INTRODUCTION TO QUANTUM MECHANICS – ADVANCED EXAMPLES II

4TH LECTURE
FROM THE COURSE
QUANTUM PHYSICS OF LOW DIMENSIONAL STRUCTURES

QPLDS

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CONTENTS

THE OVER-SUBTLE ENERGY SPLITTING OF THE HYDROGEN BASIC-STATE UNDER INFLUENCE OF THE EXTERNALLY APPLIED MAGNETIC FIELD

The Hamiltonian

$$H = A\hat{\sigma}^{el}\hat{\sigma}^{p} - \mu_{el}\hat{\sigma}^{el}\vec{H}^{(mag)} - \mu_{p}\hat{\sigma}^{p}\vec{H}^{(mag)}$$

and for the magnetic field oriented along the z-direction

$$H = A\hat{\sigma}^{el}\hat{\sigma}^{p} - \mu_{el}\sigma_z^{el}H_z^{(mag)} - \mu_{p}\sigma_z^{p}H_z^{(mag)}$$

For the same base as in the previous example

$$\chi_{-1/2}(el)\chi_{-1/2}(p) \quad \chi_{-1/2}(el)\chi_{1/2}(p) \quad \chi_{1/2}(el)\chi_{-1/2}(p) \quad \chi_{1/2}(el)\chi_{1/2}(p)$$

the interactions energy matrix is

$$H_{ik} = \begin{bmatrix} A+(\mu_{el}+\mu_p)H_z^{(mag)} & 0 & 0 & 0 \\ 0 & -A+(\mu_{el}-\mu_p)H_z^{(mag)} & 2A & 0 \\ 0 & 2A & -A+(\mu_{el}-\mu_p)H_z^{(mag)} & 0 \\ 0 & 0 & 0 & A-(\mu_{el}+\mu_p)H_z^{(mag)} \end{bmatrix}$$

and from the eigen-state equation

$$\sum_k H_{ik}\alpha_k = E^{(i)}\alpha_i$$

result following eigen-values (energy levels)

triplet state

$$E^{(1)} = A - (\mu_{el} + \mu_p) H_z^{(mag)}$$

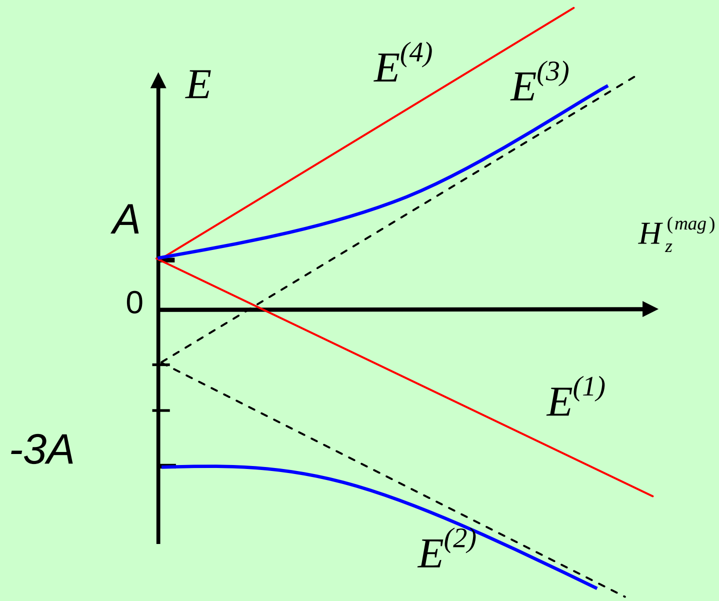
$$E^{(3)} = A(-1 + 2\sqrt{1 + (\mu_{el} - \mu_p)^2 (H_z^{(mag)})^2 / 4A^2}$$

$$E^{(4)} = A + (\mu_{el} + \mu_p) H_z^{(mag)}$$

singlet state

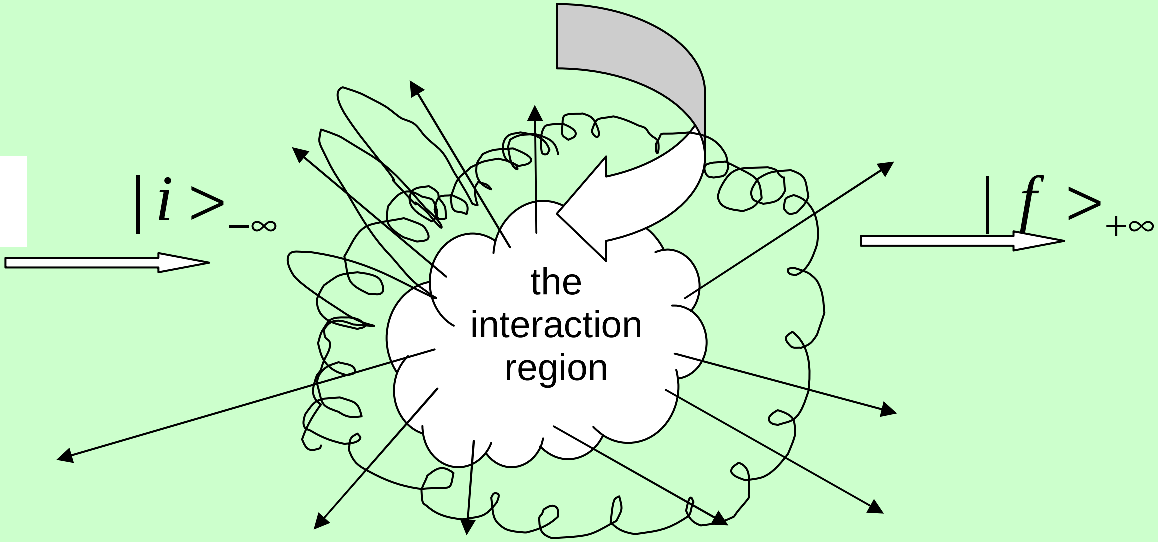
$$E^{(2)} = -A(1 + 2\sqrt{1 + (\mu_{el} - \mu_p)^2 (H_z^{(mag)})^2 / 4A^2}$$

Thus, the final energy diagram looks as follows



THE SCATTERING OPERATOR, THE TRANSITION MATRIX AND THE EVOLUTION OPERATOR (again)

The problem is don't know too much about



The solution is to use the scattering operator ***S*** (and matrix as well)
$|f>=S|i>$ (the final state is obtained from the initial state and these states are well known)

The final state can be expressed in the orthonormal base

$$\sum |m><m|f>=S|i>$$

Thus, for the arbitrary state $|n>$, after the $|i>$ and before the $|f>$, the following matrix element for the S operator can calculated

$$\boxed{<n|f> = <n|S|i>}$$

Formally, the $\underline{<n|S|i>}$ expression is named "S-matrix" or scattering matrix

and this can be used to calculate the probability of the $|n>$ state occurrence (the transition probability)

$$\boxed{P_{n(i)} = |<n|S|i>|^2 = |S_{ni}|^2 = S_{in}^{+}S_{ni}}$$

as well as the total probability of the transition from a given $|i>$ state to all possible $|n>$ states equals to

$$\sum_n P_{n(i)} = \sum_n S_{in}^{+}S_{ni} = 1$$

Another operator is associated with the *S* operator. This is the transition operator *T*:

$$\boxed{S = 1 + T}$$

Using the language of the *T* operator the transition probability equals

$$P_{n(i)} = |<n|S|i>|^2 = |<n|1+T|i>|^2 = |<n|1|i> + <n|T|i>|^2 =$$

$$= |1\underbrace{<n|i>}_{0} + <n|T|i>|^2 = |<n|T|i>|^2$$

Assuming conservation of the energy during collision $E_i = E_n = E_f = const$ the T operator can be written as

$$\boxed{T \overset{def}{=} -2\pi i\delta(E_n - E_i)\mathrm{T}}$$

and probability transition equals

$$P_{n(i)} = \frac{2\pi}{\hbar} |<n|\mathrm{T}|i>|^2 \ \delta(E_n - E_i) 2\pi\hbar\delta(E_n - E_i)$$

Next, taking advantage from the following δ -Dirac property

$$2\pi\hbar\delta(E_n - E_i) = \int_{-\infty}^{+\infty} e^{i(E_n - E_i)t/\hbar} dt$$

and assuming $E_n = E_i$ we obtain

$$P_{n(i)} = \frac{2\pi}{\hbar} |< n | \mathrm{T} | i >|^2 \ \delta(E_n - E_i) \int_{-\infty}^{+\infty} dt$$

and finally the probability of transition per unit of time equals

$$\boxed{P_{n(i)} = \frac{2\pi}{\hbar} |< n | \mathrm{T} | i >|^2 \ \delta(E_n - E_i)}$$

The formalism shown above has to be used in cases where “classical” wave-equation can not be applied due to dynamic nature <u>collisions</u>.

Some remarks about THE EVOLUTION OPERATOR used in Tomonaga picture in order to describe <u>collisions</u>

against to use Schrödinger wave-equation:

$$-\frac{\hbar}{i}\frac{\partial}{\partial t} | t >= H | t >$$

we apply Tomonaga state-vectors

$$| t >_T = e^{iH^{(0)} t/\hbar} | t >$$

and following wave-equation

$$-\frac{\hbar}{i}\frac{\partial |t>_T}{\partial t} = H_1 |t>_T$$

where we took advantage from a split of the Hamiltonian into non-interacting and interacting parts

$$H = H^{(0)} + H^{(1)}(t)\,.$$

We also introduced Tomonaga evolution operator G_T

$$|t>_T = G_0^+ |t> = G_0^+ G |t_0> = G_T |t_0>$$

which, after substitution to the wave-equation, yielded the equation of motion for this operator, namely

$$-\frac{\hbar}{i}\frac{\partial G_T}{\partial t} = H_1 G_T$$

HOWEVER

As the process of interaction can lead to quite different state AFTER the collision, the Tomonaga has to be splitted into BEFORE and AFTER time-zones

$$G_T = G_T(t, t_0)$$

$$G_+(t) = G_T(t, -\infty) \qquad G_-(t) = G_T(t, +\infty)$$

From the above result

$$|t>_T = G_+(t)\,|-\infty>_T = G_+(t)\,|i>$$

$$|t>_T = G_-(t)\,|+\infty>_T = G_-(t)\,|f>$$

with the following boundary conditions $G_+(-\infty) = G_-(+\infty) = I$

and what important

$$-\frac{\hbar}{i}\frac{\partial G_+}{\partial t} = H_1 G_+ \quad \text{and} \quad -\frac{\hbar}{i}\frac{\partial G_-}{\partial t} = H_1 G_-$$

what can be simply integrated leading to followings

$$G_+(t) = I - \frac{i}{\hbar}\int_{-\infty}^{t} H_1(t')\,G_+(t')\,dt'$$

$$G_-(t) = I + \frac{i}{\hbar}\int_{t}^{+\infty} H_1(t')\,G_-(t')\,dt'$$

THE QUAESTION IS: how the *S*-matrix formalism, which described collisions far away from the “dangerous” zone, is associated with the Tomonaga approach and the $G_+(t)$, G_- evolution operators?

THE ANSWER IS SIMPLE:

$$S = G_{+}(+\infty) = G_{T}(+\infty, -\infty), \quad S^{-1} = S^{+} = G_{-}(-\infty) = G_{T}(-\infty, +\infty)$$

as

$|+\infty>_T = S\,|-\infty>_T, \quad |-\infty>_T = S^{-1}\,|+\infty>_T$, respectively.

These topics will be continued…later, and now:

SOME FINAL REMARKS ABOUT MIXED STATES AND ABOUT A STATE OF THE SPIN POLARIZATION IN ELECTRON BEAM

But before this, some remarks about density matrix formalism

Some time ago we introduced the statistical operator (*SO*), both for the pure and mixed states, which was used in calculation of the average value of any observable

$$<O>_{ps} = <ps|O|ps> = \ldots = <k|O|ps><ps|k> = Tr[O \cdot SO_{ps}]$$

or shortly

$$\boxed{<O>_{ps} = Tr[O \cdot SO_{ps}]}$$

where the tricky statistical operator occurred

$$SO_{ps} = |ps><ps|$$

FACTS are as follows:

a) the *SO* can not be described directly using any integral-like, analytical formalism,

b) …and the same for the state vector $|\, ps >$.

BUT, as the $|\, ps >$ state can be written in, for example, the location representation, in where $< x \,|\, ps >= \Psi(x,t)$ is the wave function involved in the Schrödinger equation, THUS the *SO* can be expressed in the location representation by

$$|\, ps >< ps \,| \quad \rightarrow \quad < k \,|\, ps >< ps \,|\, l >= SO_{kl} = \rho_{kl}$$

what defines the density matrix ρ_{kl}.

The $|\, k >$ is the base vector, while the $< k \,|\, ps >$ equals c_k, the coefficient used in expression for the $|\, ps >$ as a series of base vectors. Thus

pure state

$$\rho_{kl} = c_k c_l^* = SO_{kl}$$

$$< O >= \sum_k \sum_l < k \,|\, O \,|\, l > c_k c_l^* = \sum_k \sum_l O_{kl} c_k c_l^*$$

mixed state

$$\rho_{kl}^{(mx)} = \sum_i p_i c_k^{(i)} c_l^{(i)*}$$

$$< O >_{mx} = \sum_k \sum_l \sum_i p_i < k | O | l > c_k^{(i)} c_l^{(i)*} = \sum_k \sum_l \sum_i p_i O_{kl} c_k^{(i)} c_l^{(i)*}$$

THE TWO IMPORTANT THINGS TO REMEMBER ARE

$$\boxed{< k | ps >< ps | l > = \rho_{kl}}$$

$$\boxed{Tr\rho = 1}$$

$\boxed{< O > = Tr(\rho O)}$ - independently from a pure state or a mixed state

THE TWO?!

THUS, WHICH ONE IS OBVIOUS?

Let's train and derive something more before a specific example

As the density matrix is obviously related do statistical operator, then

$$Tr[\rho F_k] = < F_k >$$

And we can repeat this $N^2 - 1$ times, if we deal with N^2 independent operators, thus, with the $(N \times N)$ ρ-matrix problem ("-1" comes from the use of $Tr\rho = 1$ condition). THIS TECHNIQUE IS CALLED THE <u>EXPANSION ORTHONORMAL METHOD</u> OF THE DENSITY MATRIX DETERMINATION

The definition: if we have any observable (*O*) with *N* linearly independent eigen-vectors (a base), then it is possible to have N^2 linearly independent orthonormal operators in a sense that:

$$\boxed{Tr[F_k F_l] = \delta_{kl}}$$

And the observable *O* (the operator) can be expressed as linear combination of these operators

$$O = \sum_{k=1}^{N^2} \alpha_k F_k \Rightarrow OF_l = \sum_{k=1}^{N^2} \alpha_k F_k F_l \Rightarrow$$

$$OF_l = \sum_{k=1}^{N^2} \alpha_k F_k F_l \; / \quad Tr \Rightarrow$$

$$Tr[OF_l] = \sum_{k=1}^{N^2} \alpha_k \underbrace{Tr[F_k F_l]}_{\delta_{kl}}$$

from where results

$$\alpha_k = Tr[O\,F_k]$$

The role as α_k has, can be played by density matrix ρ_k, namely

$$\rho = \sum_{k=1}^{N^2} \rho_k F_k$$

and $\rho_k = Tr[\rho\,F_k] = < F_k >$ (comp. with $\alpha_k = Tr[O\,F_k]$)

It is possible to recalculate the $\rho = \sum_{k=1}^{N^2} \rho_k F_k$ equation in an another base of $|n>$ vectors:

$$\rho_{mn} = \sum_{k=1}^{N^2} < F_k >< m | F_k | n > \qquad (\rho_{mn} =< m | \rho | n >)$$

The average value of an arbitrary observable *O* equals

$$< O >= Tr[\rho O] = \sum_i \sum_k \rho_i \alpha_k F_i F_k = \sum_i \sum_k \rho_i \alpha_k \delta_{ik} = \sum_i \rho_i \alpha_i$$

SIMPLIFICATIONS

a special case

$$Tr[F_k] = 0, \quad k = 1, 2, ..., N^2 - 1$$

(vanishing trace – Pauli matrixes are likely useful here? J)

including the last operator (in order to have “full set” of N^2 operators)

$$F_0 \overset{def}{=} \frac{1}{\sqrt{N}} I \qquad \rho_0 = Tr[\rho F_0] = \frac{1}{\sqrt{N}} Tr[\rho] = \frac{1}{\sqrt{N}}$$

assuming Schrödinger picture

$$\frac{\partial F_i}{\partial t} = 0$$ (observable is independent on time)

and taking derived in the first lecture equation of the statistical operator evolution

$$-\frac{\hbar}{i}\frac{\partial SO_{mx}(t)}{\partial t} = \left[H, SO_{mx}(t)\right]$$

we have (after substitution $\rho_k = Tr[\rho F_k] = < F_k >$)

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\left(\sum_k \rho_k F_k\right) = \left[H, \sum_k \rho_k F_k\right] \quad / \sum_i F_i \delta_{ik} \quad \textit{from the left side}$$

$$-\frac{\hbar}{i}\sum_i F_i \delta_{ik}\left(\sum_k F_k \frac{\partial}{\partial t}\rho_k\right) = \sum_i F_i \delta_{ik}\left[H, \sum_k \rho_k F_k\right]$$

$$\sum_i \sum_k F_i F_k \delta_{ik} \frac{\partial}{\partial t}\rho_k = \frac{i}{\hbar}\sum_i F_i \delta_{ik}\left[\sum_k \rho_k F_k, H\right]$$

$$\delta_{ik}\frac{\partial}{\partial t}\rho_k = \frac{i}{\hbar}\sum_i F_i \delta_{ik}\left[\sum_k \rho_k F_k, H\right] \qquad \left(\sum_i \sum_k F_i F_k \delta_{ik} = Tr[F_i F_k] \overset{def}{=} \delta_{ik}\right)$$

$$\frac{\partial}{\partial t}\rho_i = \frac{i}{\hbar}\sum_k \rho_k \sum_i F_i \delta_{ik}\left[F_k, H\right] \qquad ([a+b,c]=[a,c]+[b,c])$$

$$\boxed{\frac{d\rho_i}{dt} = \frac{i}{\hbar}\sum_k \rho_k Tr\{F_i[F_k, H]\}}$$

or the same more compactly:

$$\frac{d\rho_i}{dt} = \sum_k F_{ik}\rho_k \qquad F_{ik} = \frac{i}{\hbar}Tr\{H[F_i, F_k]\}$$

remembering about the boundary condition at $t = t_0 : \rho_i(t_0) = < F_i >_{t=t_0}$

<u>In summary (density matrix formalism enables):</u>

$$< O > = \sum_i \rho_i \, \alpha_i$$

$$\rho_i = < F_i >$$

$$\alpha_i = Tr[O\, F_i]$$

SPIN POLARIZATION OF ELECTRON BEAM

The phenomenon with the two possible states: $N = 2$.
Number of independent parameters: $N^2 - 1 = 3$.
So, we have 3 Pauli matrixes and we need fourth operator ~*I*.

$Tr[\sigma_k] = 0, \quad k = 1,2,3$ (comp. $Tr[F_k] = 0, \quad k = 1,2,...,N^2 - 1$)

$Tr[\sigma_i \sigma_k] = 2\delta_{ik}, \quad k = 1,2,3$ (comp. $Tr[F_k F_l] = \delta_{kl}$)

$F_0 = \frac{\sqrt{2}}{2} I, \quad F_k = \frac{\sqrt{2}}{2} \sigma_k$ (comp. $F_0 \overset{def}{=} \frac{1}{\sqrt{N}} I$ and $Tr[F_k F_l] = \delta_{kl}$)

$\rho = \rho_0 F_0 + \sum_{k=1}^{3} \rho_k F_k$ (comp. $\rho = \sum_{k=1}^{N^2} \rho_k F_k$)

$\rho_0 = \frac{\sqrt{2}}{2} < I >, \quad \rho_k = \frac{\sqrt{2}}{2} < \sigma_k >$ (comp. $\rho_k = Tr[\rho F_k] = < F_k >$)

This is spin polarization vector definition

$$\vec{P} \overset{def}{=} < \vec{\sigma} >$$

$$\rho = \frac{1}{2}(I + \sum_{k=1}^{3} P_k \sigma_k)$$

$$\rho = \frac{1}{2}(I + \vec{P} \bullet \vec{\sigma})$$

Taking advantage from

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

we obtain

$$\rho = \frac{1}{2}\begin{bmatrix} 1+P_z & P_x - iP_y \\ P_x + iP_y & 1-P_z \end{bmatrix}$$

or after diagonalization

$$\rho = \frac{1}{2}\begin{bmatrix} 1+P & 0 \\ 0 & 1-P \end{bmatrix}, \quad P = \pm|\vec{P}|$$

If $P = \pm 1$ then we have the pure state

If $-1 < P < 1$ the beam is the mixed state, especially for $P = 0$ there is no spin-polarization, and, this is a mixed state.

LET'S SIMPLIFY THE PHENOMENON BY ORIENTATION OF THE POLARIZATION ALONG ONE OF THE MAIN DIRECTION (z-axis)

$\vec{P} = [0, 0, P = P_z]$

Probability of finding the pure $|+1/2>$ state equals

$$p_{1/2} = \frac{1}{2}(1+P)$$

Probability of finding the pure $|-1/2>$ state equals

$$p_{-1/2} = \frac{1}{2}(1-P)$$

If $P=1$ then $p_{1/2}=1, \quad p_{-1/2}=0$

If $P=-1$ then $p_{1/2}=0, \quad p_{-1/2}=1$

If $P=0$: $p_{1/2} = p_{-1/2} = \frac{1}{2}$ (non-polarized beam) and the density matrix for this state equals:

$$\rho_{np} = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}$$

Look for a moment for the pure state (this can be expressed by the base vectors of the σ_z operator), which is similar, in some sense, to a mixed state

this is a state of maximum interference

$$| ps>_{pure} = \frac{\sqrt{2}}{2} |+1/2> + \frac{\sqrt{2}}{2} |-1/2>$$

and calculate statistical operator in this base $SO = | ps >< ps |$

$$< ps | = \frac{\sqrt{2}}{2} <+1/2| + \frac{\sqrt{2}}{2} <-1/2|$$

$$SO = 1/2 |1/2><1/2| + 1/2 |1/2><-1/2| + 1/2 |-1/2><1/2| + 1/2 |-1/2><-1/2|$$

and density matrix using of course $|+1/2>, |-1/2>, <+1/2|, <-1/2|$ states:

$$\rho_{\sigma_z} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$ (comp. $\rho_{mn} = \sum_{k=1}^{N^2} < F_k >< m | F_k | n >$)

And more differences between this pure and mixed states are seen in expectation values for Pauli matrixes:

for the pure state

$$<\sigma_x>_{\sigma_z} = Tr[\rho_{\sigma_z}\sigma_x] = 1$$

$$<\sigma_y>_{\sigma_z} = Tr[\rho_{\sigma_z}\sigma_0] = 0$$

$$<\sigma_z>_{\sigma_z} = Tr[\rho_{\sigma_z}\sigma_z] = 0$$

for the mixed state

$$<\sigma_x>_{np} = <\sigma_y>_{np} = <\sigma_z>_{np} = 0$$