Yukawa effective potential ($\ell = 1$) and the variational method

Reminder:

If we want to solve the TDSE:

$$\hat{H}\psi(r,\theta,\phi) = -\frac{\hbar^2}{2m}\nabla^2\psi(r,\theta,\phi) + V(r)\psi(r,\theta,\phi) = E\psi(r,\theta,\phi),$$

with a radially-symmetric potential $V(r)$, we can introduce a variable $u(r)$ so that $\psi(r,\theta,\phi) = Y_\ell^m(\theta,\phi)u(r)/r$. This will lead to the 'reduced radial equation' which is covered well in Griffiths if you're looking for a refernece. When introducing $u(r)$, the Hamiltonian acts on the wave-function as,

$$\hat{H}[\psi(r,\theta,\phi)] = \hat{H}[Y_\ell^m(\theta,\phi)r^{-1}u(r)] = r^{-1}Y_\ell^m(\theta,\phi)\hat{H}_u[u(r)],$$

where,

$$\hat{H}_u[u(r)] = -\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[\frac{\ell(\ell+1)}{2mr^2} + V(r)\right]u(r).$$

This is like moving to the rotating frame in classical mechanics. When we make this change of variables, we get an effective potential:

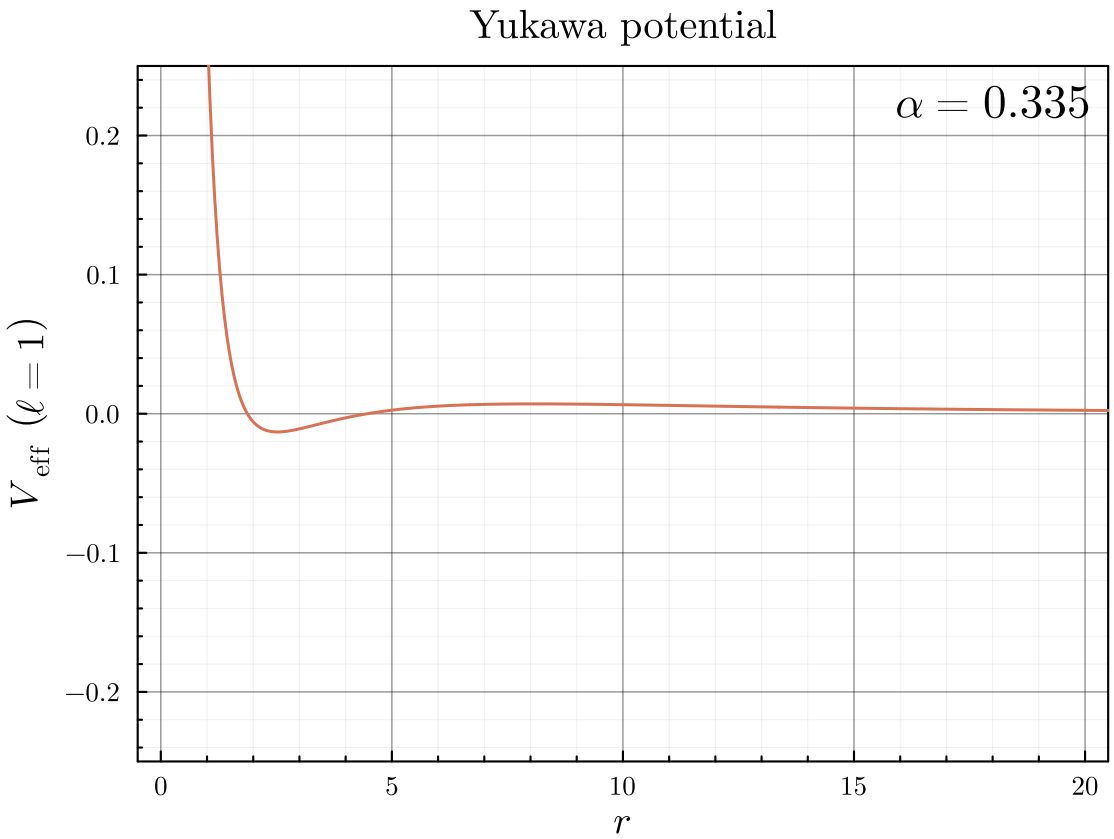
$$V_{\text{eff.}}(r) = \frac{\ell(\ell+1)}{2mr^2} + V(r).$$

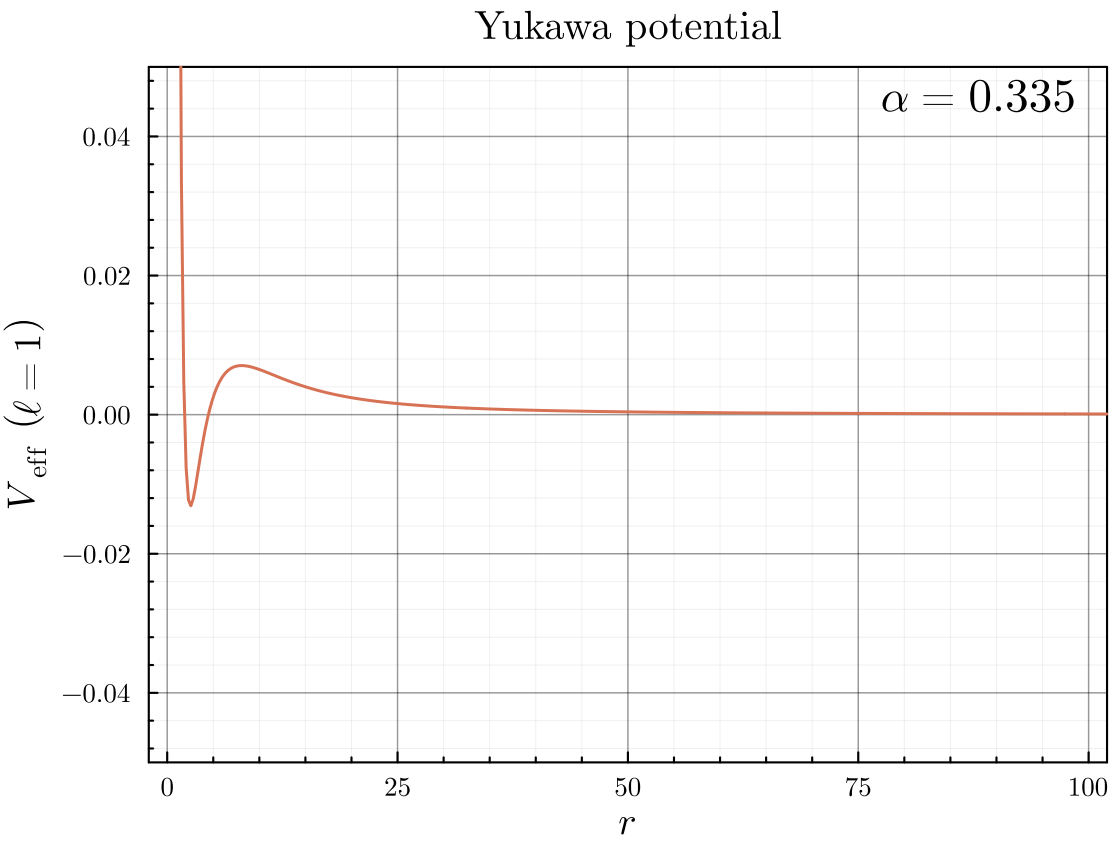
This means that when we compute the expected energy, we get a simplified integral,

$$\begin{aligned}\langle\psi|\hat{H}|\psi\rangle &= \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty}\psi(r,\theta,\phi)^*\hat{H}[\psi(r,\theta,\phi)]r^2\sin\theta dr d\theta d\phi \\ &= \int_0^{2\pi}\int_0^{\pi}|Y_\ell^m(\theta,\phi)|^2\sin\theta d\theta d\phi\int_0^{\infty}u(r)^*\hat{H}_u[u(r)]r^{-2}r^2dr \\ &= \int_0^{\infty}u(r)^*\hat{H}_u[u(r)]dr.\end{aligned}$$

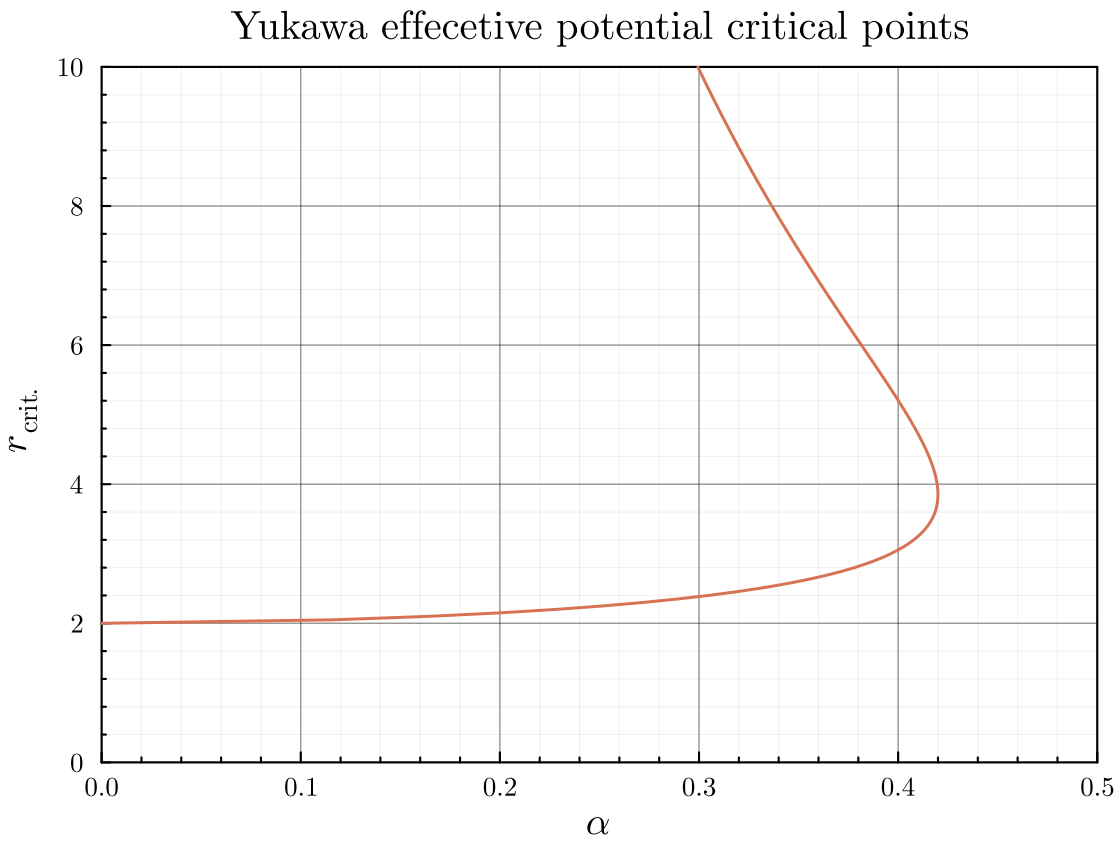
Features of the $\ell = 1$ Yukawa effective potential

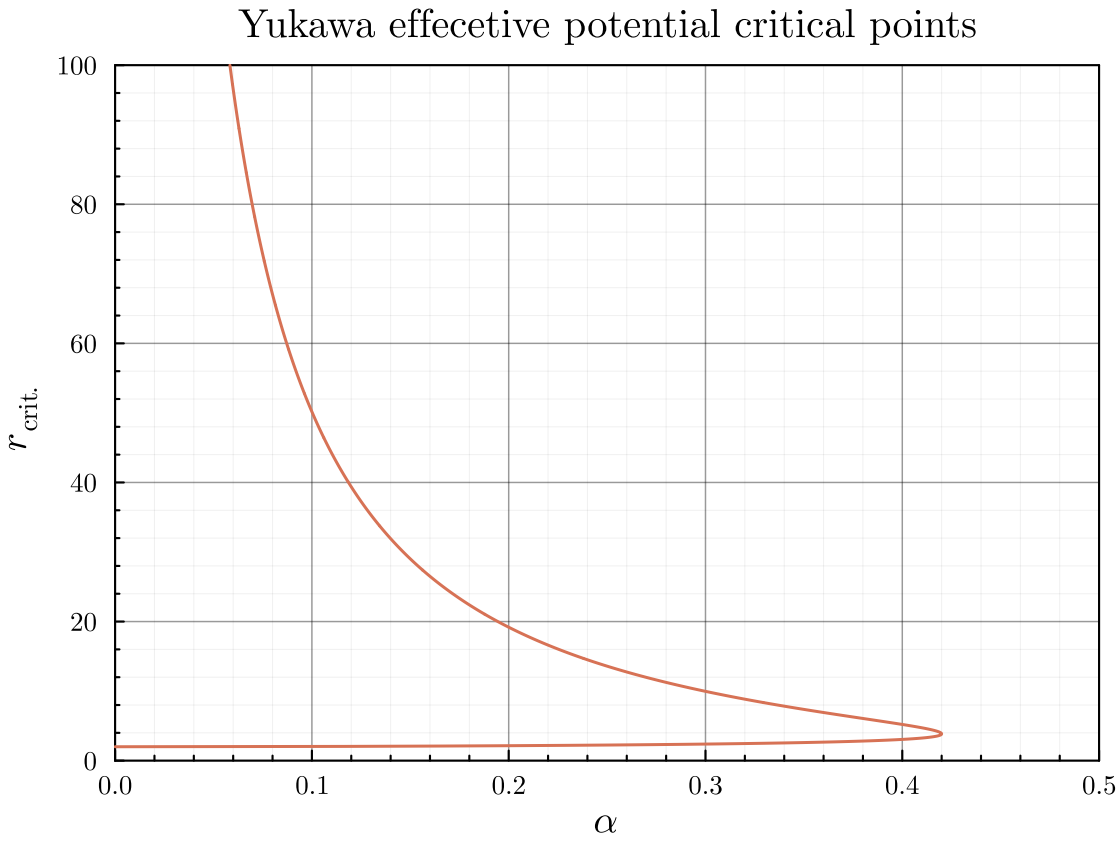
Yukawa potential at different scales:

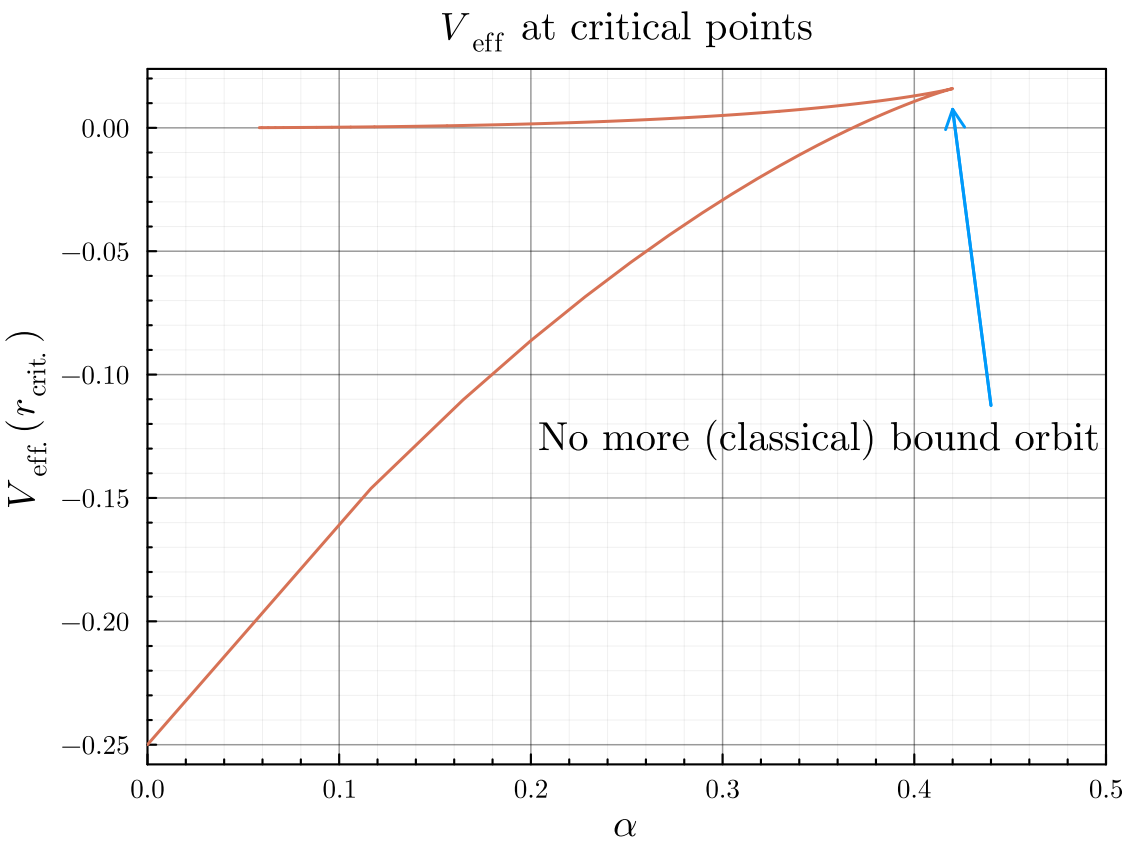




Yukawa potential critical points


Yukawa effecetive potential critical points
10
8
6
4
2
0
$r_{\text{crit.}}$
0.0
0.1
0.2
0.3
0.4
0.5
α


Yukawa effecetive potential critical points
100
80
60
40
20
0
$r_{\text{crit.}}$
0.0
0.1
0.2
0.3
0.4
0.5
α



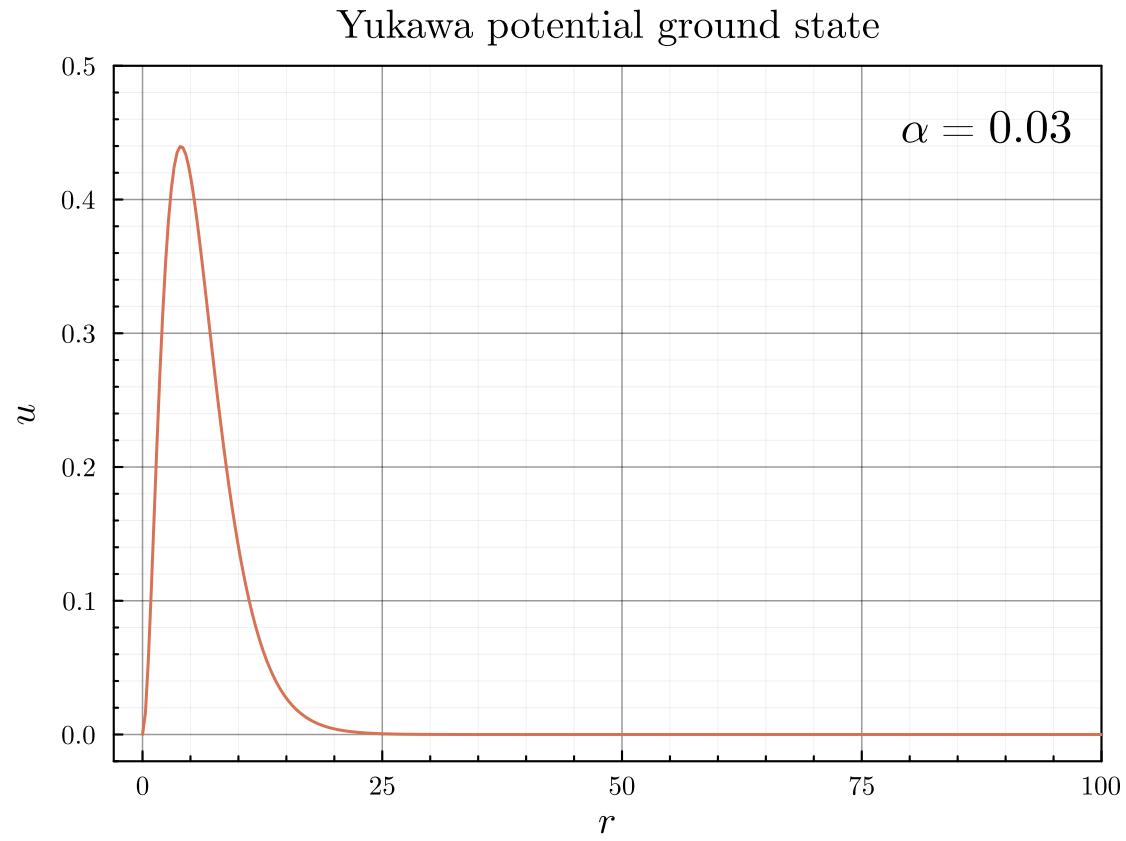
Exact ground states

Here, we compute exact ground states using 'exact diagonalization.' Exact diagonalization is the procedure in which you represent the Hamiltonian as a matrix acting on a discretized lattice and find the states and energies by computing eigenvectors and eigenvalues.

Let's play with choices of r_{max} to see how it effects our results

```
begin
    rmin = 5e-3;
    rmax = 1.0e3;
    # rmax = 2.0e1;
    Δrgoal = 0.3;
    nPts = Int(round((rmax-rmin)/Δrgoal));
    Δr = ((rmax-rmin)/(nPts-1));
end;
```

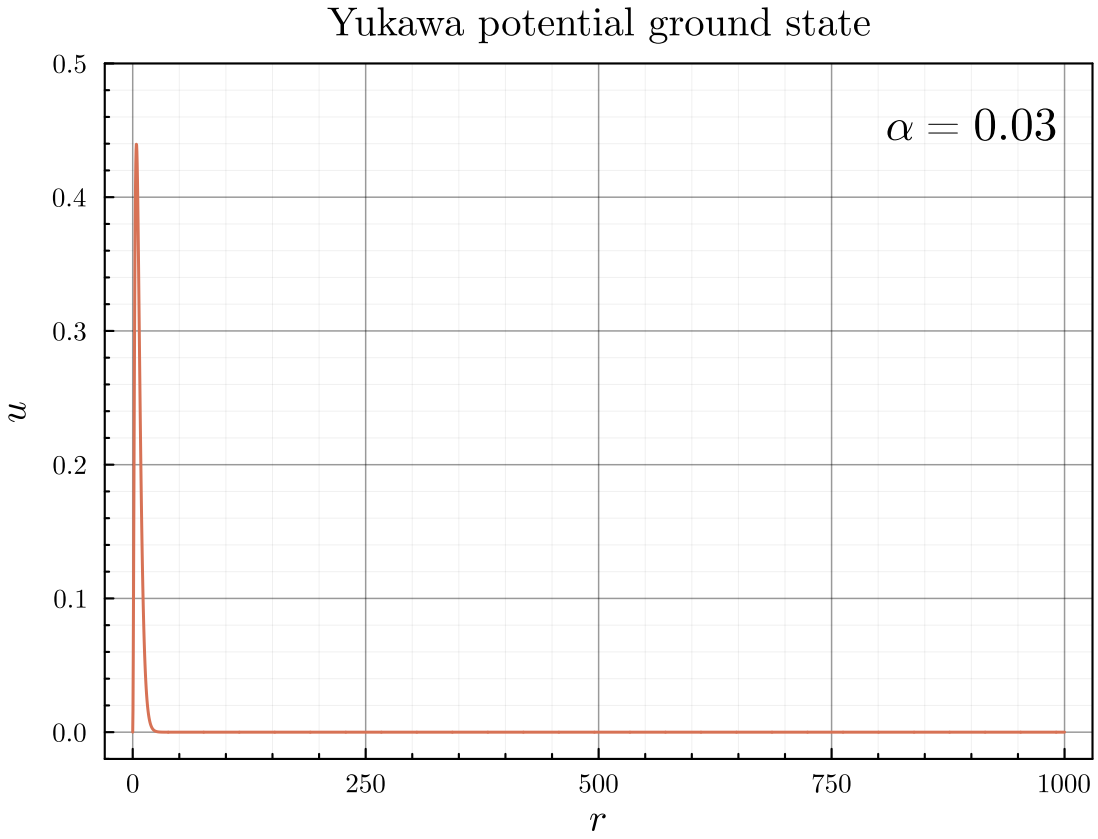
For large values of α, a bound state is not formed. However, when we choose rmax too small, we don't see this behavior. Try it!

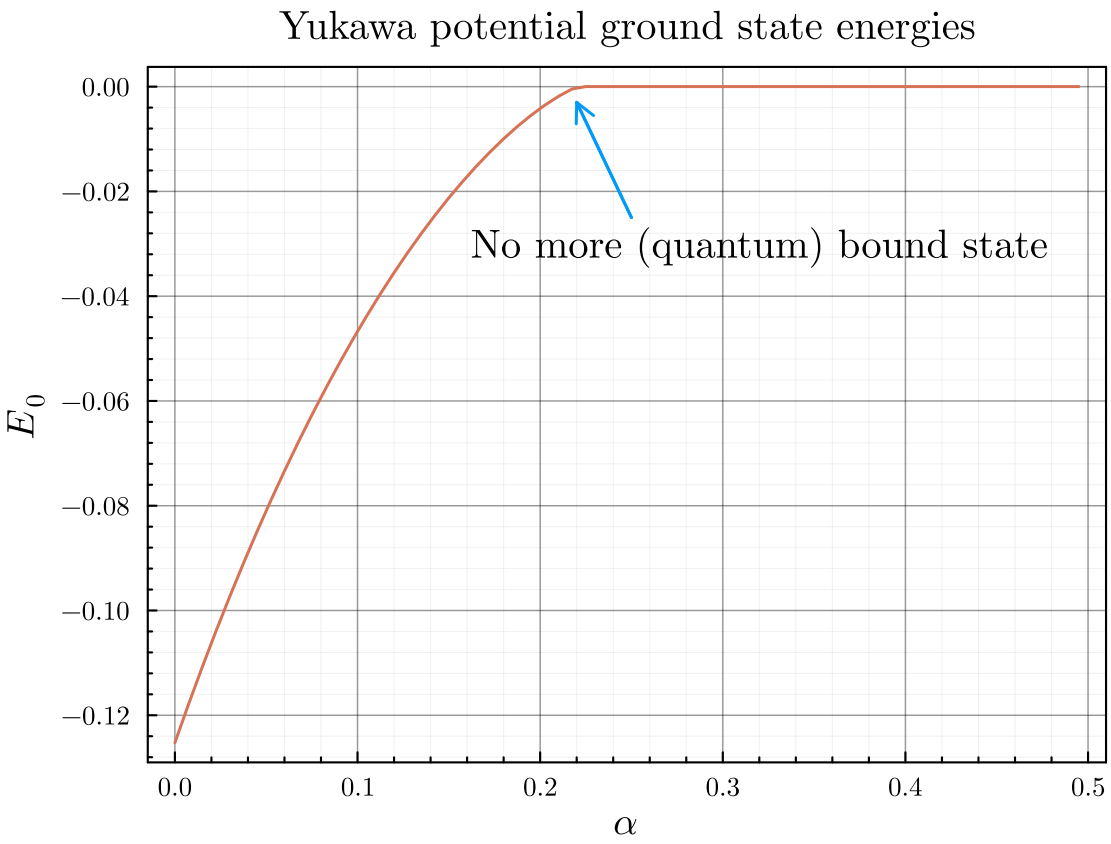


Exact diagonalization struggles to capture an unbound state because it enforces that the wave function is equal to zero at the boundaries (called Dirichlet boundary conditions). This means that there is effectively an infinite potential wall at `r_min` and `r_max`.

However, if we choose `r_max` large enough, we can avoid some problems and capture the disappearance of the bound state, but we will never be able to capture the true unbound state.

Alternatively, you could implement periodic boundary conditions which does not add an infinite potential wall but does add other features. Periodic boundary conditions would produce essentially the same results as Dirichlet boundary conditions in this particular problem because $V_{\text{eff}} \to \infty$ at $r \to 0$.



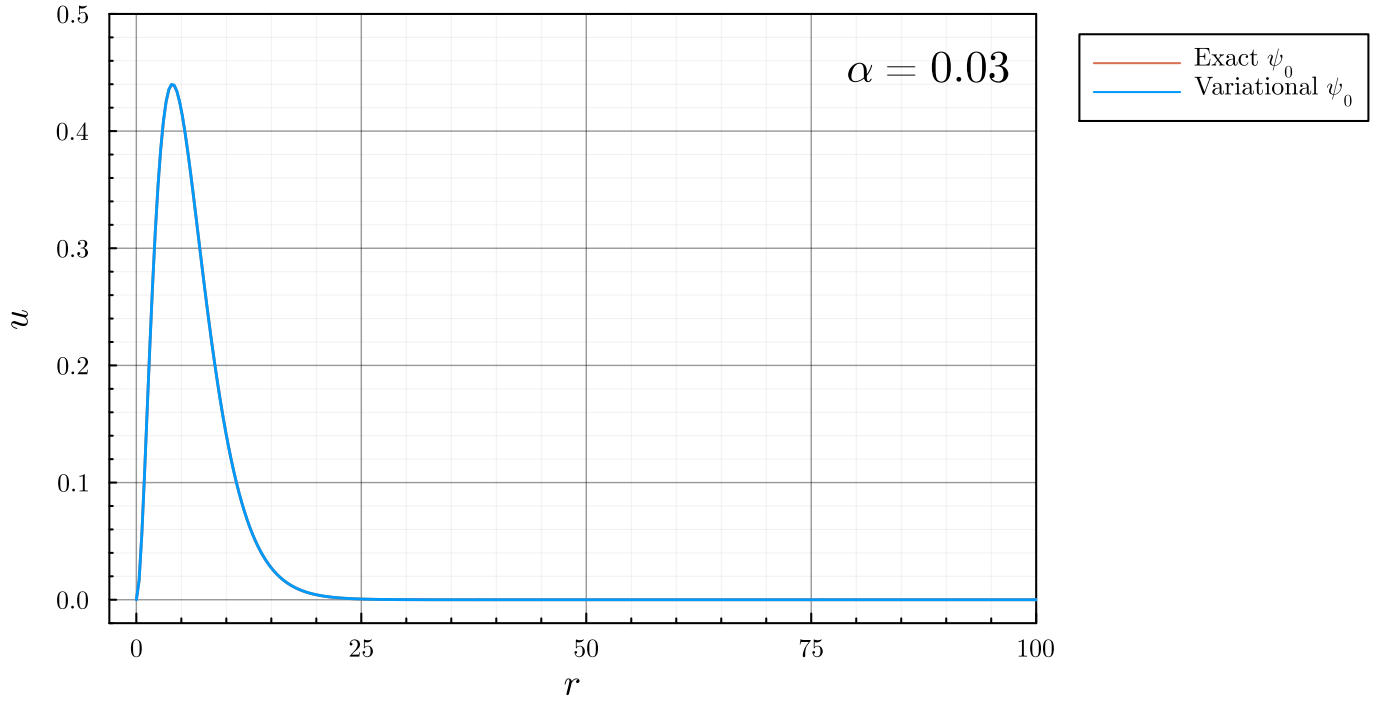


Notice that when we choose x_max too small, we don't see the hard boundary defining the disappearance of the ground state

Variational ground states and the effect of system size

An example ansatz is $u(r) \propto r^2 e^{-ar-br^2}$, so

$$\psi(r,\theta,\phi) = Y_1^0(\theta,\phi) r^{-1} u(r) \propto \cos\theta r e^{-ar-br^2}.$$



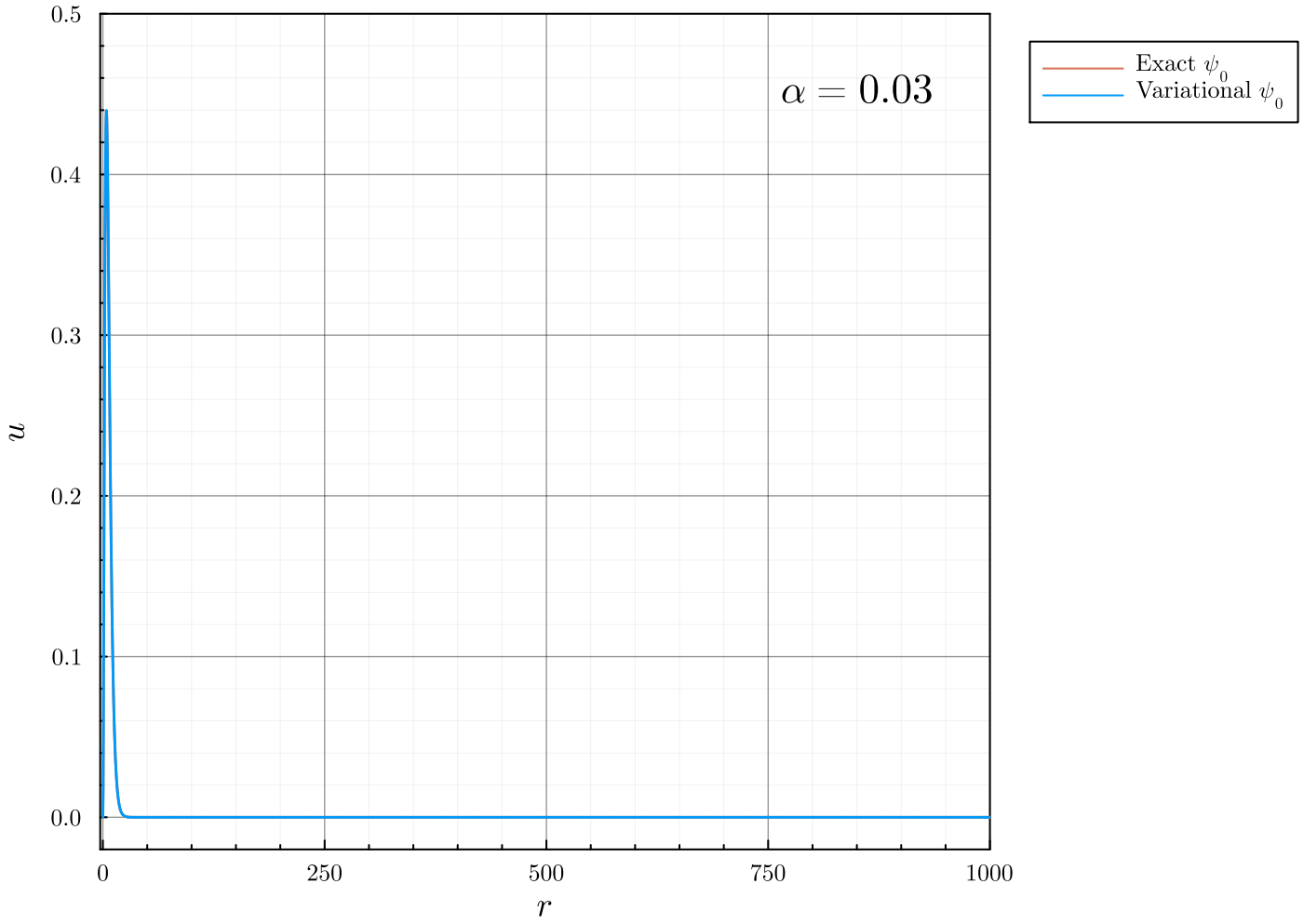
For α = 0.03,

The variational energy is: -0.09736

The exact energy is: -0.09736

The relative error is: 0.0005%

The state fidelity is: 1.0


$\alpha = 0.03$
Exact ψ_0
Variational ψ_0
u
r
0.0
0.1
0.2
0.3
0.4
0.5
0
250
500
750
1000