چاه پتانسیل دو گانه و کاربردهای آن چیست؟

آیا ملکول آمونیاک یک ملکول قطبی است؟

آیا ملکول آمونیاک را می توان همچون یک چاه دوگانه در نظر گرفت؟

ایزومرهای اپتیکی چیست؟

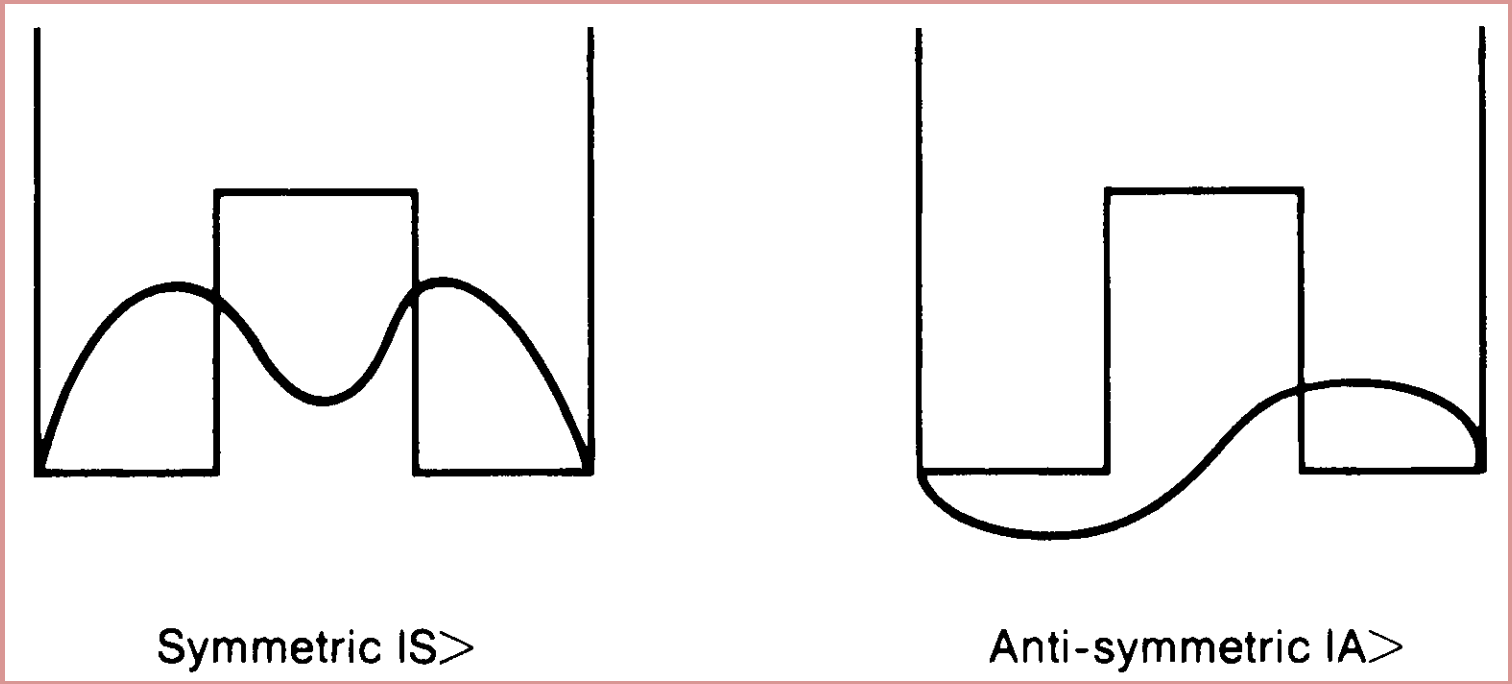
قاعده انتخاب پاریته چیست؟

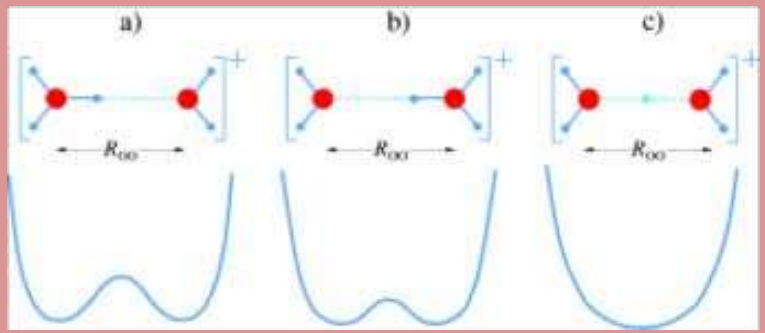
آیا این یک قاعده صرفا تجربی است یا مبنای نظری هم دارد؟

چرا قلب انسان در سمت چپ واقع شده است؟

Symmetrical Double-Well Potential

As an elementary but instructive example, we consider a symmetrical double-well potential:





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Symmetry breaking in symmetric and asymmetric double-well potentials

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Motivated by recent experimental studies of matter waves and optical beams in double-well potentials, we study the corresponding solutions of the nonlinear Schrödinger equation. Using a Galerkin-type approach, we obtain a detailed handle on the nonlinear solution branches of the problem, starting from the corresponding linear ones, and we predict the relevant bifurcations for both attractive and repulsive nonlinearities. The dynamics of the ensuing unstable solutions is also examined. The results illustrate the differences that arise between the steady states and the bifurcations emerging in symmetric and asymmetric double wells.

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Energy splitting in symmetric double-well potentials

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We extend the analytical transfer matrix method to solve the energy splitting in an arbitrary symmetric double-well potential. Dispersion equations corresponding to the split energy levels are presented in a very explicit form. Numerical calculation shows that the proposed method can give extremely accurate results for symmetric double-well potentials.

The Hamiltonian is obviously invariant under parity.

In fact, the two lowest lying states are as shown in Figure 4.3, we can see by working out the explicit solutions involving sine and cosine in classically allowed regions and sinh and cosh in the classically forbidden region.

The solutions are matched where the potential is discontinuous; we call them the symmetrical state $|S\rangle$ and the antisymmetrical state $|A\rangle$.

Of course, they are simultaneous eigenkets of H and π.

Calculation also shows that

$$E_A > E_S$$

which we can infer from the Fig. by noting that the wave function of the antisymmetrical state has a greater curvature.

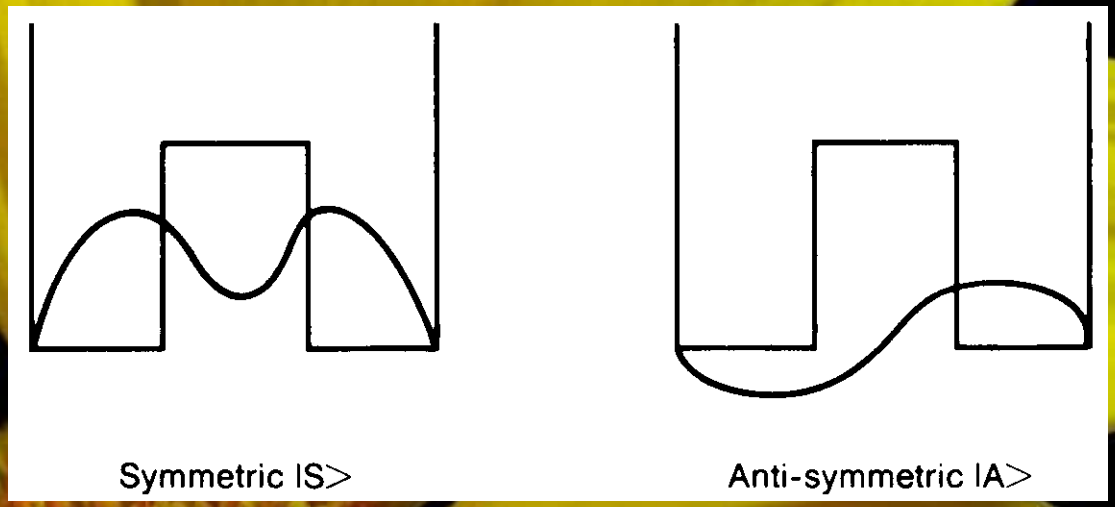
The energy difference is very tiny if the middle barrier is high, a point which we will discuss later.

We can form

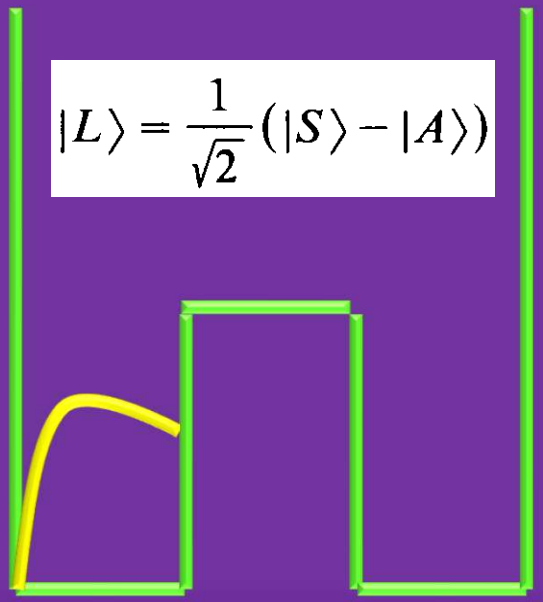
$$|R\rangle = \frac{1}{\sqrt{2}}(|S\rangle + |A\rangle)$$

$$|L\rangle = \frac{1}{\sqrt{2}}(|S\rangle - |A\rangle)$$

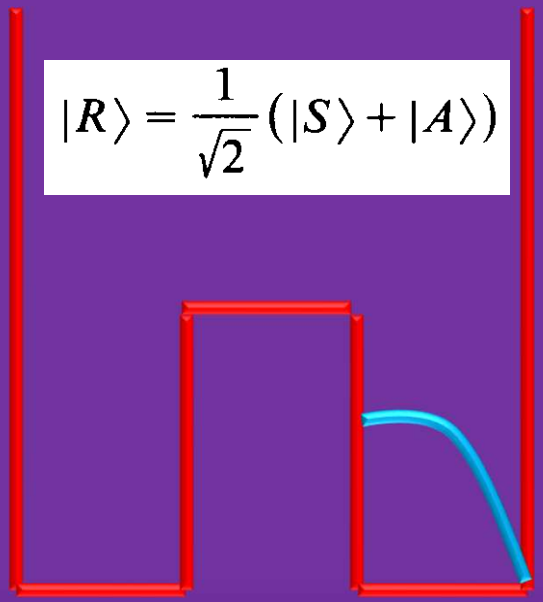
The wave functions of |R> and |L> are largely concentrated in the right-hand side and the left-hand side, respectively.



$$|L\rangle = \frac{1}{\sqrt{2}}(|S\rangle - |A\rangle)$$



$$|R\rangle = \frac{1}{\sqrt{2}}(|S\rangle + |A\rangle)$$

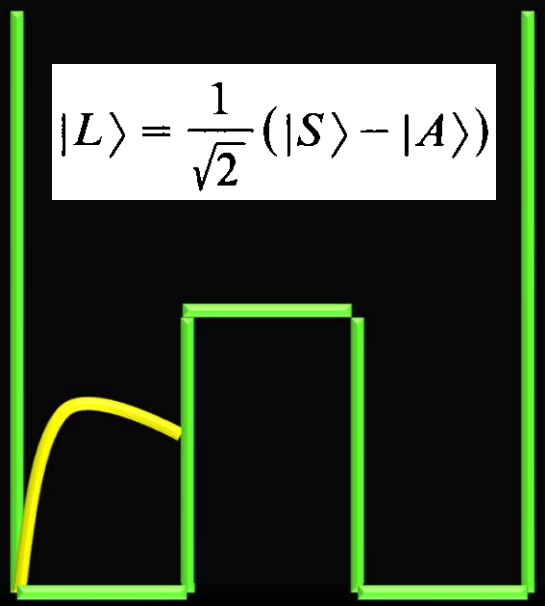


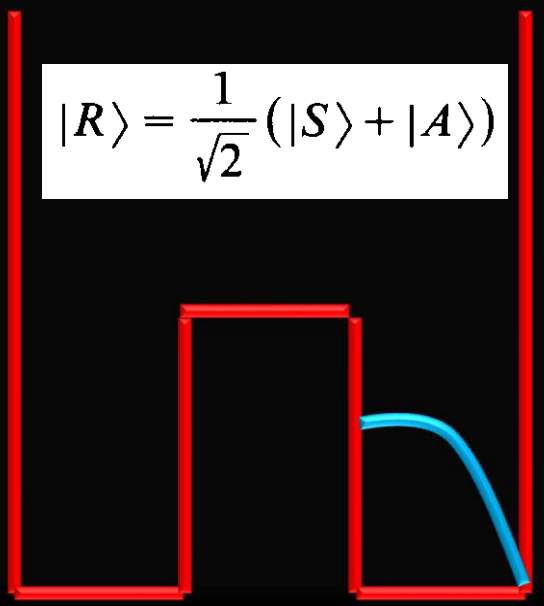
They are obviously not parity eigenstates; in fact, under parity |R> and |L> are interchanged.

π

$$|L\rangle = \frac{1}{\sqrt{2}}(|S\rangle - |A\rangle)$$

$$|R\rangle = \frac{1}{\sqrt{2}}(|S\rangle + |A\rangle)$$

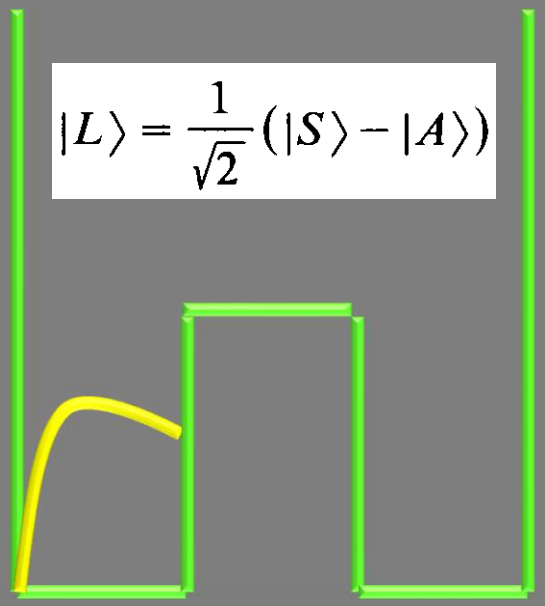


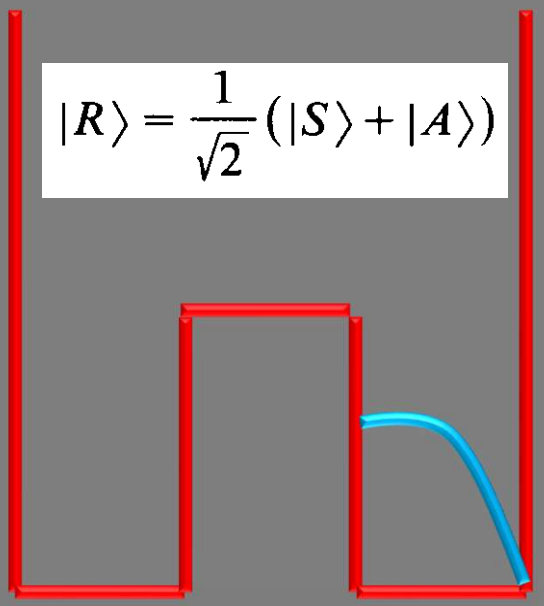


π

$$|L\rangle = \frac{1}{\sqrt{2}}(|S\rangle - |A\rangle)$$

$$|R\rangle = \frac{1}{\sqrt{2}}(|S\rangle + |A\rangle)$$





Note that they are not energy eigenstates either.

Indeed, they are classical examples of nonstationary states.

To be precise, let us assume that the system is represented by |R> at t = 0.

At a later time, we have

$$|R, t_0 = 0; t\rangle = \frac{1}{\sqrt{2}}\left(e^{-iE_s t/\hbar}|S\rangle + e^{-iE_A t/\hbar}|A\rangle\right)$$

$$= \frac{1}{\sqrt{2}} e^{-iE_s t/\hbar}\left(|S\rangle + e^{-i(E_A - E_S)t/\hbar}|A\rangle\right).$$

$$|R, t_0 = 0; t\rangle = \frac{1}{\sqrt{2}}\left(e^{-iE_S t/\hbar}|S\rangle + e^{-iE_A t/\hbar}|A\rangle\right)$$

$$= \frac{1}{\sqrt{2}} e^{-iE_S t/\hbar}\left(|S\rangle + e^{-i(E_A - E_S)t/\hbar}|A\rangle\right).$$

At time $t = \frac{T}{2} \equiv \frac{2\pi\hbar}{2(E_A - E_S)}$, the system is found in pure |L>.

At t = T, we are back to pure |R>, and so forth.

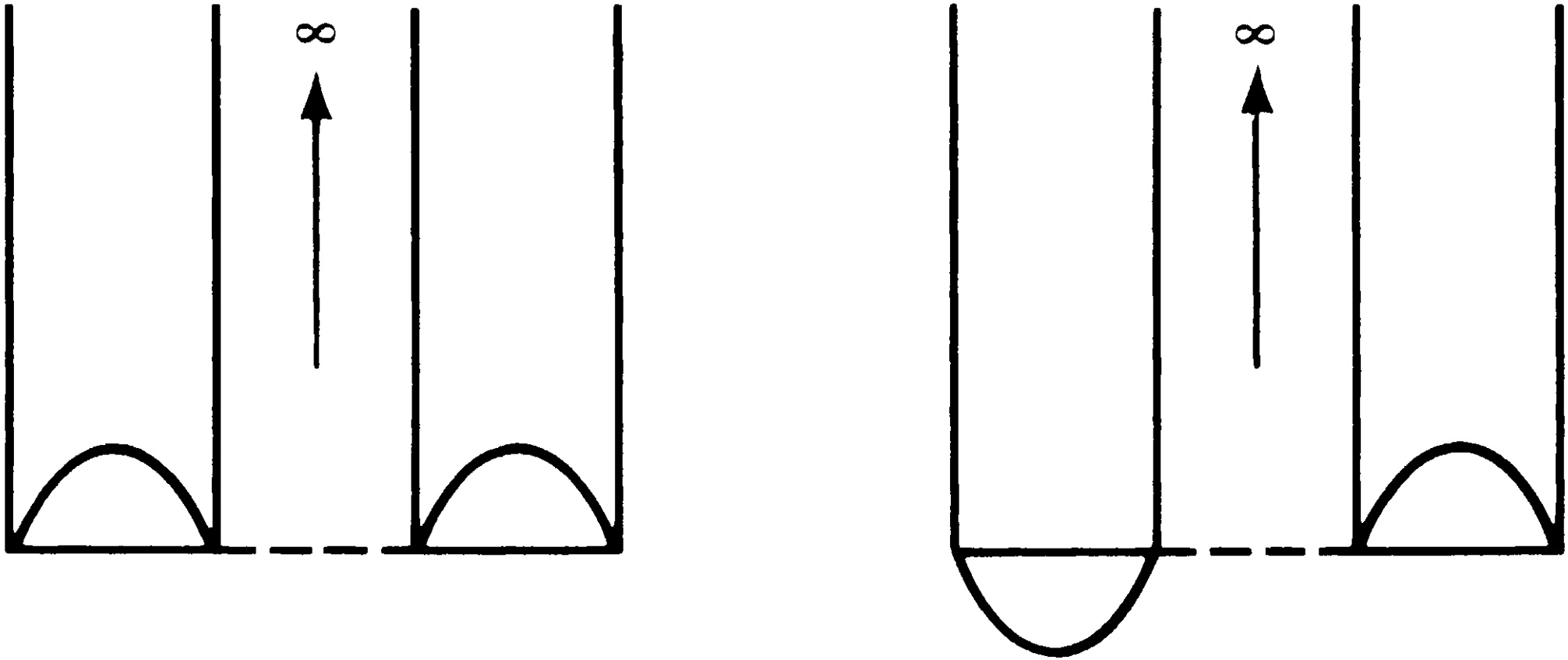
Thus, in general, we have an oscillation between |R> and |L> with angular frequency

$$\omega = \frac{(E_A - E_S)}{\hbar}$$

This oscillatory behavior can also be considered from the viewpoint of tunneling in quantum mechanics.

A particle initially confined to the right-hand side can tunnel through the classically forbidden region (the middle barrier) into the left-hand side, then back to the right-hand side, and so on.

But now let the middle barrier become infinitely high:



The |S> and |A> states are now degenerate, so |R> and |L> are also energy eigenkets even though they are not parity eigenkets.

$$H|S\rangle = E_S|S\rangle$$

$$H|A\rangle = E_A|A\rangle$$

If the symmetric double-well is infinite, then the system is degenerate: $E_S = E_A = E$

$$H|R\rangle = H\frac{1}{\sqrt{2}}(|S\rangle + |A\rangle) = \frac{1}{\sqrt{2}}(E_S|S\rangle + E_A|A\rangle)$$

$$H|R\rangle = E\frac{1}{\sqrt{2}}(|S\rangle + |A\rangle) = E|R\rangle$$

Similarly we can show that

$$H|L\rangle = E\frac{1}{\sqrt{2}}(|S\rangle - |A\rangle) = E|L\rangle$$

Once the system is found in |R>, it remains so forever (oscillation time between |S> and |A> is now ∞).

$$t = \frac{T}{2} \equiv \frac{2\pi\hbar}{2(E_A - E_S)}$$

$$E_S = E_A = E$$

Because the middle barrier is infinitely high, there is no possibility for tunneling.

Thus when there is degeneracy, the physically realizable energy eigenkets need not be parity eigenkets.

We have a ground state which is asymmetrical despite the fact that the Hamiltonian itself is symmetrical under space inversion, so with degeneracy the symmetry of H is not necessarily obeyed by energy eigenstates |S> and |A>.

This is a very simple example of broken symmetry and degeneracy.

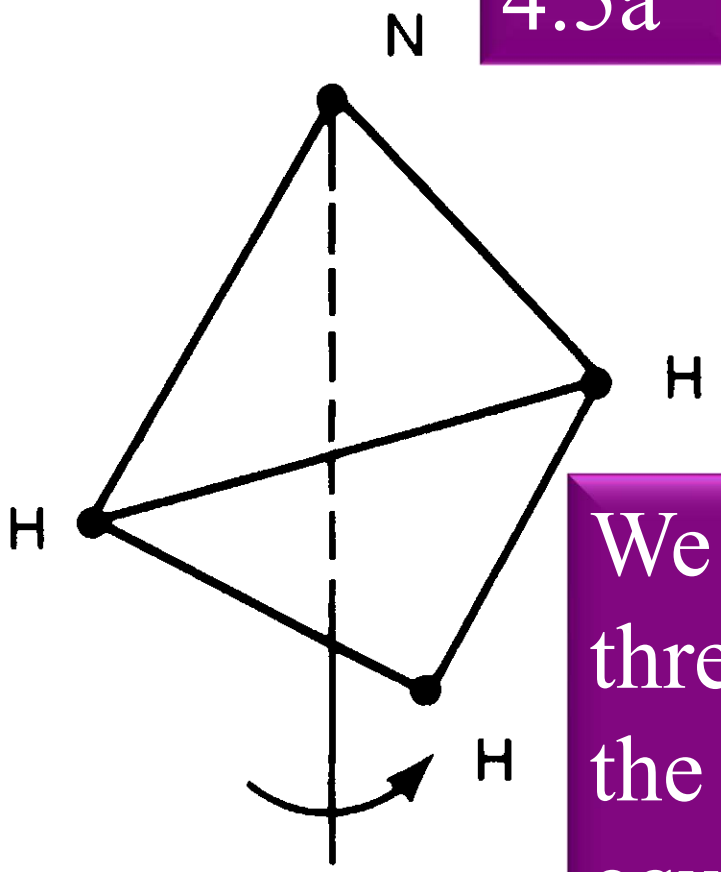
Nature is full of situations analogous to this.

Consider a ferromagnet.

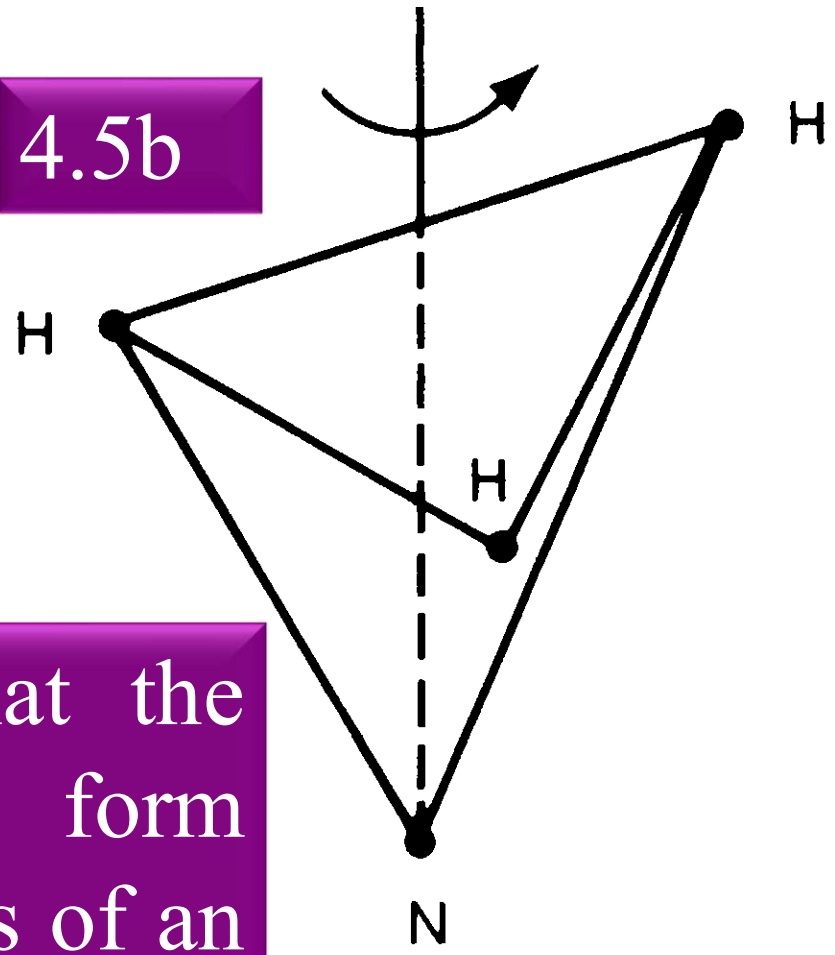
The basic Hamiltonian for iron atoms is rotationally invariant, but the ferromagnet clearly has a definite direction in space; hence, the (infinite) number of ground states is not rotationally invariant, since the spins are all aligned along some definite (but arbitrary) direction.

A textbook example of a system that illustrates the actual importance of the symmetrical double well is an ammonia molecule, NH_3:

4.5a



4.5b

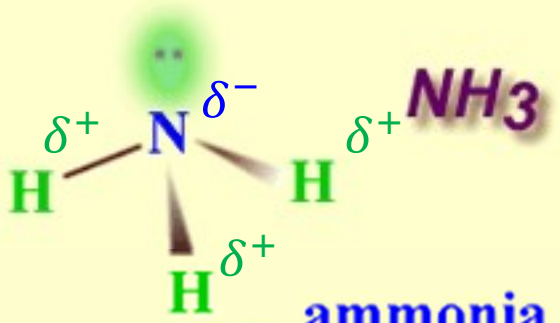


We imagine that the three H atoms form the three corners of an equilateral triangle.

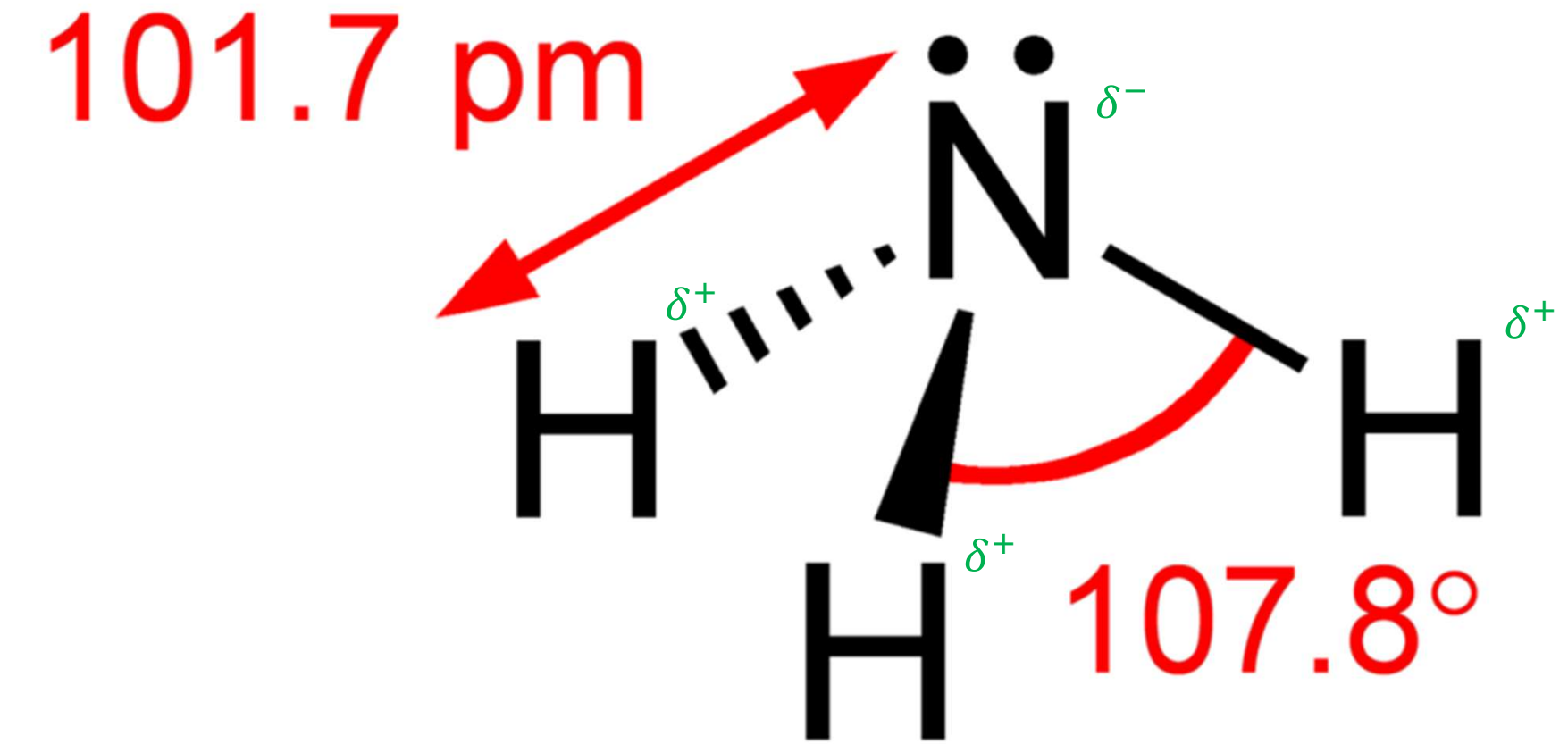
The N atom can be up or down, where the directions up and down are defined because the molecule is rotating around the axis as shown above.

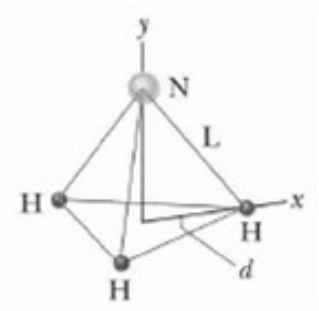
$^{7}N: 1s^2 2s^2 2p^6$

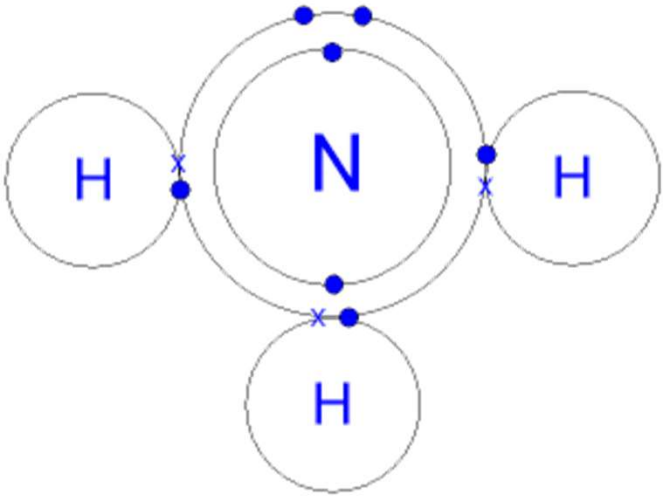
$^{1}H: 1s^1$



ammonia


101.7 pm
δ−
δ+
δ+
δ+
107.8°


y
N
L
H
x
H
H
d


H
N
H
H

Ammonia is a polar molecule because the different electronegativity's of the nitrogen and the hydrogen molecules makes the hydrogen slightly positive and the nitrogen slightly negative. However there are 2 valance electrons of the nitrogen atom which are not bonded to anything, which are called lone pairs.

The lone pairs means that the ammonia molecule is not symmetrical therefore the electronegativity's do not cancel eachother, creating a polar molecule.

So the up and down are meaningful, because the ammonia is a **polar and rotating** molecule.

The up and down positions for the N atom are analogous to R and L of the double-well potential.

The parity and energy eigenstates are superpositions of Figure 4.5a and Figure 4.5b in the sense of |R> and |L>, respectively.

$$|R\rangle = \frac{1}{\sqrt{2}}(|S\rangle + |A\rangle)$$

$$|L\rangle = \frac{1}{\sqrt{2}}(|S\rangle - |A\rangle)$$

the energy difference between the simultaneous eigenstates of energy and parity correspond to an oscillation frequency of 24,000 MHz—a wavelength of about 1 cm, which is in the microwave region.

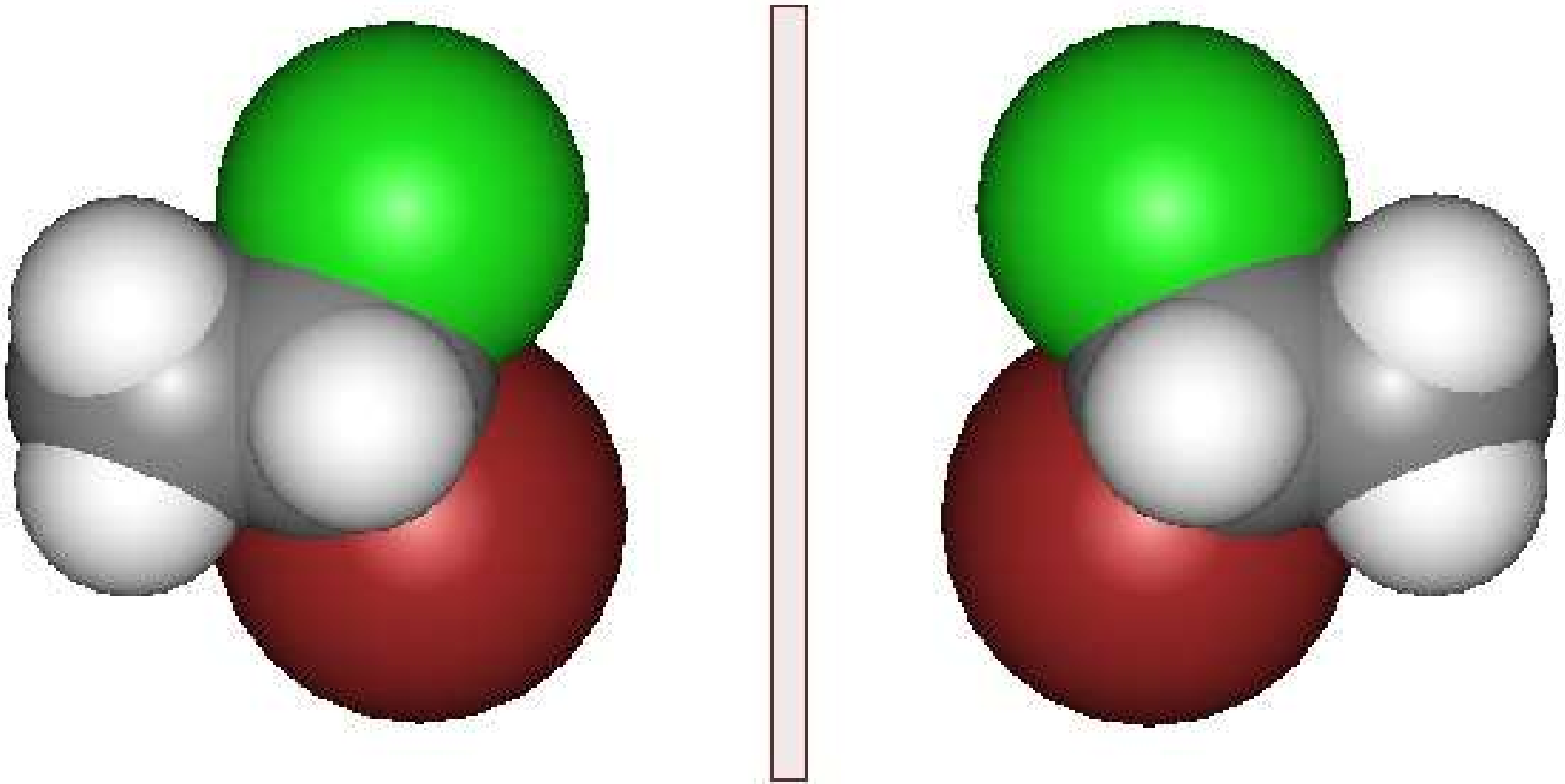
In fact, NH_3 is of fundamental importance in maser physics.

There are naturally occurring organic molecules, such as sugar or amino acids, which are of the R-type (or L-type) only.

Such molecules which have definite handedness are called **optical isomers**.

In many cases the oscillation time is practically infinite—on the order of 10^4-10^6 years—so R-type molecules remain right-handed for all practical purposes.

For more information on optical isomers see the following link:
http://www.chemguide.co.uk/basicorg/isomerism/optical.html



It is amusing that if we attempt to synthesize such organic molecules in the laboratory, we find equal mixtures of R and L.

Why we have a preponderance of one type is nature's deepest mystery.

Is it due to a genetic accident, like the spiral shell of a snail or the fact that our hearts are on the left-hand side?

Parity-Selection Rule

Suppose |α> and |β> are parity eigenstates

$$\pi|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle$$

$$\pi|\beta\rangle = \varepsilon_\beta|\beta\rangle$$

where ε_α and ε_β are the parity eigenvalues (± 1).

We can show that $\langle\beta|\mathbf{X}|\alpha\rangle = 0$ unless $\varepsilon_\alpha = -\varepsilon_\beta$.

In other words, the parity-odd operator x connects states of opposite parity.

The proof of this follows:

$$\langle \beta|\mathbf{x}|\alpha\rangle = \langle \beta|\pi^{-1}\pi\,\mathbf{x}\,\pi^{-1}\pi|\alpha\rangle = \varepsilon_\alpha\varepsilon_\beta(-\langle \beta|\mathbf{x}|\alpha\rangle)$$

which is impossible for a finite nonzero $\langle\beta|\mathbf{X}|\alpha\rangle = 0$ unless ε_α *and* ε_β are opposite in sign, since:

$$\langle\beta|\mathbf{X}|\alpha\rangle\left(1+\varepsilon_\alpha\varepsilon_\beta\right) = 0$$

$$if\ \langle\beta|\mathbf{X}|\alpha\rangle \neq 0 \quad \Rightarrow \quad 1+\varepsilon_\alpha\varepsilon_\beta = 0$$

$$\varepsilon_\alpha\varepsilon_\beta = -1$$

ε_α *and* ε_β are 1 or -1, hence

$$\varepsilon_\alpha = -\varepsilon_\beta$$

Perhaps the reader is familiar with this argument from $\int \psi_\beta^* \mathbf{X} \psi_\alpha d\tau = 0$ if ψ_α and ψ_β have the same parity.

This selection rule, due to Wigner, is of importance in discussing radiative transitions between atomic states. As we will discuss in greater detail later, radiative transitions take place between states of opposite parity as a consequence of multipole expansion formalism. This rule was known phenomenologically from analysis of spectral lines, before the birth of quantum mechanics, as **Laporte's rule**. It was Wigner who showed that Laporte's rule is a consequence of the parity-selection rule.

If the basic Hamiltonian H is invariant under parity, nondegenerate energy eigenstates [as a corollary of (4.2.43)] cannot possess a permanent electric dipole moment:

$$\langle n|\mathbf{x}|n\rangle = 0. \tag{4.2.44}$$

This follows trivially from (4.2.43), because with the nondegenerate assumption, energy eigenstates are also parity eigenstates [see (4.2.32) and (4.2.33)]. For a degenerate state, it is perfectly all right to have an electric dipole moment. We will see an example of this when we discuss the linear Stark effect in Chapter 5.

Our considerations can be generalized: Operators that are odd under parity, like $\mathbf{p}$ or $\mathbf{S}\cdot\mathbf{x}$, have nonvanishing matrix elements only between states of opposite parity. In contrast, operators that are even under parity connect states of the same parity.

$$\mathbf{H}|\mathbf{n}\rangle = \mathbf{E_n}|\mathbf{n}\rangle \ (4.2.32)$$

$$\int \psi_\beta^* \mathbf{X} \psi_\alpha d\tau = 0 \ (4.2.43)$$

$$\pi \tfrac{1}{2}(1 \pm \pi)|n\rangle = \pm \tfrac{1}{2}(1 \pm \pi)|n\rangle \ (4.2.33)$$

Parity Nonconservation

The basic Hamiltonian responsible for the so-called weak interaction of elementary particles is not invariant under parity. In decay processes we can have final states which are superpositions of opposite parity states. Observable quantities like the angular distribution of decay products can depend on pseudoscalars such as $\langle \mathbf{S} \rangle \cdot \mathbf{p}$. It is remarkable that parity conservation was believed to be a sacred principle until 1956, when Lee and Yang speculated that parity is not conserved in weak interactions and proposed crucial experiments to test the validity of parity conservation. Subsequent experiments indeed showed that observable effects do depend on pseudoscalar quantities such as correlation between $\langle \mathbf{S} \rangle$ and $\mathbf{p}$. Because parity is not conserved in weak interactions, previously thought "pure" nuclear and atomic states are, in fact, parity mixtures. These subtle effects have also been found experimentally.