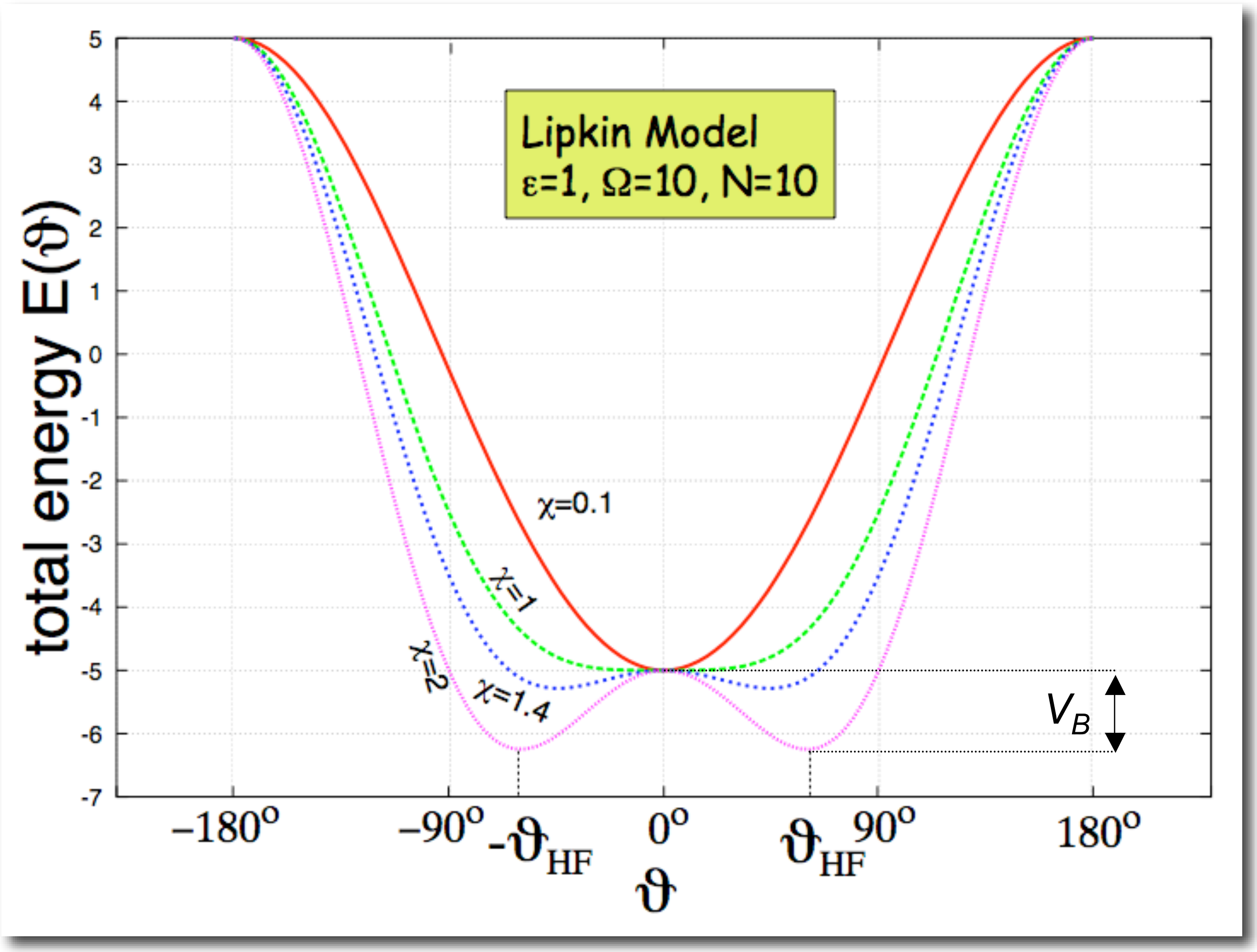


$$E_{HF} = \begin{cases} -\frac{\varepsilon}{2}\Omega & \text{for} \quad \chi < 1 \\ -\frac{\varepsilon}{4}\Omega\left(\chi + \frac{1}{\chi}\right) & \text{for} \quad \chi \geq 1 \end{cases}$$

Barrier height: $$V_B = \frac{\varepsilon}{4}\Omega\left(\chi + \frac{1}{\chi} - 2\right)$$

Deformation parameter

$$\hat{Q} \equiv \hat{K}_x = \frac{1}{2}\left(\hat{K}_+ + \hat{K}_-\right)$$

$$q \equiv \langle \tau | \hat{Q} | \tau \rangle = \frac{1}{2}\Omega \sin\theta \cos\phi$$

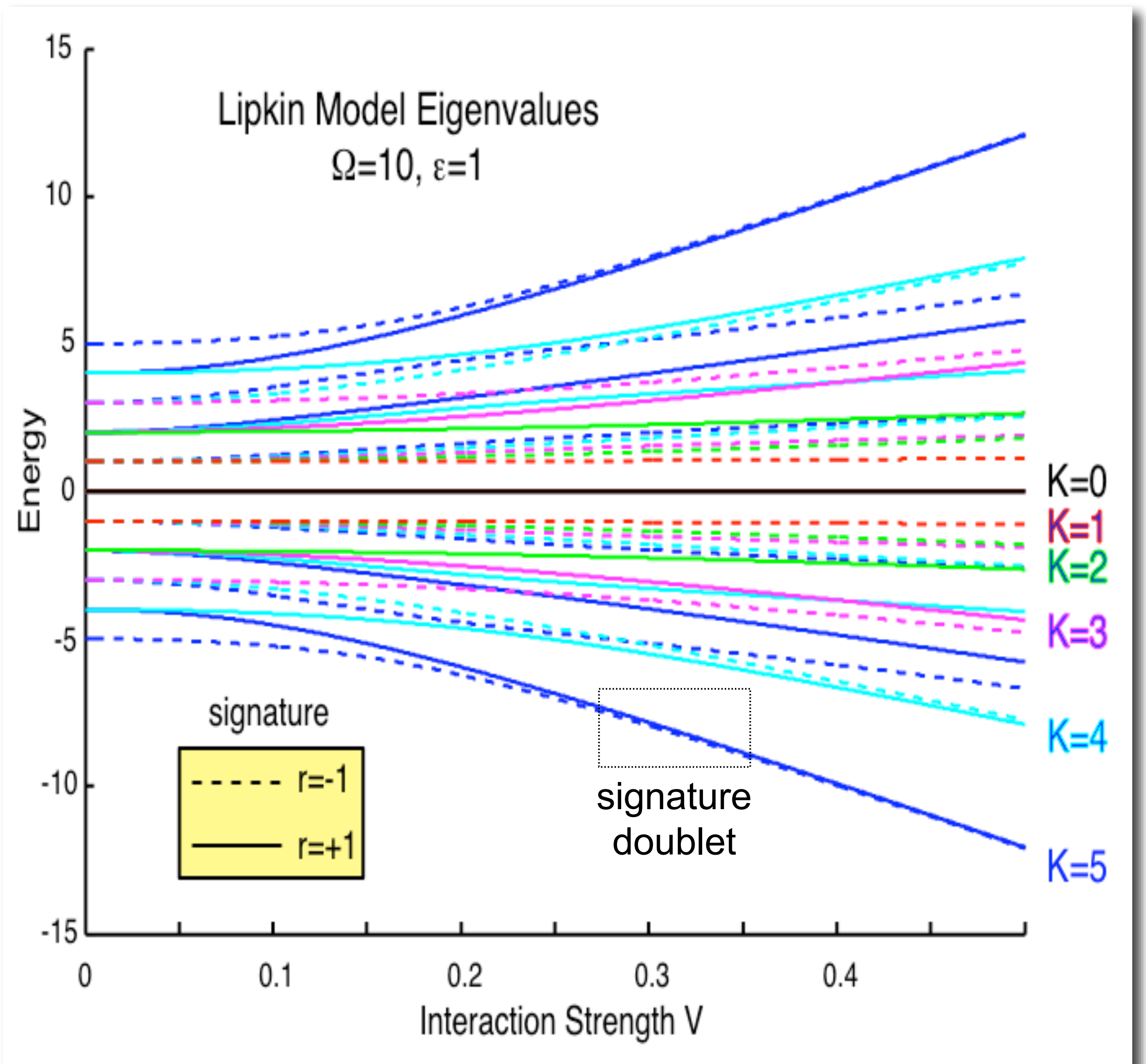
Deformation parameter
of the Lipkin Model

$$q_{HF} = \begin{cases} 0 & \text{for} \quad \chi < 1 \\ \frac{\Omega}{2}\sqrt{1 - \frac{1}{\chi^2}} & \text{for} \quad \chi \geq 1 \end{cases}$$

For *q=0* one is dealing with the “spherical” system
For *q>0* one is dealing with the “deformed” system

For the exact solution, *q*=0 (why?)

Homework: calculate $\sqrt{\langle \hat{Q}^2 \rangle}$ in the LM ground state. Compare with the HF deformation.



Lipkin Model Eigenvalues
Ω=10, ε=1
Energy
Interaction Strength V
15
10
5
0
-5
-10
-15
0
0.1
0.2
0.3
0.4
K=0
K=1
K=2
K=3
K=4
K=5
signature
r=-1
r=+1
signature doublet

Signature of the Hartree-Fock State

$$\hat{R} = e^{i\pi \hat{K}_o}$$

$$\begin{aligned}
\langle \tau | \hat{R} | \tau \rangle &= \frac{1}{(1+|\tau|^2)^\Omega} \left(e^{-\frac{i\pi}{2}} + e^{\frac{i\pi}{2}} |\tau|^2 \right)^\Omega \\
&= i^\Omega \left(\frac{|\tau|^2 - 1}{|\tau|^2 + 1} \right)^\Omega \\
&= (-i)^\Omega \cos^\Omega \theta \\
&= (-i)^\Omega \frac{1}{\chi^\Omega} = e^{-i\pi \frac{\Omega}{2}} \frac{1}{\chi^\Omega}
\end{aligned}$$

Ground-state signature

- Signature is broken in the deformed HF solution
- At large value of χ signature is maximally broken! (complete alignment of quasi-spin along the x-axis!)

Note that $\hat{R}^2 = (-1)^N$

Therefore, **for an even number of fermions**,

$$\hat{R}^2 = 1,\ \hat{R}^{-1} = \hat{R},\ \hat{R}^{+} = \hat{R}$$

$$\begin{aligned}
\hat{R}|\tau\rangle &= \frac{1}{(1+|\tau|^2)^{\Omega/2}} \hat{R} e^{\tau \hat{K}_+} \hat{R}^{-1} \hat{R} |\Omega/2, -\Omega/2\rangle \\
&= e^{-i\pi \frac{\Omega}{2}} \frac{1}{(1+|\tau|^2)^{\Omega/2}} e^{-\tau \hat{K}_+} |\Omega/2, -\Omega/2\rangle \\
&= e^{-i\pi \frac{\Omega}{2}} |-\tau\rangle
\end{aligned}$$

Consequently, under the signature operation

$$\theta \to -\theta,\ q \to -q$$

Let us now introduce the operator

$$\hat{P}_r = \frac{1}{2}\left(1 + r\hat{R}\right)$$

$$\hat{P}_r^2 = \frac{1}{4}\left(1 + 2r\hat{R} + r^2\hat{R}^2\right) = \hat{P}_r$$

=1

Therefore, P_r is a projector!

$$\hat{R}\hat{P}_r = \hat{R}\frac{1}{2}\left(1 + r\hat{R}\right) = r\hat{P}_r$$

or

$$\hat{R}|\Psi_r\rangle = r|\Psi_r\rangle$$

where

$$|\Psi_r\rangle \equiv \hat{P}_r|\Psi\rangle$$

We demonstrated that P_r projects on good signature (or: restores signature symmetry)

The **projected energy** can be written as

$$E_r \equiv \frac{\langle\Psi_r|\hat{H}|\Psi_r\rangle}{\langle\Psi_r|\Psi_r\rangle}$$

In the following, we assume that $\langle\Psi|\Psi\rangle = 1$

$$\begin{aligned}
\langle\Psi_r|\Psi_r\rangle &= \langle\Psi|\hat{P}_r^2|\Psi\rangle \\
&= \langle\Psi|\hat{P}_r|\Psi\rangle \\
&= \frac{1}{2}\left(1 + r\langle\Psi|\hat{R}|\Psi\rangle\right)
\end{aligned}$$

$$\begin{aligned}
\langle\Psi_r|\hat{H}\Psi_r\rangle &= \langle\Psi|\hat{P}_r\hat{H}\hat{P}_r|\Psi\rangle \\
&= \langle\Psi|\hat{H}\hat{P}_r|\Psi\rangle \\
&= \frac{1}{2}\left(\langle\Psi|\hat{H}|\Psi\rangle + r\langle\Psi|\hat{H}\hat{R}|\Psi\rangle\right)
\end{aligned}$$

Let us consider projected product states:

$$|\Psi\rangle = |\tau\rangle, \quad |\Psi_r\rangle = \hat{P}_r|\tau\rangle$$

We first note that the **projected product states are not product states!**

$$\begin{aligned} |\Psi_r\rangle &= \frac{1}{2}\left(|\tau\rangle + re^{-i\pi\frac{\Omega}{2}}|-\tau\rangle\right) \\ &= \frac{1}{2}\left(|\tau\rangle + rr_{g.s.}|-\tau\rangle\right) \end{aligned}$$

Consequently, the projected ground-state (excited state) wave function is the symmetric (antisymmetric) combination of product states representing motion in the right and left potential well. By projecting out good signature, one is going beyond the class of product states of the Hartree-Fock method. Consequently, the projected energy will be lower than that of HF.

Let us evaluate the matrix elements needed to compute the projected energy

$$\begin{aligned} \langle\Psi_r|\Psi_r\rangle &= \frac{1}{2}\left(1 + r\langle\tau|\hat{R}|\tau\rangle\right) \\ &= \frac{1}{2}\left(1 + rr_{g.s.}\cos^{\Omega}\theta\right) \end{aligned}$$

$$\begin{aligned} \langle\Psi_r|\hat{H}|\Psi_r\rangle &= \frac{1}{2}\left(\langle\Psi|\hat{H}|\Psi\rangle + r\langle\Psi|\hat{H}\hat{R}|\Psi\rangle\right) \\ &= \frac{1}{2}\left[E(\tau) + rr_{g.s.}\langle\tau|\hat{H}|-\tau\rangle\right] \end{aligned}$$

Homework:

1) using the method of SU(2) generating functions, calculate

$$\langle \tau | \tau' \rangle \text{ and } \langle \tau | \hat{H}_{LM} | \tau' \rangle$$

for arbitrary values of τ and τ'.

2) Put τ'=- τ and compute the projected energy for the ground state and for the first excited state with $r=-r_{g.s.}$

3) Assume two cases:

   a) Projection *after* variation (PAV), i.e., $\tau = \tau_{HF}$

   b) Projection *before* variation (VAP), i.e., the projected energy is minimized with respect to τ

4) For various values of χ compare HF energy, exact energy, PAV energy, and VAP energy of the Lipkin Model.

5) What can you conclude from this calculation?