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Symmetrical Double-Well Potential and its Application

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Abstract

In this work, the Schroedinger equation with one dimensional double-well potential have been derived for obtaining the explicit solutions in classically allowed regions and for the ones in the classically forbidden region. The solutions are matched where the potential is discontinuous. The oscillatory behavior of symmetrical double-well potential is also considered from the view point of tunneling in quantum mechanics. Angular frequency of changing double-well potential states is computed in this work. The quantum tunneling in a double-well potential appears in a variety of physical cases.

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Introduction

Three scientists have been awarded the 2018 Nobel prize in physics for creating tools from beams of laser. Quantum mechanics of Laser/Maser operation is based on the simple concept of double-well potential.

The symmetrical double-well potential is one of the most important potentials in quantum mechanics. It consists of a potential with two minima separated by a barrier. It is of continuing interest in many contemporary areas of physics. In the classical limit one expects that an initial state prepared in one well is stable. Quantum tunneling allows the possibility to escape from one side to the other passing under the classically forbidden region. Canonical examples are a nitrogen atom in ammonia molecule or an electron in a double quantum dot.

One of the applications of the double-well potential involves the working of Ammonia MASER. The mechanism of oscillating wave function is a very good explanation for the inversion of ammonia molecule. In an ammonia molecule, NH_3, the three H atoms form the three corners of an equilateral triangle. The three H atoms in ammonia also form a plane. The N atom can be up or down.

Feynman used the ammonia molecule to illustrate the principle of superposition of states in quantum mechanics. In systems like ammonia there are two degenerate states; the system can reside in a superposition of both, and, most importantly, can tunnel from one to the other. Tunneling is omnipresent in quantum mechanics, and is the key ingredient in modern applications such as solid state devices: solar cells and microscopes.

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The system of particles in a double well potential can be used as quantum logic gates for ultracold atoms confined in optical lattices which are fundamental building blocks. A regular array of cold atoms in an optical lattice serves as the quantum register. There are many other applications of double-well potential, such as the atomic clock and optical pumping. In fact, four Noble Prizes in physics have been awarded to those whose exploited double-well potential of some form.

Derivation of Symmetrical Double-Well Potential

A one-dimensional symmetric rectangular double-well potential given by

$$V = \begin{cases} \infty & |x| > a + b \\ 0 & a < |x| > a + b \\ V_0 & |x| < a \end{cases}$$

is shown in figure (1). Symmetric and antisymmetric wave functions are studied in the three regions. The most general solution of the Schroedinger equation in each region is a linear combination of sine and cosine or sinh and cosh functions. Quantum mechanics requires that the piecewise wave function and its first derivative must be continuous. In this case, these conditions reduce to the following equations.

In region I, $V = 0$ for $-(a+b) < x < -a$.

In region II, $V = V_0$ for $-a < x < a$.

In region III, $V = 0$ for $a < x < (a+b)$.

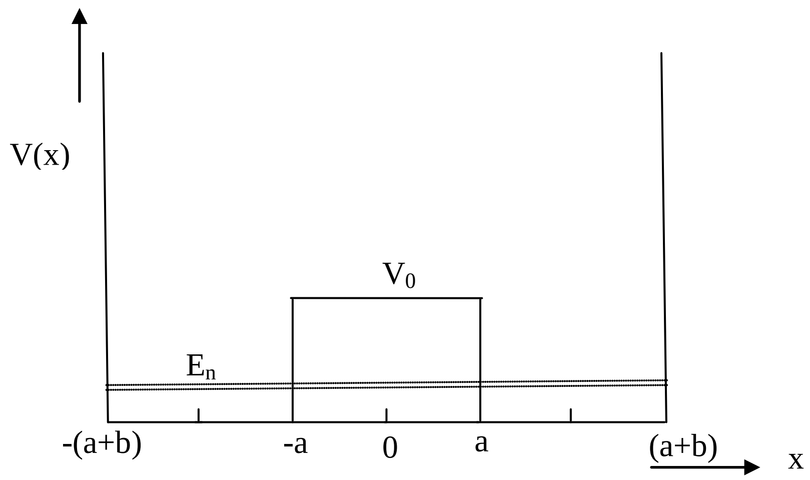

Figure 1. The symmetrical rectangular double-well potential

Approximation of the energies

The two solutions are

$$\frac{k_S}{K_S} = -\tan k_S b \ \tanh K_S a$$

$$\frac{k_A}{K_A} = -\frac{\tan k_A b}{\tanh K_A a}$$

where

$$K_{S,A} = \sqrt{\frac{2m(V_0 - E_{S,A})}{\hbar^2}}$$

$$k_{S,A} = \sqrt{\frac{2mE_{S,A}}{\hbar^2}}$$

For two cases,
$$-\frac{k_S}{K_S \tan k_S b} = \tanh K_S a \tag{1}$$

$$-\frac{k_A}{K_A \tan k_A b} = \frac{1}{\tanh K_A a} \tag{2}$$

On right side,

$$\tanh Ka = \frac{e^{Ka} - e^{-Ka}}{e^{Ka} + e^{-Ka}}$$

$$= 1 - 2e^{-2Ka}$$

$$= 1 - 2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}\left(1 + \sqrt{\frac{2ma^2V_0}{\hbar^2}}\left(\frac{E}{V_0}\right)\right)} \tag{3}$$

On the left sides, both are taken the form as

$$-\frac{k}{K \tan kb}$$

Notice that for large κa, this ratio must be close to 1.

First,
$$\frac{k}{K} = \frac{\sqrt{\frac{2mE}{\hbar^2}}}{\sqrt{\frac{2m(V_0 - E)}{\hbar^2}}}$$

$$= \sqrt{\frac{E}{V_0}}\left(1 + \frac{E}{2V_0}\right) \tag{4}$$

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Since there will be slightly more than one lobe of the sine in the right well, the wavelength for either case will be slightly greater than 2b. Then

$$\lambda \;>\; 2b$$

$$k = \frac{2\pi}{\lambda}$$

$$k < \frac{\pi}{b}$$

By setting $kb \;=\; \pi - \varepsilon$

The tangent becomes

$$\tan\, kb = \tan(\pi - \varepsilon)$$

$$= -\tan\varepsilon \qquad (5)$$

Thin terms of E/V_0 would like to be expressed, but it is not possible:

$$\varepsilon \;=\; \pi - kb$$

$$= \pi - \sqrt{\frac{2mb^2E}{\hbar^2}} \qquad (6)$$

and the small ratio depends only on b, while V_0 may be varied independently. So there really are two independent small parameters. Let

$$\sqrt{\frac{2mb^2E_0}{\hbar^2}} = \pi$$

$$\varepsilon = \pi - \sqrt{\frac{2mb^2(E_0+\Delta)}{\hbar^2}}$$

$$= -\frac{mb^2\Delta}{\pi\hbar^2} \qquad (7)$$

Put it all together:

$$-\frac{k_S}{K_S\,\tan k_S b} = \tanh K_S a$$

$$\sqrt{\frac{E}{V_0}}\left(1+\frac{E}{2V_0}\right) = \tan\varepsilon\left(1 - 2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}} - 2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\left(\frac{E}{V_0}\right)\right)$$

$$\tan\varepsilon = \sqrt{\frac{E}{V_0}}\left(1+\frac{E}{2V_0}\right)\left(1 + 2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}} + 2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\left(\frac{E}{V_0}\right)\right) \qquad (8)$$

Expanding in $\frac{E}{V}$,

$$\tan\varepsilon_S = \sqrt{\frac{E}{V_0}}\left(1+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+\frac{E}{V_0}\left(\frac{1}{2}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\right)\right) \tag{9}$$

Compare the antisymmetric case:

$$-\frac{k_A}{K_A\tan k_A b}=\frac{1}{\tanh K_A a}$$

$$\tan\varepsilon_A = \sqrt{\frac{E}{V_0}}\left(1+\frac{E}{2V_0}\right)\left(1-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\left(\frac{E}{V_0}\right)\right)$$

$$\tan\varepsilon_A = \sqrt{\frac{E}{V_0}}\left(1-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+\frac{E}{V_0}\left(\frac{1}{2}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\right)\right) \tag{10}$$

Therefore, comparing of equations (9) and (10) is needed:

$$\tan\varepsilon_S = \sqrt{\frac{E_S}{V_0}}\left(1+\frac{E_s}{2V_0}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+\frac{E_S}{V_0}\left(e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\right)\right)$$

$$\tan\varepsilon_A = \sqrt{\frac{E_A}{V_0}}\left(1+\frac{E_A}{2V_0}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}-\frac{E_A}{V_0}\left(e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\right)\right)$$

Now, for sufficiently large V_0

$$2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}} >> \frac{E_S}{V_0}\left(e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\sqrt{\frac{2ma^2V_0}{\hbar^2}}\right)$$

and the latter can be dropped. The point is, it is $2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}$ that creates the first difference between the two expressions.

Then,

$$\tan\varepsilon_S = \sqrt{\frac{E_S}{V_0}}\left(1+\frac{E_S}{2V_0}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right) \tag{11}$$

$$\tan\varepsilon_A = \sqrt{\frac{E_A}{V_0}}\left(1+\frac{E_A}{2V_0}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right) \tag{12}$$

where to lowest order, $\tan\varepsilon_S = -\dfrac{mb^2\Delta_S}{\pi\hbar^2}$ (13)

$$\tan\varepsilon_A = -\frac{mb^2\Delta_A}{\pi\hbar^2} \tag{14}$$

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It may also be written as $$E_S = E_0 + \Delta_S \tag{15}$$

$$E_A = E_0 + \Delta_A \tag{16}$$

Therefore, $$-\frac{mb^2\Delta_S}{\pi\hbar^2} = \sqrt{\frac{E_0+\Delta_S}{V_0}}\left(1+\frac{E_0+\Delta_S}{2V_0}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)$$

$$= \sqrt{\frac{E_0}{V_0}}\left(1+\frac{E_0}{2V_0}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+\frac{\Delta_S}{2E_0}\right) \tag{17}$$

$$-\frac{mb^2\Delta_A}{\pi\hbar^2} = \sqrt{\frac{E_0}{V_0}}\left(1+\frac{E_0}{2V_0}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+\frac{\Delta_A}{2E_0}\right) \tag{18}$$

Collecting Δ terms,

$$-\Delta_S\left(\frac{mb^2}{\pi\hbar^2}+\frac{1}{2E_0}\sqrt{\frac{E_0}{V_0}}\right) = \sqrt{\frac{E_0}{V_0}}\left(1+\frac{E_0}{2V_0}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right) \tag{19}$$

$$-\Delta_A\left(\frac{mb^2}{\pi\hbar^2}+\frac{1}{2E_0}\sqrt{\frac{E_0}{V_0}}\right) = \sqrt{\frac{E_0}{V_0}}\left(1+\frac{E_0}{2V_0}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right) \tag{20}$$

or, since $$E_0 = \frac{\pi^2\hbar^2}{2mb^2}$$

$$-\frac{\pi\Delta_S}{2E_0}\left(1+\frac{1}{\pi}\sqrt{\frac{E_0}{V_0}}\right) = \sqrt{\frac{E_0}{V_0}}\left(1+\frac{E_0}{2V_0}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right) \tag{21}$$

$$-\frac{\pi\Delta_A}{2E_0}\left(1+\frac{1}{\pi}\sqrt{\frac{E_0}{V_0}}\right) = \sqrt{\frac{E_0}{V_0}}\left(1+\frac{E_0}{2V_0}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right) \tag{22}$$

$$-\frac{\pi\Delta_S}{2E_0} = \sqrt{\frac{E_0}{V_0}}\left(1-\frac{1}{\pi}\sqrt{\frac{E_0}{V_0}}\right)\left(1+\frac{E_0}{2V_0}+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right) \tag{23}$$

$$-\frac{\pi\Delta_A}{2E_0} = \sqrt{\frac{E_0}{V_0}}\left(1-\frac{1}{\pi}\sqrt{\frac{E_0}{V_0}}\right)\left(1+\frac{E_0}{2V_0}-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right) \tag{24}$$

Now define $$\frac{\pi\Delta}{2E_0} = \sqrt{\frac{E_0}{V_0}}\left(1-\frac{1}{\pi}\sqrt{\frac{E_0}{V_0}}\right)\left(1+\frac{E_0}{2V_0}\right)$$

$$= \sqrt{\frac{E_0}{V_0}}\left(1-\frac{1}{\pi}\sqrt{\frac{E_0}{V_0}}+\frac{E_0}{2V_0}+.....\right)$$

$$= \sqrt{\frac{E_0}{V_0}}+..... \tag{25}$$

Then, keeping only the lowest order,

$$\Delta_S = -(\Delta+...)\left(1+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+...\right) \tag{26}$$

$$\Delta_A = -(\Delta+...)\left(1-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}+...\right) \tag{27}$$

There are small corrections to both Δ and to the exponential terms, but they are small by comparison. By taking V_0 as large as we like, those corrections as small as we like can be made. So the final energy difference is

$$E_A - E_S = (E_0+\Delta_A) - (E_0+\Delta_S)$$

$$= -\Delta\left(1-2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)+\Delta\left(1+2e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}}\right)$$

$$= \frac{8}{\pi}E_0\sqrt{\frac{E_0}{V_0}}e^{-2a\sqrt{\frac{2mV_0}{\hbar^2}}} \tag{28}$$

where E_0 is the ground state energy of the corresponding infinite square well.

Oscillatory Behavior of Symmetrical Double-Well Potential

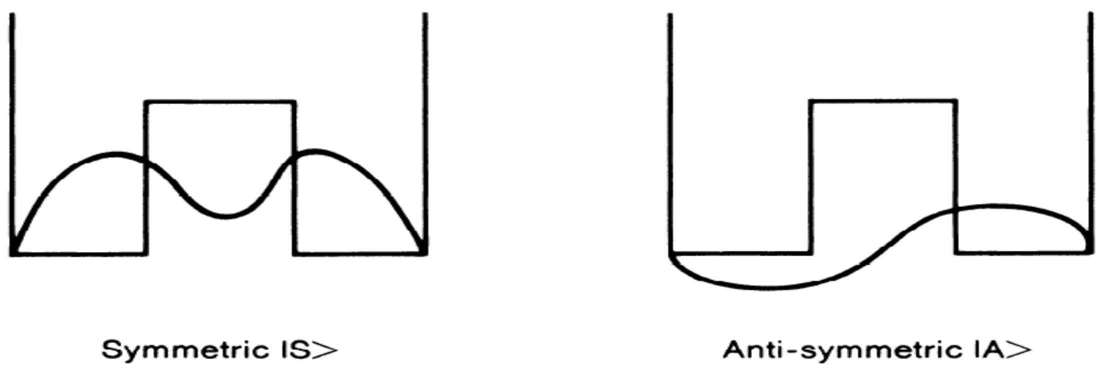

Figure 2. The symmetrical double-well potential with the two lowest lying states

The two lowest lying states in a symmetrical double-well potential is shown in figure (2). By using the explicit solutions involving sine and cosine in classically allowed regions and sinh and cosh in the classically forbidden region is explored. The solutions are matched where the potential is discontinuous; they are called the symmetrical state $|S\rangle$ and the anti-

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symmetrical state $|A\rangle$. Of course, they are simultaneous eigenkets of H and π. The derivation of symmetrical double-well potential in above section shows that

$$\mathbf{E_A > E_S}. \tag{29}$$

Figure (2) also indicates that the wave function of the antisymmetrical state has a greater curvature. The energy difference is very tiny if the middle barrier is high.

Angular Frequency of Double-Well Potential

It can be formed as
$$\left|R\right\rangle = \frac{1}{\sqrt{2}}\left(\left|S\right\rangle + \left|A\right\rangle\right) \tag{30a}$$

and
$$\left|R\right\rangle = \frac{1}{\sqrt{2}}\left(\left|S\right\rangle - \left|A\right\rangle\right) \tag{30b}$$

The wave functions of (30a) and (30b) are largely concentrated in the right-hand side and the left-hand side, respectively. They are obviously not parity eigenstates; in fact, under parity $\left|R\right\rangle$ and $\left|L\right\rangle$ are interchanged. Note that they are not parity eigenstates either. Indeed, they are classical examples of nonstationary states. To be precise, assume that the system is represented by $\left|R\right\rangle$ at t = 0. At a later time,

$$\left|R, t_0 = 0; t = 0\right\rangle = U(t, t_0)\left|R, t_0 = 0\right\rangle$$

$$U(t, t_0) = e^{-\frac{iHt}{\hbar}}$$

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

$$= \frac{1}{\sqrt{2}} e^{\frac{-iE_S t}{\hbar}}\left(\left|S\right\rangle + e^{\frac{-i(E_A - E_S)t}{\hbar}}\left|A\right\rangle\right) \tag{31}$$

Since, $\omega = \dfrac{E_A - E_S}{\hbar}$, $\dfrac{2\pi}{T} = \dfrac{E_A - E_S}{\hbar}$, $T = \dfrac{2\pi\hbar}{E_A - E_s}$

At $t = \dfrac{T}{2}$, $t = \dfrac{\pi\hbar}{E_A - E_S}$

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

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

$$= e^{\frac{-iE_S\pi}{E_A - E_S}} |L\rangle$$

$$\sim |L\rangle$$

At $t = \frac{T}{2}$, the system is found pure $|L\rangle$.

At $t = T = \frac{2\pi\hbar}{E_A - E_s}$

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

$$= \frac{1}{\sqrt{2}} e^{\frac{-iE_S 2\pi}{E_A - E_S}} \left(|S\rangle + e^{-i2\pi} |A\rangle \right)$$

$$= e^{\frac{-iE_S 2\pi}{E_A - E_S}} |R\rangle$$

$$\sim |R\rangle$$

At t = T, they are back to pure $|R\rangle$.

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

$$\omega = \frac{E_A - E_S}{\hbar} \tag{32}$$

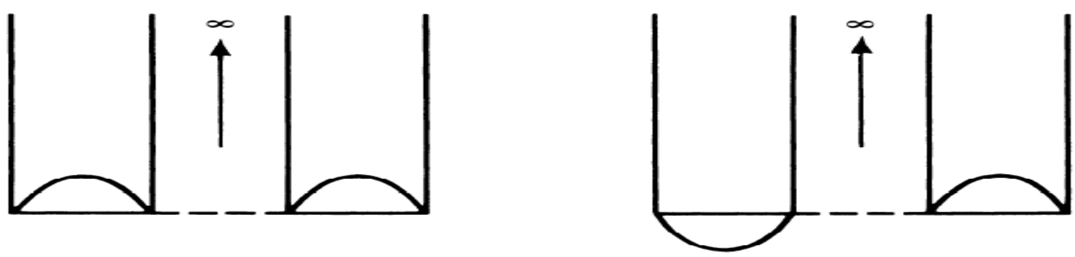

Figure 3. The symmetrical double-well potential with an infinitely high middle barrier

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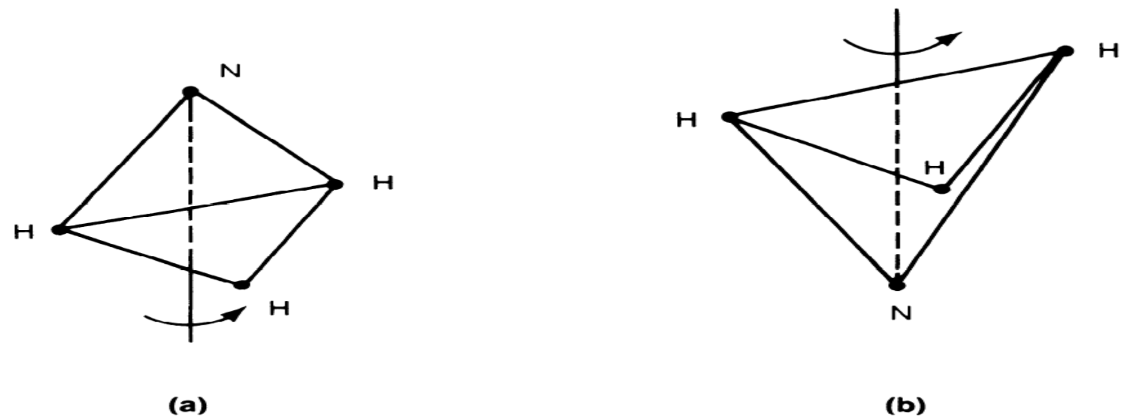

Figure 4. An ammonia molecule, NH_3

Conclusion

The oscillatory behavior can also be considered from the view point of tunneling in quantum mechanics. A particle initially confined to the right-hand side can tunnel through the classically forbidden region into the left-hand side, than back to the right-hand side, and so on. But now let the middle barrier becomes infinitely high; see figure (3). The $|S\rangle$ and $|A\rangle$ states are now degenerate, so equations of (30a) and (30b) are also energy eigenkets even though they are not parity eigenkets. Once the system is found in $\left|R\right\rangle$, it remains so forever. A ground state 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 $|S\rangle$ and $|A\rangle$.

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.

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

In an ammonia molecule, NH_3 as shown in figure (4), the three H atoms form the three corners of an equilateral triangle. The up and down positions for the N atom are analogous to ***R*** and ***L*** of the double-well potential. At a given time the nitrogen can be above the plane or below it. A nitrogen atom sets 0.04 nm above the plane of the hydrogens. The N-H distance (which makes an angle of 68º with the symmetry axis) is 0.10 nm. This generates a potential well with a double minimum, and the lowest state in each side of the well has an effective width of about 0.03 nm. It will be interested in the motion of the nitrogen atom along a direction normal to the plane of the hydrogen atoms. This direction is to define an x-axis of coordinates, with x = 0 being at the plane of the hydrogen atoms. This motion, which can be likened to the inversion of an umbrella in a windstorm, is hindered by a potential barrier that is not overcome, but rather tunneled through.

The hindered inversion motion in NH_3 can be analyzed on the basis of symmetry arguments, and this analysis leads to a better understanding of quantum tunneling, of radiative processes, of Maser/Laser operation, and of a topic that is a bit farther afield but quite important, the band theory of solids.

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