String breaking/computing energy levels on the lattice

Marc Wagner

Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany

September 14, 2007

1 String breaking

Literature: [1].

Definition of the static quark antiquark potential

- \( V(R) = \) energy of the lowest state containing an infinitely heavy quark antiquark pair at separation \( R \) (+ dynamical quarks + gluons).

Pure Yang-Mills theory (gluons, but no dynamical quarks)

- The quark antiquark potential is linear for intermediate and large separations (confinement; cf. Figure 1).
- There is a gluonic flux tube (a string) connecting the quark and the antiquark; the profile of this flux tube is essentially independent of the separation, which leads to a linearly rising quark antiquark potential.

![Figure 1: The static quark antiquark potential in Yang-Mills theory and in QCD.](image-url)
QCD (gluons and dynamical quarks)

- The static quark antiquark potential is linear for intermediate separations, but constant for large separations (cf. Figure 1).

- When increasing the distance of the static quarks beyond a certain value $R_{\text{string breaking}}$, a light quark antiquark pair is created; the flux tube breaks and two static-light mesons appear; the attractive force between the static sources is “completely” screened by dynamical quarks, i.e. the potential for $R > R_{\text{string breaking}}$ is essentially two times the mass of the lightest static-light meson.

- The static-light spectrum, to be more precise the mass of the lightest static-light meson gives an estimate of the string breaking distance.

2 Computing energy levels on the lattice (theory)

Basic principle

- Compute the temporal correlation of a state $|\phi\rangle = \mathcal{O}|0\rangle$:

$$
\langle \phi(T)|\phi(0)\rangle = \langle \mathcal{O}(T)|\mathcal{O}(0)|0\rangle = \langle \mathcal{O}\rangle^HT\langle \mathcal{O}\rangle^H\langle 0|e^{-HT}\mathcal{O}|0\rangle = \sum_n \langle n|\phi(0)\rangle^2 e^{-(E_n-E_0)T} \quad (1)
$$

($|n\rangle$: eigenstates of the Hamiltonian $H$; $E_n$: corresponding eigenvalues).

- For large $T$

$$
\langle \phi(T)|\phi(0)\rangle \approx \left(\Omega|\phi(0)\rangle\right)^2 e^{-(E_\Omega-E_0)T}, \quad (2)
$$

where $|\Omega\rangle$ is the lowest state with $\langle \Omega|\phi\rangle \neq 0$.

- Then

$$
e^{-(E_\Omega-E_0)a} = \frac{e^{-(E_\Omega-E_0)(T+a)}}{e^{-(E_\Omega-E_0)T}} \approx \frac{\langle \phi(T+a)|\phi(0)\rangle}{\langle \phi(T)|\phi(0)\rangle} \quad (3)
$$

and

$$
E_\Omega - E_0 \approx E_\Omega^\phi(T+a) = -\frac{1}{a} \ln \left( \frac{\langle \phi(T+a)|\phi(0)\rangle}{\langle \phi(T)|\phi(0)\rangle} \right). \quad (4)
$$

($a$: lattice spacing).
An example of how to choose $|\phi\rangle$ (quark antiquark potential)

- Create a state with a static quark antiquark pair:

$$|\phi\rangle = \bar{Q}(x)U(x,y)Q(y)|0\rangle.$$ \hfill (5)

- One can show that this state contains a static antiquark at $x$ and a static quark at $y$, and that it has vanishing overlap to all other states with different “heavy quark number”.

- To preserve gauge invariance, a parallel transporter (a gluonic string) has been included:

$$U(x,y) = P\left\{ \exp \left( i \int_x^y dz_j A_j(z) \right) \right\}$$ \hfill (6)

($P$ denotes path ordering).

- Integrating out the static quarks (the corresponding propagator can be calculated analytically) yields the well known Wilson loop:

$$\langle \phi(T)|\phi(0)\rangle = \#\langle W_{(R,T)} \rangle = \frac{1}{3} \text{Tr} \left( P\left\{ \exp \left( i \oint dz_\mu A_\mu(z) \right) \right\} \right)$$ \hfill (7)

(the path of integration is shown in Figure 2).

Figure 2: Unsmeared and smeared Wilson loops.
3 Computing energy levels on the lattice (practical issues)

- In lattice calculations it is not possible to measure \( \langle \phi(T)|\phi(0) \rangle \) for large \( T \):
  - Lattices have a finite (rather small) extension.
  - Due to the exponential fall off, \( \langle \phi(T)|\phi(0) \rangle \) is very small for large \( T \). Therefore, relative statistical errors are huge.
- Solution: choose \( |\phi\rangle \) such that it is close to the state you want to measure, i.e. \( \langle \Omega|\phi\rangle \approx 1 \). Then (2) is already valid for rather small \( T \).
- How can we determine such a state \( |\phi\rangle \)?
  - Physical arguments/expectations: usually one has a rough picture of how the corresponding state might look like; for example for the static quark antiquark potential the lowest state is expected to contain two static point-like sources connected by a gluonic flux tube with a certain diameter; therefore, it is better to use smeared Wilson loops instead of ordinary unsmeared Wilson loops, which are “too thin” (cf. Figure 2).
  - Use a variational technique.

A variational technique

- Use a whole set of states \( |\phi_j\rangle \), instead of only a single state \( |\phi\rangle \), and determine that linear combination
  \[
  |\psi\rangle = \alpha_j|\phi_j\rangle,
  \]  
  which has maximum overlap to \( |\Omega\rangle \) (to be more precise, determine that linear combination, for which \( \mathcal{E}_\Omega^{\psi}(T + a) \) is minimal for given \( T \)).
- To determine the “best state” \( |\psi\rangle \), compute the correlation matrix
  \[
  C_{jk}(T) = \langle \phi_j(T)|\phi_k(0) \rangle
  \]  
  and solve the generalized eigenvalue problem
  \[
  C_{jk}(T + a)\alpha_k^{(n)} = C_{jk}(T)\alpha_k^{(n)}\lambda^{(n)} \quad \text{(no sum over } n) \tag{10}
  \]
  (in the following we consider the eigenvalues sorted according to \( \lambda^{(1)} \leq \lambda^{(2)} \leq \ldots \leq \lambda^{(N)} \); reality and positivity can be shown by multiplying (10) with \( (\alpha_j^{(n)})^* \)). \( |\psi\rangle \) is given by (8) with \( \alpha_j = \alpha_j^{(N)} \) and the corresponding minimal energy is
  \[
  \mathcal{E}_\Omega^{\psi}(T + a) = -\frac{1}{a} \ln \left( \frac{\langle \psi(T + a)|\psi(0) \rangle}{\langle \psi(T)|\psi(0) \rangle} \right) = -\frac{1}{a} \ln \left( \frac{(\alpha_j^{(N)})^* C_{jk}(T + a)\alpha_k^{(N)}}{(\alpha_j^{(N)})^* C_{jk}(T)\alpha_k^{(N)}} \right) = -\frac{1}{a} \ln \left( \lambda^{(N)} \right). \tag{11}
  \]
**“Proof”**:  

- To determine the best state $|\psi\rangle$, minimize $E_\Omega^\psi(T + a)$ with respect to $\alpha_n^*$:  
  \[
  \frac{\partial}{\partial \alpha_n} E_\Omega^\psi(T + a) = \frac{\partial}{\partial \alpha_n^*} \left(- \frac{1}{a} \ln \left( \frac{\langle \psi(T + a)|\psi(0)\rangle}{\langle \psi(T)|\psi(0)\rangle} \right) \right) = \frac{\partial}{\partial \alpha_n^*} \left(- \frac{1}{a} \ln \left( \frac{\alpha^* C_{jk}(T + a) \alpha_k}{\alpha^* C_{jk}(T) \alpha_k} \right) \right) = - \frac{1}{a} \frac{C_{nk}(T + a) \alpha_k}{\langle \alpha|C(T + a)|\alpha\rangle} + \frac{1}{a} \frac{C_{nk}(T) \alpha_k}{\langle \alpha|C(T)|\alpha\rangle} = 0. \tag{12}
  \]
  This is equivalent to
  \[
  C_{nk}(T + a) \alpha_k = C_{nk}(T) \alpha_k \frac{\langle \alpha|C(T + a)|\alpha\rangle}{\langle \alpha|C(T)|\alpha\rangle} = \lambda. \tag{13}
  \]
  For $\lambda = \text{constant}$ this is a generalized eigenvalue problem. The solutions $\alpha_k^{(n)}$, $\lambda^{(n)}$, $n = 1, \ldots, N$, are consistent with the full equation, since
  \[
  \frac{\langle \alpha^{(n)}|C(T + a)|\alpha^{(n)}\rangle}{\langle \alpha^{(n)}|C(T)|\alpha^{(n)}\rangle} = \lambda^{(n)}. \tag{14}
  \]
  Note that this line of reasoning is not waterproof, since it does not include solutions with non-constant $\lambda$.

- Further remarks:
  
  - Determine the best state $|\psi\rangle$ at rather small $T$. This is more stable from a numerical point of view.
  
  - In principle, the whole low lying spectrum can be obtained via
    \[
    E_{\Omega^{(n)}} - E_0 \approx - \frac{1}{a} \ln \left( \lambda^{(N - n)} \right). \tag{15}
    \]
    if sufficiently many states $|\phi_j\rangle$ are used ($\Omega^{(n)}$ are low lying states, which have non-vanishing overlap to span $\{ |\phi_j\rangle \}$, and $E_{\Omega^{(0)}} < E_{\Omega^{(1)}} < E_{\Omega^{(2)}} < \ldots$ are their corresponding energies).
  
  - In the limit $N \to \infty$ the generalized eigenvalue problem (10) is just a diagonalization of the Hamiltonian.
  
  - To get an idea of the quality of the extracted energy $E_\Omega^\psi$, one can compute the overlap of $|\psi\rangle$ and $|\Omega\rangle$ by considering the following expression for large $T$:
    \[
    \frac{|\langle \Omega|\psi\rangle|^2}{\langle \psi|\psi\rangle} = \frac{|\langle 0|\psi\rangle|^2 e^{-(E_\Omega - E_0)(T + a)}}{\langle \psi|\psi\rangle e^{-(E_\Omega - E_0)(T + a)}} \approx \frac{\langle \psi(T + a)|\psi(0)\rangle}{\langle \psi(T + a)|\psi(0)\rangle e^{-((E_\Omega - E_0)a)/(T + a)/a}} \approx \frac{\langle \psi(T + a)|\psi(0)\rangle}{\langle \psi(T + a)|\psi(0)\rangle} \frac{T}{a}. \tag{16}
    \]
    ((2) and (4) have been used). Note that this is only possible, if $|\psi\rangle$ is normalized, since $\langle \psi|\psi\rangle$ is hardly accessible in numerical computations.
4 Numerical results for the static quark antiquark potential

- Computation of the static quark antiquark potential:
  - Twisted mass formulation, 2+1+1 flavors, 89 configurations at $\beta = 3.5, L^3 \times T = 24^3 \times 48, \kappa = 0.16480, \mu = 0.004, \mu = 0.11, \epsilon = 0.09$.
  - Wilson loops with five different smearing levels, i.e. $N = 5$.

- Figure 3a shows $E^{\psi}_\Omega$ as a function of $T$ for different quark separations $R$ (the best state $|\psi\rangle$ has been determined at $T = 2$).

- Figure 3b shows the static quark antiquark potential $V$ as a function of $R$ ($V(R) = E^{\psi}_\Omega(R, T = 5)$) together with a least squares fit with $V(R) = V_0 - \alpha/R + \sigma R$, from which one can determine e.g. $r_0$.

- Figure 3c shows the overlap of $|\psi\rangle$ and $|\Omega\rangle$ according to (16) as a function of $T$ for different quark separations $R$.

- Note that the rather weak overlap for large $R$ (cf. Figure 3c) is consistent with the lower plateaux quality in Figure 3a.

Figure 3: a) $E^{\psi}_\Omega$ as a function of $T$ for different quark separations $R$. b) $V$ as a function of $R$. c) Overlap of $|\psi\rangle$ and $|\Omega\rangle$ as a function of $T$ for different quark separations $R$. 
Where is string breaking?

- With the method discussed above (using smeared Wilson loops to extract the static quark antiquark potential) one does not observe string breaking. The reason is a bad choice of states $|\phi_j\rangle$: the overlap of $|\phi_j\rangle$ and $|\Omega\rangle$ is acceptable as long as $R \lesssim R_{\text{string breaking}} \approx 2.2 \times r_0$, but there is essentially no overlap, as soon as the string is broken (the corresponding state $|\Omega\rangle$ is expected to be a two meson state then).

- Solution: do not only use “string states” (5) but also “two meson states”, e.g.

$$|\phi_j\rangle = \bar{Q}(x)\gamma_5 q(x)\bar{\eta}(y)\gamma_5 Q(y)|0\rangle$$

(17)

and smeared versions therefrom; when using the variational method, there should be sufficient overlap both below and above the string breaking distance $R_{\text{string breaking}}$ (the corresponding correlation matrix is sketched in Figure 4).

![Figure 4: The correlation matrix to compute string breaking.](image)

References