Nuclear Shell Model

(A computational approach)

Guglielmo Pasa

v. 0.1 (18 avril 2019)

Table des matières

Chapitre 1

Introduction

1.1 Liquid Drop

1.1.1 The origin

The liquid drop model of the atomic nucleus assumes that nuclear matter is a kind of liquid in which we find volume forces, surface tension forces as well as pair-force between the particles of the liquid nuclear matter.

The atomic mass is a number A in atomic units which is the number of nucleons (protons and nuetrons) into the nucleus, so it is a whole integer. The number of protons in a nucleus is Z. The number of neutron into a nucleus is N. We have then

$$A = Z + N.$$

In atomic physics, A and N have rather limited consequences, except for the stability of the nucleus. The whole of chemistry is determined by Z, since the coupling of the electrons to the nucleus is due to the electromagnetic field generated by the protons. On a second approximation, neutrons also have an importance due to their magnetic moment and their impact on the reduced mass of the system.

In nuclear physics, the electrons are neglected, since they can seldom interact with nuclear matter with regular atomic energies, except for very heavy nuclei, for which the electron are very close to the nucleus and can be captured.

One of the main assumption is that nuclear matter is incompressible, as experiments shows that nuclear density is quite constant into the nucleus and that the nuclear radius increases such that

$$A \propto R^3 \;\Leftrightarrow R \propto A^{\frac{1}{3}}$$

Surface-tension forces varies as the surface of the drop so the force is proportional to $R^2 \propto A^{\frac{2}{3}}$.

1.2 Square well

1.3 Rounded square well

1.4 Spin-orbit coupling

Spin-orbit coupling gives the Fine structure in the atomic spectra. The degeneracies in $n\ell$ levels of the H atom are then split into nj with $j = \ell + \frac{1}{2}$ and $j = \ell - \frac{1}{2}$.

This is due to the orbital motion of the electron around the nucleus which generates a magnetic field on the electron that interacts with the spin magnetic moment of the electron. The magnetic field is produced by the movement of the electron around the nucleus that can be seen, in the rest frame of the electron, as the movement of the nucleus around the electron. The movement of the nucleus which is positively charged, generates a magnetic field B at the position of the electron. If $\vec{v}$ is the speed of the electron, then

$$\vec{B} = \frac{\vec{v} \times \vec{E}}{c^2}$$

The magnetic moment of the electron on its orbit can be calculated quasi-classicaly as

$$\mu_L = -e\frac{\omega}{2\pi}\pi r^2 = -e\frac{\frac{v}{r}}{2\pi}\pi r^2 = -e\frac{pr}{2m} = -e\frac{L}{2m}$$

where $\omega = \frac{v}{r}$ is the angular speed of the electron and r the radius of its orbit. So that we can write

$$\mu = -e\frac{1}{2m}(g_L\vec{L} + g_s\vec{s})$$

where we have introduced $g_L = 1$ the orbital gyromagnetic factor and a similar contribution to the spin with $g_s = 2$. The Pauli equation or the classical limit of the Dirac equation gives for the total angular momentum $L + 2s$, that is $\frac{g_s}{g_L} = 2$.

The spin magnetic moment of the electron is

$$\vec{\mu}_s = -\frac{g_s e}{2m}\vec{s}$$

with $g_s = 2$ in the Dirac theory (the first order correction gives $g_s = 2 + \frac{\alpha}{\pi} = 2.0023$ with α the fine structure constant). Since the electric field is the derivative of the potential $\vec{E} = -\nabla V$, we can write the energy of the spin-orbit coupling as

$$\Delta E_{SO} = \frac{1}{c^2}(\vec{v} \times \vec{E}) \cdot \vec{\mu}_s$$

that is

$$\Delta E_{SO} = \frac{g_s e}{2mc^2}(\vec{v} \times \nabla V) \cdot \vec{s}$$

1.5 Nuclear Shell Model

Chapitre 2

Simple Models

2.1 Introduction

In spherical coordinates the laplacian is

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}$$

The non-relativistic Schrœdinger equation for the one-nucleon state is then

$$E\Psi(r,\theta,\phi) = \left[-\frac{\hbar^2}{2m}\Delta + U(r)\right]\Psi(r,\theta,\phi)$$

with

$$\Psi(r,\theta,\phi) = R(r)Y_{lm}(\theta,\phi)$$

where the normalized spherical harmonics are

$$Y_{lm}(\theta,\phi) = \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell+m)!}{(\ell-m)!}}P_\ell^m\big(\cos(\theta)\big)e^{im\phi}$$

and P_ℓ^m are the associated Legendre polynomials

$$P_\ell^m(x) = (-1)^m(1-x^2)^{\frac{m}{2}}\frac{d^m}{dx^m}P_\ell(x)$$

and P_ℓ is the Legendre polynomial given by the Rodrigue formula

$$P_\ell(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n$$

and is a solution of the equation

$$\left[(1-x^2)\frac{d^2}{dx^2} - 2x\frac{d}{dx} + \ell(\ell+1)\right]P_\ell = 0.$$

The spherical harmonics satisfy the orthogonality relation

$$\int_0^\pi d\theta\int_0^{2\pi} d\phi\; Y^*_{m,l}(\theta,\phi)Y_{m',l'}(\theta,\phi)\sin(\theta) = \delta_{mm'}\delta_{ll'}.$$

The radial equation is then

$$ER_\ell(r) = \left[-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} + U(r)\right]R_\ell(r)$$

Define ϵ, ν, x and y by

$$E = \frac{\hbar^2}{2mR^2}\epsilon, \qquad U(r) = \frac{\hbar^2}{2mR^2}\nu(r), \qquad x = \frac{r}{R}, \qquad R_\ell(r) = u_\ell(x)$$

we get the radial equation

$$\epsilon u_\ell(x) = \left[-\frac{1}{x^2}\frac{\partial}{\partial x}\left(x^2\frac{\partial}{\partial x}\right) + \frac{\ell(\ell+1)}{x^2} + \nu(x)\right]u_\ell(x)$$

that is

$$\left[-x^2\frac{\partial^2}{\partial x^2} - 2x\frac{\partial}{\partial x} + \ell(\ell+1) + x^2(\nu(x)-\epsilon)\right]u_\ell(x) = 0.$$

2.2 Infinite spherical square well

In the case of an infinite square well potential

$$U(r) = \begin{cases} 0 & \text{if} : r \leqslant R \\ \infty & \text{if} : r > R \end{cases}$$

This can be achieved by demanding that

$$R_\ell(r) = 0, \quad \text{for } r \geqslant R$$

or

$$u_\ell(x) = 0, \quad \text{for } x \geqslant 1.$$

The radial equation is then

$$\left[-x^2\frac{\partial^2}{\partial x^2} - 2x\frac{\partial}{\partial x} + \ell(\ell+1) - x^2\epsilon\right]u_\ell(x) = 0.$$

which can be put in the form

$$x^2u_\ell'' + 2xu_\ell' + [\epsilon x^2 - \ell(\ell+1)]u_\ell = 0$$

This is the spherical Bessel differential equation. The solutions are the spherical Bessel functions of the first kind $j_\ell(z)$ and of the second kind $y_\ell(z)$, where $z = x\sqrt{\epsilon}$.

Since the spherical Bessel functions of the second kind diverge at $z = 0$, the only acceptable solutions are the spherical Bessel functions of the first kind

$$j_\ell(z) = \sqrt{\frac{\pi}{2z}}J_{\ell+\frac{1}{2}}(z).$$

The quantization condition comes then by imposing the boundary condition (at $z = x\sqrt{\epsilon} = \sqrt{\epsilon}$ for $x = 1$)

$$j_\ell(\sqrt{\epsilon}) = 0$$

So $\sqrt{\epsilon}$ must be a zero of the spherical Bessel function of the first kind, which are the same as the zero of the Bessel function of the first kind $J_{\ell+\frac{1}{2}}$.

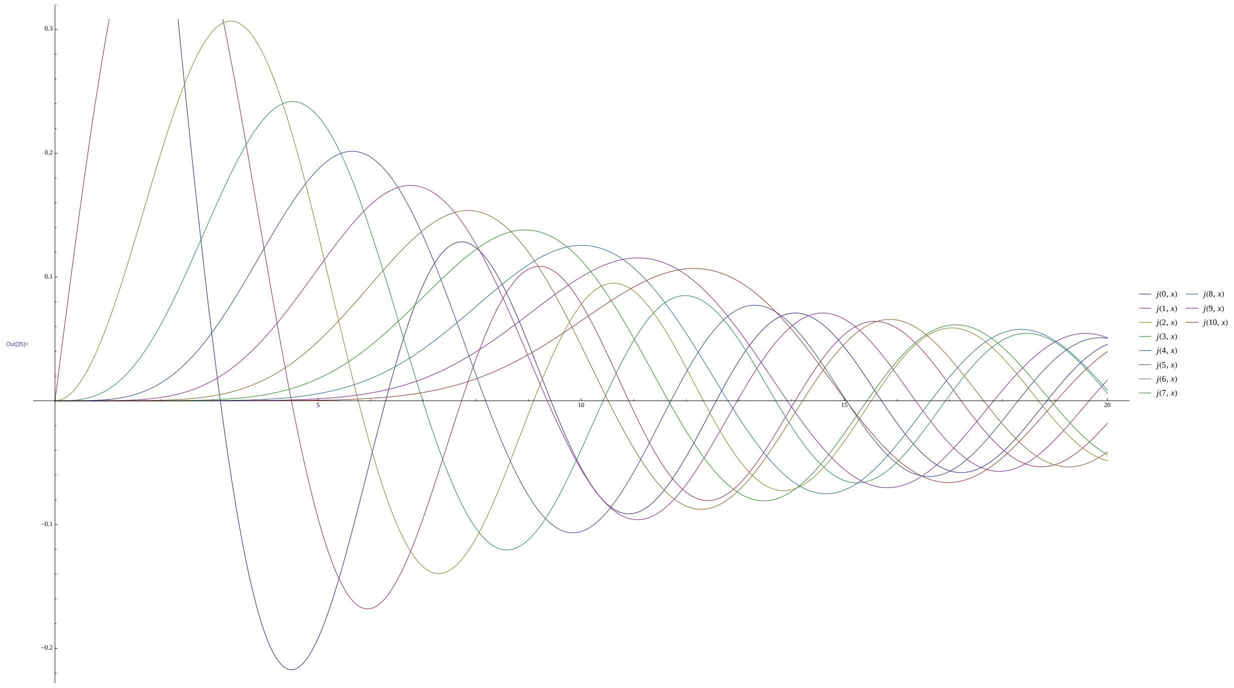

FIGURE 2.1 – Spherical Bessel functions of the first kind j_ℓ for $\ell = 0 \ldots 10$. The zeroes give the value of $\sqrt{\epsilon}$.

n	ℓ	state
1	0	$1s$
1	1	$1p$
1	2	$1d$
2	0	$2s$
1	3	$1f$
2	1	$2p$
1	4	$1g$
2	2	$2d$

n	ℓ	state
1	5	$1h$
3	0	$3s$
2	3	$2f$
1	6	$1i$
3	1	$3p$
1	7	$1k$
2	4	$2g$
3	2	$3d$

TABLE 2.1 – The first states of the infinite square well with increasing energies. The states are labeled by the angular momentum quantum number ℓ, and the order number n of the zero for that ℓ. States that are very close in energy have the same color.

2.3 Spherical harmonic oscillator

This time we take the potential

$$U(r) = \frac{1}{2} m \Omega^2 r^2$$

so that the radial equation, with $\omega^2 = \frac{m^2 R^4 \Omega^2}{\hbar^2}$, becomes

$$\epsilon u_\ell(x) = \left[-\frac{1}{x^2} \frac{\partial}{\partial x} \left(x^2 \frac{\partial}{\partial x} \right) + \frac{\ell(\ell+1)}{x^2} + \omega^2 x^2 \right] u_\ell(x)$$

By substituting $y_\ell = x u_\ell$ and rewriting the equation with y_ℓ we have

$$\begin{cases} u' &= \frac{y'}{x} - \frac{y}{x^2} \\ u'' &= \frac{y''}{x} - 2\frac{y'}{x^2} + 2\frac{y}{x^3} \end{cases}$$

so that

$$\epsilon\frac{y_\ell}{x} = \left[-\frac{2}{x}\left(\frac{y_\ell'}{x} - \frac{y_\ell}{x^2}\right) - \frac{y_\ell''}{x} + 2\frac{y_\ell'}{x^2} - \frac{2}{x^3}y_\ell + \frac{\ell(\ell+1)}{x^2}\frac{y_\ell}{x} + \omega^2 x^2\frac{y_\ell}{x}\right]$$

we obtain then the radial equation, on multiplying by x and dividing by ω and substituting $z = x\sqrt{\omega}$

$$y_\ell'' + \left(\frac{\epsilon}{\omega} - z^2 - \frac{\ell(\ell+1)}{z^2}\right) y_\ell = 0$$

where now $y_\ell = y_\ell(z)$.

This is an equation of the form

$$y'' + \left(4n + 2\alpha + 2 - x^2 + \frac{1 - 4\alpha^2}{4x^2}\right) y = 0$$

whose solution are expressed with the associated Laguerre functions $L_n^\alpha(x)$ by

$$y(x) = e^{-\frac{x^2}{2}} x^{\alpha+\frac{1}{2}} L_n^{(\alpha)}(x^2).$$

provided the following conditions are satisfied

$$\begin{cases} \dfrac{1-4\alpha^2}{4} & = -\ell(\ell+1) \\ 4n + 2\alpha + 2 & = \dfrac{\epsilon}{\omega} \end{cases} \Leftrightarrow \begin{cases} \alpha & = \ell + \frac{1}{2} \\ \epsilon & = \omega(4n + 2\ell + 3) \end{cases}$$

This means that the energy is quantized by the number

$$k = (2n + \ell)$$

as

$$\epsilon = \omega(2k + 3)$$

and the eigenfunctions take the form

$$y_{n,\ell}(z) = e^{-\frac{z^2}{2}} z^\ell L_n^{(\ell+\frac{1}{2})}(z^2).$$

n	ℓ	k	state
0	0	0	$1s$
0	1	1	$1p$
0	2	2	$1d$
1	0	2	$2s$
0	3	3	$1f$
1	1	3	$2p$
2	0	4	$3s$
1	2	4	$2d$
0	4	4	$1g$

n	ℓ	k	state
2	1	5	$3p$
1	3	5	$2f$
0	5	5	$1h$
3	0	6	$4s$
2	2	6	$3d$
1	4	6	$2g$
0	6	6	$1i$

k	states	n_{states}	$n_{\text{cumulative}}$
0	$1s$	2	2
1	$1p$	6	8
2	$2s$, $1d$	$2 + 10 = 12$	20
3	$2p$, $1f$	$6 + 14 = 20$	40
4	$3s$, $2d$, $1g$	$2 + 10 + 18 = 30$	70
5	$3p$, $2f$, $1h$	$6 + 14 + 22 = 42$	112
6	$4s$, $3d$, $2g$, $1i$	$2 + 10 + 18 + 26 = 56$	168

2.4 Spherical finite square well

We assume that nucleons are bound by an average potential that is spherically symmetric and has the shape of a square well of depth $-V$ constant for a distance $r = R$, R being the nuclear radius

$$U(r) = \begin{cases} -V & \text{if} : r \leqslant R \\ 0 & \text{if} : r > R \end{cases}$$

The value of the potential V is of order of some tens of MeV (typically $V = 40$ MeV and $R \simeq 10^{-15}$ m).

Let us look for bound states, for which

$$-V < E < 0.$$

Then, with $\epsilon = -\alpha^2$

$$\nu(r) = \begin{cases} -\nu_0^2 & \text{if } 0 \leqslant x \leqslant 1 \\ 0 & \text{if } x > 1 \end{cases} \qquad -\nu_0^2 < -\alpha^2 < 0.$$

So, for a finite square well potential, we recover a two domain equation

$$\begin{cases} \left[x^2 \frac{\partial^2}{\partial x^2} + 2x\frac{\partial}{\partial x} - \ell(\ell+1) + x^2(\nu_0^2 - \alpha^2)\right] u_\ell(x) & = 0, \quad 0 \leqslant x \leqslant 1 \\ \\ \left[x^2 \frac{\partial^2}{\partial x^2} + 2x\frac{\partial}{\partial x} - \ell(\ell+1) - \alpha^2 x^2\right] u_\ell(x) & = 0 \quad x > 1 \end{cases}$$

Which are spherical Bessel equations. If we define $\beta^2 + \alpha^2 = \nu_0^2$ [1] and

$$z = \begin{cases} x\beta & \text{if } 0 \leqslant x \leqslant 1 \\ x\alpha & \text{if } x > 1 \end{cases}$$

the equations can be written

$$\begin{cases} \left[z^2 \frac{\partial^2}{\partial z^2} + 2z\frac{\partial}{\partial z} + (z^2 - \ell(\ell+1))\right] u_\ell(z) = 0 \quad \text{inside} \\ \\ \left[z^2 \frac{\partial^2}{\partial z^2} + 2z\frac{\partial}{\partial z} - (z^2 + \ell(\ell+1))\right] u_\ell(z) = 0 \quad \text{outside} \end{cases}$$

the first equation is the *spherical Bessel equation* and the second equation is the *modified spherical Bessel equation*, the respective solutions which converge in their respective domain are the *spherical Bessel function of the first kind* and the *modified spherical Bessel function of the second kind*

$$u_\ell(z) = \begin{cases} A_\ell \, j_\ell(z) & \text{inside} \\ \\ B_\ell \, k_\ell(z) & \text{outside} \end{cases}$$

The spherical Bessel functions and modified spherical Bessel functions can be expressed with their cylindrical counterparts of half integer order

$$j_\ell(z) = \sqrt{\frac{\pi}{2z}} J_{\ell+\frac{1}{2}}(z), \qquad k_\ell(z) = \sqrt{\frac{2}{\pi z}} K_{\ell+\frac{1}{2}}(z)$$

1. The number α^2 give the depth of the energy level relative to the free state $E = 0$ (it is the ionization energy), and β^2 gives the height of the energy from the bottom of the level.

So the radial solution is of the form

$$
R_\ell(x) = \begin{cases} A_\ell \, j_\ell(x\beta) & \text{if } 0 \leqslant x \leqslant 1 \\ \\ B_\ell \, k_\ell(x\alpha) & \text{if } x > 1 \end{cases}
$$

For $x \leqslant 1$ we have excluded the spherical Bessel function of the second kind y_ℓ since it diverges at the origin and for $x > 1$ we have excluded the modified spherical Bessel function of the first kind i_ℓ since it diverges at infinity.

Continuity at $x = 1$ requires that

$$
A_\ell \, j_\ell(\beta) = B_\ell \, k_\ell(\alpha) \quad \Rightarrow \quad B_\ell = A_\ell \frac{j_\ell(\beta)}{k_\ell(\alpha)}
$$

and continuity of the first derivative requires

$$
A_\ell \, \beta \, j'_\ell(\beta) = B_\ell \, \alpha \, k'_\ell(\alpha)
$$

that is

$$
\beta \, j'_\ell(\beta) = \alpha \, k'_\ell(\alpha) \frac{j_\ell(\beta)}{k_\ell(\alpha)}
$$

or

$$
\sqrt{\nu_0^2 - \alpha^2} \, \frac{j'_\ell(\sqrt{\nu_0^2 - \alpha^2})}{j_\ell(\sqrt{\nu_0^2 - \alpha^2})} = \alpha \, \frac{k'_\ell(\alpha)}{k_\ell(\alpha)}
$$

which provides the quantization conditions for the eigenstates and eigen-energies $\epsilon_{n\ell}$.

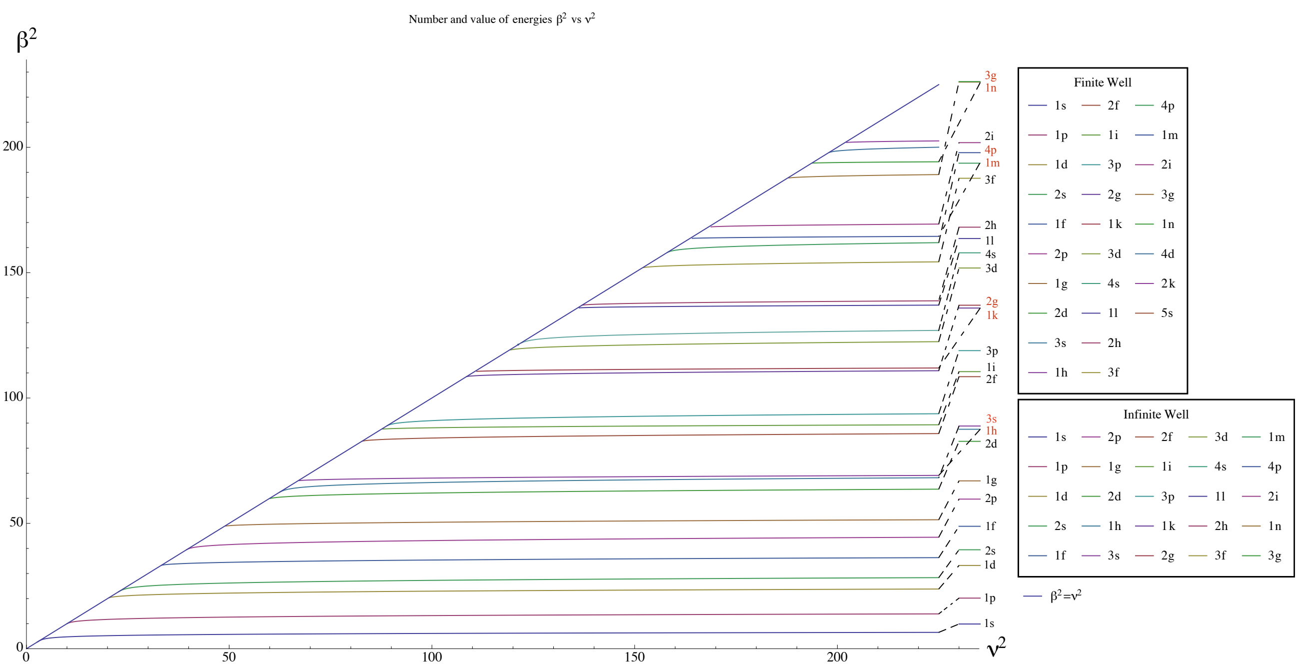

Figure 2.2 – Evolution of Energy levels with the height of the finite square well potential, for a depth up to $\nu = 15$. Notice how the levels $3s$ and $1h$ are reversed, as are the levels $2g$ and $1j$, $1l$ and $4p$, $3g$ and $1m$, compared to the infinitely deep well.

To compare the eigenenergies with the case of the infinite-height square potential, we have plotted the evolution of β^2 (the height of the eigenvalue of Energy from the bottom of the well) with the

n	ℓ	state	infinite well
1	0	$1s$	$1s$
1	1	$1p$	$1p$
1	2	$1d$	$1d$
2	0	$2s$	$2s$
1	3	$1f$	$1f$
2	1	$2p$	$2p$
1	4	$1g$	$1g$
2	2	$2d$	$2d$
3	0	$3s$	$1h$
1	5	$1h$	$3s$
2	3	$2f$	$2f$
1	6	$1i$	$1i$
3	1	$3p$	$3p$

n	ℓ	state	infinite well
1	7	$2g$	$1k$
2	4	$1k$	$2g$
3	2	$3d$	$3d$
4	0	$4s$	$4s$
1	8	$1l$	$1l$
2	5	$2h$	$2h$
3	3	$3f$	$3f$
4	1	$4p$	$1m$
1	9	$1m$	$4p$
2	6	$2i$	$2i$
1	10	$1n$	$3g$
3	4	$3g$	$1n$

TABLE 2.2 – The first states of the infinite square well with increasing energies. The states are labeled by the angular momentum quantum number ℓ, and the order number n of the zero for that ℓ. States that are very close in energy have the same color. The states $3g$ and $1m$ are very close.

depth ν^2. We see that the lowest lying levels do increase gently with ν^2 to reach the value of the limiting case of infinite depth. The labels of the states are written next to the plot.

The sequence of states is give in table 2.2

The picture 2.3 gives a more comprehensive view with $\nu_{\text{max}} = 30$.

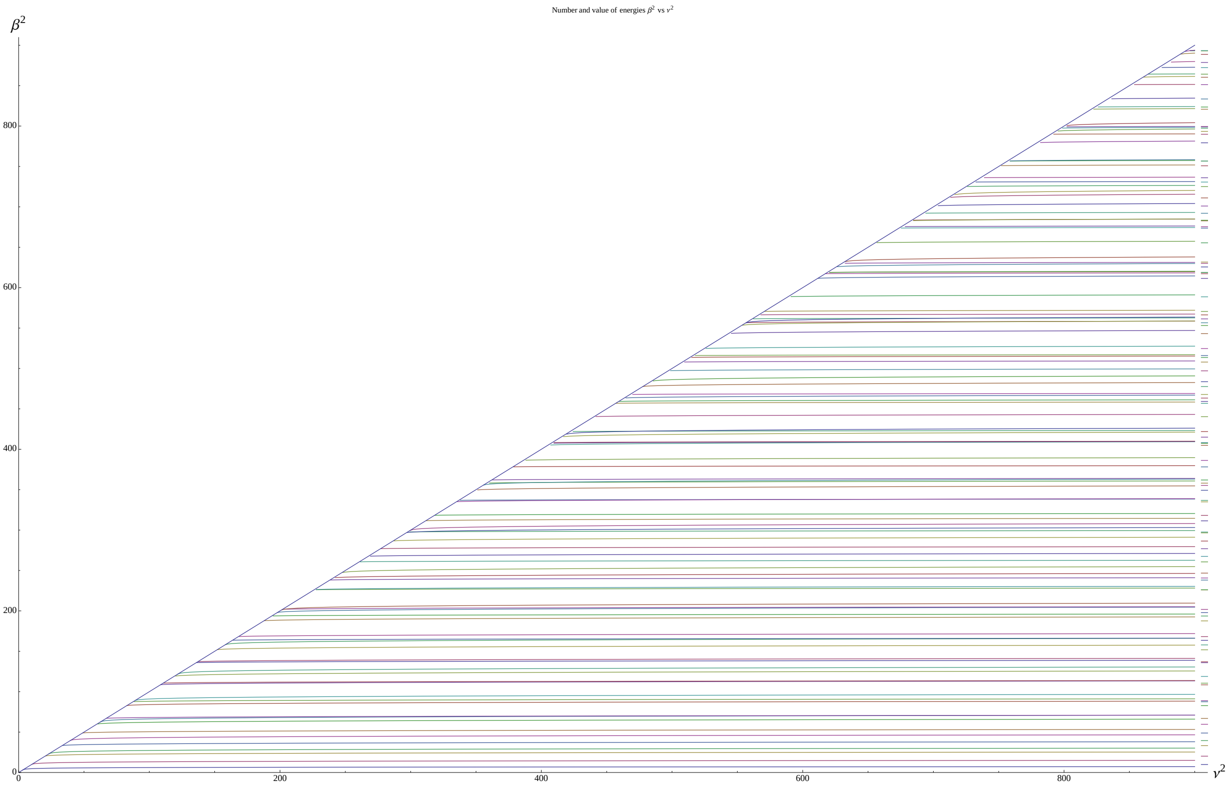

FIGURE 2.3 – Evolution of Energy levels with the height of the finite square well potential, for a depth up to $\nu = 30$.

Chapitre 3

Spin-orbit coupling

3.1 Introduction

3.2 Spin-orbit effect

Index