SU(3)$(-colour) *Gauge Theory*, a non-Abelian group
- Gives each *Quark* a *Colour Charge*
- In the *Simple Quark Model*, *Mesons* are bound states of a quark and antiquark $q\bar{q}$
- While *Baryons* (or antibaryons) are composed of three quarks (or antiquarks) qqq (or $\bar{q}\bar{q}\bar{q}$)
- Full QCD is hard! The $\mathcal{L}$agrangian

$$\mathcal{L} = \frac{1}{2}\sum_{f=1}^{6}\left[i\bar{q}_f(x)\gamma^\mu \overleftrightarrow{D}_\mu q_f(x) - m_f\bar{q}_f(x)q_f(x)\right] - \frac{1}{4}\sum_{a=1}^{8}\left[G^a_{\mu\nu}G^{\mu\nu a}\right] \quad (1)$$

where the sum over f is the sum over the quark flavours u, d, s, c, b and t, and the

$$G^a_{\mu\nu} = \partial_\mu B^a_\nu(x) - \partial_\nu B^a_\mu(x) + g f_{abc} B^b_\mu(x) B^c_\nu(x) \quad (2)$$

- Thus move to the lattice!
- On the lattice, quarks live on the lattice sites, and gluons live in the lattice spacings, known as *Link Matrices* $U_\mu \in SU(3)$
- Brings its own problems (*Fermion Doubling*, systematic errors, etc.) but allows us to perform non-perturbative QCD calculations
- Requires a *Wick Rotation*

$$t \to i\tau$$

and we work on a *Euclidean Lattice*

- Hence we are working with a statistical mechanical system, which has an associated *Path Integral*

$$\int_{-\infty}^{\infty} \mathscr{D}q \, \exp\left[-\int_{t'}^{t''} \mathrm{d}t \mathcal{L}(q, \dot{q})\right] \tag{3}$$

- And so *Monte Carlo Simulation* is very useful!

- Simple quark model gives a rich theory of *Quarkonia*; the h_c, J/ψ, χ_0, χ_1 and χ_2 etc.
- However some states are unexplained!
- For a quark-antiquark pair, with *Total Spin* S and *Orbital Angular Momentum* L the *Total Spin* J is

$$\vec{J} = \vec{L} + \vec{S} \tag{4}$$

while the *Parity* P and *Charge Conjugation* C quantum numbers are

$$P = (-1)^{L+1} \quad \text{and} \quad C = (-1)^{L+S} \tag{5}$$

- Whence we get a strict set of allowed quantum states

$$\begin{array}{cccc} 0^{-+}, & & 2^{-+}, & \cdots \\ & 1^{--}, & 2^{--}, & 3^{--}, \cdots \\ 0^{++}, & 1^{++}, & 2^{++}, & 3^{++}, \cdots \\ & 1^{+-}, & & 3^{+-}, \cdots \end{array} \tag{6}$$

and so on

- But what about the missing states you ask?!
- Namely, those states J^{+-} for J even and J^{-+} for J odd, known as *Exotic States*
- Have been experimental hints of these at Belle and BaBar; the $X(3872)$, $Y(4620)$, and even charged Z states

Bound Quark-Antiquark States
Possible Explanations I

- There are various non-QCD extensions to the simple quark model

- The *MIT Bag Model*, where *Confinement* is replicated by requiring that the colour current through some surface vanishes

$$n^\mu J^a_\mu = 0 \qquad \text{where} \qquad J^a_\mu = (\bar{q_r}, \bar{q_g}, \bar{q_b})\, \lambda^a \gamma_\mu \begin{pmatrix} q_r \\ q_g \\ q_b \end{pmatrix} \tag{7}$$

- Even better is the *Gluon Flux-Tube Model*!

- Gluon self-interactions are taken into account, and we get a spectrum closer to that of full QCD. This is because even in the absence of quarks there is still a non-trivial pure Yang-Mills theory which has it's own spectrum of states

Bound Quark-Antiquark States
Possible Explanations II

- In contrast to the Abelian case of an electromagnetic field say, the colour fields are constrained to strings
- These are our link matrices U_μ joining quarks on the lattice. The purely gluonic states correspond to closed loops of links

- In contrast to the Abelian case of an electromagnetic field say, the colour fields are constrained to strings
- These are our link matrices U_μ joining quarks on the lattice. The purely gluonic states correspond to closed loops of links
- The flux-tube is in fact more like a flux sausage than a string

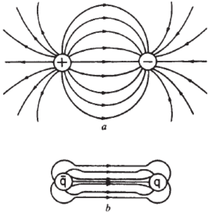


Figure: (a) electric field lines between a positive and a negative electric charge and (b) colour field lines between a quark and an antiquark. Adapted from [13] with kind permission, copyright (1979) Nature

- *Born-Oppenheimer Approximation* is valid as the gluons move so fast that their effect can be taken as an effective potential. This produces an interaction strength that increases linearly with quark separation such that the string tension remains constant as the quark-antiquark pair are pulled apart
- Model then reproduces quark confinement as the energy needed to separate a quark-antiquark pair is infinite.
- At a large distances it becomes energetically more favourable to create a quark-antiquark pair out of the vacuum rather than increase the length of the flux tube

- *Born-Oppenheimer Approximation* is valid as the gluons move so fast that their effect can be taken as an effective potential. This produces an interaction strength that increases linearly with quark separation such that the string tension remains constant as the quark-antiquark pair are pulled apart
- This model then reproduces quark confinement as the energy needed to separate a quark-antiquark pair is infinite.
- At a large distances it becomes energetically more favourable to create a quark-antiquark pair out of the vacuum rather than increase the length of the flux tube, leading to two colourless mesons

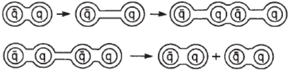


Figure: As the quarks separate the energy expanded in pulling them apart creates a quark-antiquark pair out of the vacuum resulting in two colourless mesons. Adapted from [13] with kind permission, copyright (1979) Nature

- From the Schrödinger equation

$$\mathcal{H}|\psi(\vec{r}) > = E|\psi(\vec{r}) > \tag{8}$$

by the method of separation of variables such that

$$\psi(\vec{r}) = R(r)\Phi(\phi)\Theta(\theta) \tag{9}$$

for a spherically symmetrical potential $V(r)$ we can get the equation for the radial wavefunction $R(r)$

$$\left\{ \frac{\hbar^2}{2m} \left[-\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2 \frac{\mathrm{d}}{\mathrm{d}r} \right) + \frac{l(l+1)}{r^2} \right] + V(r) \right\} R(r) = ER(r) \tag{10}$$

or

$$\left\{ \frac{\hbar^2}{2m} \left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{l(l+1)}{r^2} \right] + V(r) \right\} U(r) = EU(r) \tag{11}$$

where $U(r) = rR(r)$

- This is valid for any spherically symmetric potential function $V(r)$
- Thus we may choose the *Cornell Potential*

$$V(r) = -\frac{\pi}{12r} + \sigma r \tag{12}$$

where σ is the string tension with $\sqrt{\sigma} \simeq 400\,\text{MeV}$

- Using C++ code we may preform computational modelling of this system
- Using the *Numerov Three-Point Algorithm*

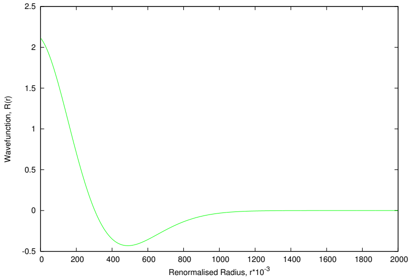
$$U_{n+1}(r) = \frac{2(1 - \frac{5}{12}l^2k_n^2)U_n(r) - (1 + \frac{1}{12}l^2k_{n-1}^2)U_{n-1}(r)}{1 + \frac{1}{12}l^2k_{n+1}^2} \tag{13}$$

we can calculate the wavefunction of $q\bar{q}$ states

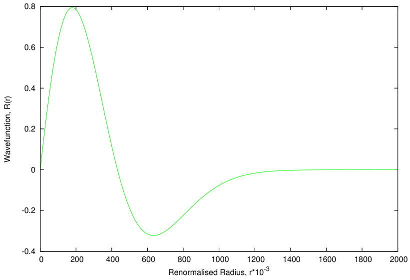
- The gluon flux-tube model potential was also simulated where here

$$V(r) = -A\frac{1}{r} + Br^2 \tag{14}$$

- A range of graphs were plotted. Here are a select few!

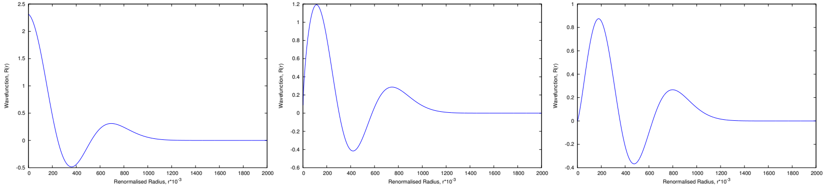


(a) $\ell = 0$ Angular Momentum



(b) $\ell = 1$ Angular Momentum

Figure: $n = 2$ States of A Charmonium in The Cornell Potential



(a) $\ell = 0$ Angular Momentum

(b) $\ell = 1$ Angular Momentum

(c) $\ell = 2$ Angular Momentum

Figure: $n = 3$ States of The Gluon-Flux Tube Model Charmonium

- Can also try to reproduce the $q\bar{q}$ specturm using the Cornell potential

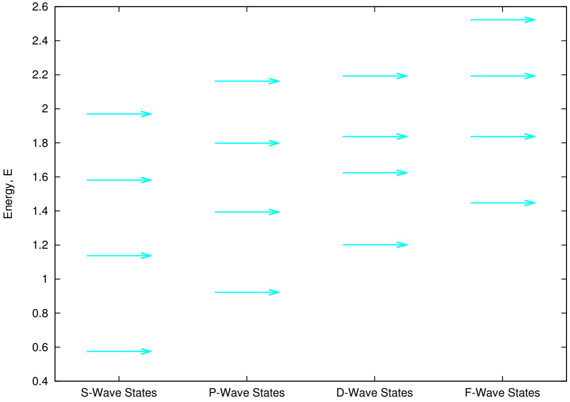


Figure: Charmonium Excitation States In The Cornell Potential

- And the Gluon Flux-Tube potential

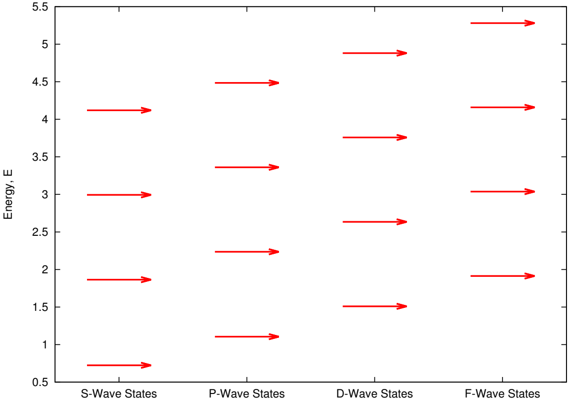


Figure: Charmonium Excitation States In The Gluon Flux-Tube Potential

- For a one-dimensional periodic set of quantum fields ϕ_k on the lattice where $k = 0, 1, 2, \ldots, N-1$ with action

$$S = \sum_{k,k'} \phi_k \Box_{k,k'} \phi_{k'} \tag{15}$$

where

$$\Box_{k,k'} = m^2 \delta_{k,k'} + (-\delta_{k,k'+1} - \delta_{k,k'-1} + 2\delta_{k,k'}) \tag{16}$$

the two-point correlation function

$$c(l) = \int_{-\infty}^{\infty} \prod_k \mathrm{d}\phi_k \, \phi_{j+l}\phi_j \exp(-S) \tag{17}$$

may be given by

$$< 0|\phi_k \phi_{k'}|0 > = \frac{\pi}{\sinh\left(2\sinh^{-1}(m/2)\right)} \exp[-2\sinh^{-1}(m/2)(z_0)] \tag{18}$$

- Seen that the two-point correlation function for a quantum chromodynamical process falls off exponentially in time with the mass of the particle

- Using the $\mathcal{H}$eisenberg picture and inserting a complete set of states $|n >< n|$ it is seen that

$$C_{ij}(t_1) = \sum_n Z_{in} Z^*_{nj} \exp(-E_n t_1) \tag{19}$$

where

$$Z_{in} = < 0|\Phi_i(t_1)|n > \qquad \text{and} \qquad Z^*_{nj} = < n|\Phi^\dagger_j(0)|0 > \tag{20}$$

- Hence fitting to an exponential decay gives the ground state energy E_1

- A fit to the randomly generated data $\bar{C_{ij}}(t_1 - t_0)$ must be calculated for the correlation functions for a given set of Quantum Chromodynamics operators by performing a *Chi-Squared Test*

- Here

$$\chi^2 = \sum_{i,j,n,t_0} \frac{\left(\bar{C_{ij}}(t_1 - t_0) - C_{ij}(E_n, Z_{in}, Z_{nj}, t_0 - t_1)\right)^2}{\sigma_{ij}^2} \tag{21}$$

where σ_{ij}^2 is the variance in the randomly generated Monte Carlo data and this must be minimised with respect to $\{E_n\}$ and $\{Z_{ij}\}$ for a global minimum

- If $\chi^2 \simeq n$ the fit is within one standard deviation of the Monte Carlo data and the energy spectrum may be confidently extracted

- The `variational_fitter` code was run to fit exponential decaying curves to a range of sets of operators from the T_1^{--} and T_1^{-+} symmetry point groups
- For all eighteen operators of the T_1^{-+} group the variational fitting was successful. This may be interpreted as a particle with mass $4.211 \pm 0.011\,\mathrm{GeV}$
- For the T_1^{--} group χ^2 was not within the acceptable range for the eight ρ and the eight ρ plus the two π operators. Hence there are no gluonic states in the T_1^{--} symmetry point group

Table: Values for m_0 of the T_1^{-+} Symmetry Point Group

	Both ρ Operators	Remaining 16 Operators	All 18 Operators
First Good Timeslice	0.7473 ± 0.002 $\simeq 4.235 \pm 0.011$ Gev	0.7480 ± 0.0046 $\simeq 4.239 \pm 0.026$ Gev	0.743 ± 0.002 $\simeq 4.211 \pm 0.011$ GeV
Largest Time Separation	(all the same separation)	(all the same separation)	0.748 ± 0.002 $\simeq 4.239 \pm 0.011$ GeV
Smallest χ^2	0.7472 ± 0.0023 $\simeq 4.234 \pm 0.013$ Gev	0.7491 ± 0.0042 $\simeq 4.245 \pm 0.024$ GeV	0.742 ± 0.003 $\simeq 4.205 \pm 0.017$ GeV

- Can calculate the radial wavefunctions using numerical methods
- The Cornell Potential and the gluon-flux tube potential may be used to reproduce the linear interaction term causing the wavefunctions to drop off quickly with increasing r
- Representative of the confinement property of Quantum Chromodynamics

Conclusions

- Analytic calculation of correlation functions is complicated to begin with
- Putting a quantum field theory on a lattice then introduces new complications
- Still possible to compute such functions analytically using the $\mathcal{F}$ourier transform representation and the $\mathcal{G}$reen function method with the $\mathcal{C}$auchy Residue Theorem
- Find that the two-point correlation functions decay exponentially in Euclidean time with the mass of the state
- Using variational fitting for the T_1^{-+} group a physical states with mass of $4.211 \pm 0.011\,\mathrm{GeV}$ was found corresponding to an exotic $c\bar{c}$ state and this is exactly where experiments at Belle and BABAR find states

- Quantum Chromodynamics is an extremely interesting theory with a huge number of research opportunities to offer

- Accurately reproducing the charmonium spectrum will require further fine tuning and optimisation of the code

- Extraction of the mass parameters of more states offers an increasing number of exotic states to be identified as physical states of the $c\bar{c}$ system

- Remains to use the `variational_fitter` code to fit the data generated using the `CUDA LQCD Correlator Calculator` software recently developed by Ó Conbhuí. This software is capable of calculating the correlation functions of quantum fields in an extremely computationally inexpensive fashion with the prospect of predicting new mesonic states

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Any Questions???

Acknowledgements
Dr. Mike J. Peardon[†]
Sr. Pol Vilaseca Marinar[‡], Mr. Graham Moir[§] and Mr. Tim Harris Sch.[§]
Mr. Pádraig Ó Conbhuí[¶] and Mr. Cian Booth[¶]
And all of the Lattice Quantum Chromodynamics undergraduate students.

- For a one-dimensional periodic set of quantum fields ϕ_k on the lattice where $k = 0, 1, 2, \dots, N-1$ with action

$$S = \sum_{k,k'} \phi_k \Box_{k,k'} \phi_{k'} \tag{22}$$

where

$$\Box_{k,k'} = m^2 \delta_{k,k'} + (-\delta_{k,k'+1} - \delta_{k,k'-1} + 2\delta_{k,k'}) \tag{23}$$

the two-point correlation function

$$c(l) = \int_{-\infty}^{\infty} \prod_k \mathrm{d}\phi_k \, \phi_{j+l} \phi_j \exp(-S) \tag{24}$$

may be given by

$$c(l) = \frac{1}{Z[0]} \frac{\partial}{\partial J_{j+l}} \frac{\partial}{\partial_j} Z[J] \bigg|_{J=0} \tag{25}$$

where $Z_0[J]$ is the generating functional, with J a source field, given by

$$Z_0[J] = \int_{-\infty}^{\infty} \mathrm{d}[\phi(x)] \exp\left(-S[\phi(x)] + \int_{-\infty}^{\infty} J(x)\phi(x) \right) \tag{26}$$

- Writing S as a matrix M and performing a $\mathcal{G}$aussian integration we find that

$$c(l) = \sqrt{\frac{\pi}{\det(M)}}\frac{1}{4}M^{-1}_{j+l,j} \tag{27}$$

- It remains to find the eigenvalues, and thus the inverse matrix elements $M^{-1}_{k,k'}$
- Reverting to four-space and using the $\mathcal{F}$ourier transform representation

$$M_{k,k'} = \int_{-\infty}^{\infty} \frac{\mathrm{d}^4 p}{(2\pi)^4}\,\tilde{M}(p)\exp[ip(k-k')] \tag{28}$$

where

$$\tilde{M}(p) = \int_{-\infty}^{\infty} M(k)\exp(-ipk)\mathrm{d}k \tag{29}$$

$$= \frac{1}{(2\pi)^4}\left(m^2 + 4\sin^2(p/2)\right) \tag{30}$$

- And a $\mathcal{G}$reen function to calculate the inverse matrix

$$M^{-1}_{k,k'} = \int_{-\infty}^{\infty} \frac{\mathrm{d}^4 p}{(2\pi)^4}\, \mathcal{G}(k) \exp[ip(k - k')] \tag{31}$$

such that

$$\Box \mathcal{G}(k) = \delta(k) \tag{32}$$

yielding

$$\mathcal{G}(k) = (2\pi)^4 \frac{1}{m^2 + 4\sin^2(p/2)} \tag{33}$$

- And the $\mathcal{C}$auchy Residue Theorem

$$\int_{\gamma} f(z)\mathrm{d}z = 2\pi i \sum_{j} n(w_j,\gamma)\mathrm{Res}_{z=w_j} f(z)$$

with
$$\mathrm{Res}_{z=w_j} f(z) = \lim_{z\to w_j} (z-w_j)\, f(z) = \frac{g(w_j)}{h'(w_j)} \quad (34)$$

to evaluate, with $z = k - k'$ for ease, the complex integral

$$M^{-1}_{k,k'} = \int_{-\infty}^{\infty} \mathrm{d}^3\vec{p}\, \exp(-i\vec{p}\cdot\vec{z}) \int_{-\infty}^{\infty} \mathrm{d}p^0\, \frac{1}{m^2 + 4\sin^2(p/2)} \exp(ip^0 z_0) \quad (35)$$

we find that

$$< 0|\phi_k \phi_{k'}|0 > = M^{-1}_{k,k'} = \frac{\pi}{\sinh\left(2\sinh^{-1}(m/2)\right)} \exp[-2\sinh^{-1}(m/2)(z_0)] \quad (36)$$