8. Modulating quantum states: Fence

We touch in this chapter the study of interactions between quantum states as they can be found in laboratory space experiments. In early days of QM they were taken as thought experiments so that the way we see quantum states necessarily differ from that produced by the founder fathers.

Here, focus is on a Fence understood as a domain mediating quantum and classical aspects simultaneously. We describe states of affair submitted to experimental scrutiny where quantum states are physical channels relating material systems. The abstract quantum states projected in configuration space can be related to wave functions constructed directly to laboratory levels; Feynman's QM is an example described in preceding chapters.

At the Fence one may assign, in a first approximation model, all mass content included in the material system so that interaction with external quantum sources may change the I-frame state of motion leading to classical accelerations that can be experimentally identified.

On the other hand, in quantum chemistry one usually refers to a one-I-frame molecular system; yet in laboratory surrounding one can fetch material systems that would play the role of fragments with respect to a 1-system with same matter (energy) content. These latter material systems with their own I-frames would contribute with asymptotic states. Understanding the "passage" from quantum states relating *many*-I-frame systems to *one*-I-frame system is still a rarely discussed issue, if at all. This is the case encountered for example in bi-molecular reactions. Internal base states remain invariant in this setup procedure.

Thus, the determination of quantum states is an issue when handling this type of situation; the game between material-system/I-frame/quantum-states must be understood and differentiated when the descriptive level is located at the laboratory space: see a recent example provided by an opto-mechanical cavity used to study dynamic back-action caused by electromagnetic forces in such cavities (Eichenfield M. et al. Nature **450** (2009) 550-555).

E&E.8-1 Why is the Fence concept so relevant?

A fundamental limit on measurement in quantum mechanics, namely Heisenberg's uncertainty principle, is a consequence of non-commutativity of canonical operators related to so-called observables. Thus, the eigenvalues of these operators *cannot simultaneously label quantum base states* of the system; there are no eigenstates for the

product operator. A quantum state can hence be either represented in the base set of one or the other only.

In its original cast, it is asserted that the product of the imprecision of measurements of conjugate observables carried out simultaneously on a system has a lower bound given by Planck's constant. The formalization in quantum mechanics reads like a product of fluctuation operators:($\hat{A}$ - ΔA) ($\hat{B}$-ΔB) ≥ h/4π, and ΔA and ΔB are standard deviations of $\hat{A}$ and $\hat{B}$ defined by $\Delta A = (<\hat{A}^2> - <\hat{A}>^2)^{1/2}$; the symbol <…> stands for mean value with respect to a *given quantum state*, and similarly for ΔB.

For the momentum and position operators one has the relation: $\Delta p_i \, \Delta q_i \geq h/4\pi$ (Cf. Eq. 4.6.1.5). These relations are usually interpreted as the limitation of state preparations or the limitation of the ideal independent measurements on identically prepared systems. From our viewpoint it is the linear superposition with amplitudes over a number of base states which would respond for such fluctuations in a natural manner.

A problem never sufficiently emphasized is that this notion is well dependent on the quantum state of the system as we saw in Sect. 4.6. If a measuring device takes the system away its quantum domain via readings of recording, then ΔA and ΔB are certainly independent of the measuring apparatus. (For a detailed discussion and references on a more general description of statistics of measurement outcomes see Ozawa, Phys. Lett. A 320 (2004) 367).

At a Fence, interaction of a well-defined quantum state with a material system "external" to the one sustaining that quantum state can be seen as leading to a new quantum state. The associated linear superposition will embody the interactions that can be cast in terms of uncertainty-like relationships.

For the latter case one has replaced the effect of a sensing (measuring) material system by the effect produced to the scattered quantum state.

Whatever you do, one will end up producing a perturbed quantum state, which means that the input linear superposition is changed into another thereby reflecting interactions. Moreover, at a Fence the change must be made compatible with conservation of linear and angular momentum and energy for the system as a whole, this simply means to include the quantum-measuring device. Remember that for abstract Hilbert space energy is a label. It is the Fence that brings us to the Laboratory world. You may call it real world. It is in this sense that the Fence concept is most relevant. At this frontier some ambiguity is unavoidable.

Last but not least, entanglement phenomenon relating one to many I-frame systems is a fundamental quantum mechanical issue at the core of present day developments in quantum cryptography, computing and information fields (see for instance Mathews, J.C.F. et al. Nature Photonics **3** (2009) 346-350). These issues are briefly mentioned here but not really studied because most of the ananyses use particle model representations. Only the lentanglement between an electromagnetic field with a two-state model system is discussed.

8.1. Entanglement: a primer

Consider the system whose elements are a quantized EM field and a two-state material system where the I-frame origin is located at **r** w.r.t. a laboratory frame. Consider the Fock space elements:

$$\exp(i\mathbf{k}_\omega.\mathbf{r}) \mid 1_\omega\rangle = \mid \mathbf{k}; n_\omega=1\rangle \quad (8.1.1a)$$

$$\exp(i\mathbf{k}_\omega'.(\mathbf{r}'-\mathbf{r}) \mid 1_\omega\rangle = \mid \mathbf{k}'; n_\omega=1\rangle \quad (8.1.1b)$$

The last base vector indicates the source of the EM-field at the origin of the I-frame for the material system.

Let indicate by |a> and |b> the base vectors for the material system, energy eigenvalues ε_a and ε_b; $\varepsilon_b - \varepsilon_a > 0$ and the energy gap corresponds to $\hbar\omega$.

Consider the base state for a beam focus onto the I-frame system:

$$\mid \mathbf{k}; n_\omega=1\rangle \otimes |a\rangle$$

For the interacting systems introduce the entangled base state:

$$\mid n_\omega=1; a\rangle \quad (8.1.2a)$$

The labels used remind us the energy information of the initial beam only. The base state is not separable ; pictorially speaking the "photon" is dissolved in the material system; it is therefore not available in the photon field. To describe this new situation a new base state indicated as is introduced:

$$\mid n_\omega=0; b\rangle \quad (8.1.2b)$$

Again, the vacuum state is "dissolved" in the material system excited state; it is not separable into constituents. These two state are associated to one-I-frame only at variance with the incoming beam plus material system state $\mid \mathbf{k}; n_\omega=1\rangle \otimes |a\rangle$. The 1-I-frame base states are used to describe time dependent entangled quantum states, $|\Psi,t\rangle$:

$$|\Psi,t\rangle = C_a(t) \mid n_\omega=1; a\rangle + C_b(t) \mid n_\omega=0; b\rangle \quad (8.1.3)$$

The quantum state is no longer a simple product. These types of states are said to be *entangled*.

The quantum state $|\Psi,t\rangle$ in the entangled base set is a periodic function:

$$|\Psi,t\rangle = \cos(ft/2\hbar) \mid n_\omega=1; a\rangle + \sin(ft/2\hbar) \mid n_\omega=0; b\rangle \quad (8.1.4)$$

The constant f couples the two base states together. In this simple model, at t=0 the amplitudes was at $|n_\omega=1; a\rangle$. In units of $(f/2\hbar)$ when the argument takes on the

value $\pi/2$ the amplitude correspond to the vector (0 1), namely $|\, n_\omega=0; b\rangle$ shows unit amplitude. In principle, if no interactions with the surrounding show up the time evolution will continue unabated.

From the laboratory side the 1-I-frame system will appear as photon emitter. Thus a base state similar to those (8.1.1b) with origin at the material I-frame and reciprocal vectors indicated by **k**' is required:

$$\exp(i\mathbf{k}_\omega'.(\mathbf{r}'-\mathbf{r})\,|\,1_\omega\rangle\otimes|a\rangle = |\,\mathbf{k}'; n_\omega=1\rangle\otimes|a\rangle \quad (8.1.1c)$$

For the time being the model handles elastic scattering situations. Because the material system compensate any change in direction the $\mathbf{k}_\omega$' vectors corresponds to a high density of states. In this sense (8.1.1c) differs from (8.1.1b). If the size of the source is small enough the photon may be emitted in any direction.

But the source corresponds to state $|\Psi,t\rangle$, an entangled state where the photon is "dissolved" in. There is no amplitude at $|\mathbf{k}'; n_\omega=0\rangle\otimes|b\rangle$.

The bases sets are now written:

$$(|\mathbf{k}; n_\omega=1\rangle\otimes|a\rangle \quad |\,\mathbf{k}; n_\omega=0\rangle\otimes|b\rangle) \qquad \text{ingoing}$$
$$(|\mathbf{k}'; n_\omega=1\rangle\otimes|a\rangle \quad |\,\mathbf{k}'; n_\omega=0\rangle\otimes|b\rangle) \qquad \text{outgoing}$$

The origin of vectors **k** and **k**' are different. The process would go from ingoing state $[1 \quad 0]_{ing}$ through $[\cos(f\omega t)\ \cos(f\omega t)]_{ent}$ to eventually end up in a quantum state $[1 \quad 0]_{out}$.

The process below is stochastic:

$$[\cos(f\omega t) \quad \sin(f\omega t)]_{ent} \rightarrow [1 \quad 0]_{out}$$

Such is the nature of spontaneous emission. For the time being we take that as a fact. We do not have the theory to calculate something that will look like an event. The process:

$$[1 \quad 0]_{ing} \rightarrow [\cos(f\omega t) \quad \sin(f\omega t)]_{ent}$$

Because one moves from a two-I-frame system (ingoing state) to one-I-frame system (entangled state) the process above shares the look of an event. It is not sure that such process will be successful. If it happens the system become homogeneous. Yet we cannot predict when the emission event will take place. As counting processes are involved frequency measures are adequate and along this line the introduction of probabilistic talk appears adequate.

Retain basically the concept of entangled state. This one is clearly sustained by the material system.

8.2. Quantum States: Diffraction & Interference

A quantum state is mathematically well defined as a linear superposition over relevant base states. The way it is articulated to specific material systems is also a fundamental aspect to be examined via a number of cases. Interactions with real space systems change quantum states. Propagation of resulting quantum states are represented in Hilbert space.

Understanding how to prepare, modulate, change, transmit and record quantum states is the task ahead for any quantum mechanical description of processes at a Fence. Let us examine some key systems where this interplay between real space and quantum configuration spaces can be analyzed with simple (and useful) model systems.

8.2.1. Single Slit Diffraction

The situation to be discussed corresponds to a quantum state $|\phi>$ projected in a **k**-base $<\mathbf{k}|\phi>$ and expanded in the base set of eq. 4.6.1.1, namely $\{\exp(i\mathbf{k}.\mathbf{r})\}$ so that the representation in real space of this quantum state is the linear superposition (Fourier transform, Cf.sect.3.2.4& 3.2.5):

$$\phi(\mathbf{r}) = 1/\sqrt{2\pi} \int_{-\infty}^{+\infty} dk \, \exp(i\mathbf{k}.\mathbf{r}) <\mathbf{k}|\phi> \qquad (8.2.1.1)$$

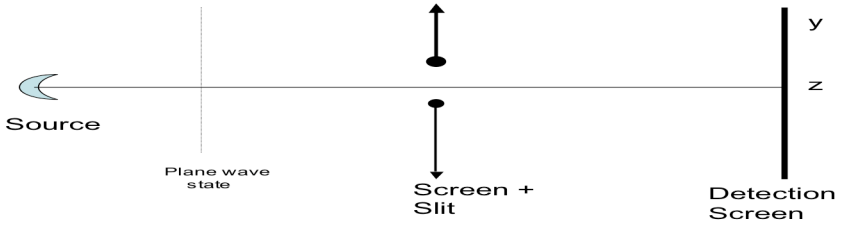
The shape of the quantum state in reciprocal space is the function $<\mathbf{k}|\phi>$ that you have constructed. Now taking those coordinates defining a screen one has to evaluate $\phi(\mathbf{r})$ on the space point belonging to the screen; this is the wave function in coordinate space only.

A plane wave state corresponds to a one-frequency quantum state $<\mathbf{k}|\phi> \delta(\mathbf{k}-\mathbf{k}_o)$ and the real space function becomes proportional to $\exp(i\mathbf{k}_o.\mathbf{r})$. In other words a propagation direction if fixed and given by the reciprocal vector $\mathbf{k}_o=(k_{1o}, k_{2o}, k_{3o})$. To get the value of the wave function at a given point in real space one simply replaces the corresponding **r**-vector. Thus, in a plane perpendicular to $\mathbf{k}_o$ this latter vector is constant so that the wave function that is characterized by such vector will be always the same. This is the main feature identifying such state.

Let us interpose a plane perpendicular to $\mathbf{k}_o=(0,0,k_o)$ having a slit as indicated in the Scheme below.

The quantum state $\phi(\mathbf{r})$, given as a plane wave, would interact with the screen including a slit. The slit is an object in real space while in quantum mechanics

focus is on the interaction with the incoming quantum state. The interaction is model by an interaction operator, $V(\mathbf{R}_i)=V(\mathbf{r})$ as we saw in Feynman's approach. The real space source of material system is assumed to produce one-I-frame system at a time; the kinetic energy operator looks like $\hat{K}(r) \rightarrow -(\hbar^2/2M_i)\ \nabla_{\mathbf{r}}^2$. The material system is hence given by the Hamiltonian of eq.(.1.7). Thus all elements required to calculate relevant quantum states are at hand.



The key is to understand that the potential standing for the hole scatters (interacts with) the incoming state yielding a *new linear superposition*. The interest focuses on detecting this new quantum state. The amplitudes in the new linear superposition, say $\Psi(\mathbf{r})$ reflects the detailed interactions. We have to obtain the base set able to describe the scattering states. To get at the core of the problem assume we have calculated such function in an exact manner; we have the set of non-zero amplitudes in the scattering base set. What is the result one ought to expect? The result expressed in intensity regime is a diffraction pattern. A whole pattern of diffraction related to the scattering of a plane wave state; a distribution of complex numbers. That's it! What about the experiment set up at the laboratory?

At a Fence one has to consider the nature of the detection device. This latter is not included among the states obtainable as solutions of eq.(8.1.7) with the potential modeling the slit. We know that the virtual pattern should elicit a diffraction pattern. Moreover, the system prepared at the source must be detectable beyond the screen+slit. This put specific requirements to the slit size, which is no problem since we are in real space conditions. For instance, preparing beams of fullerenes (C_{60}) you better adjust the slit size so that one can detect this material system at the right hand side the diffracting screen. Material system and quantum state you cannot get one without the other!

A common detecting device registers *events* (clicks) at the surface of a specially prepared screen. These events can be collected one-by-one if the intensity from the source is controlled to get that result.

Suddenly a question pops up from a student in the audience:

Student: Can you tell us where and when a particular event would take place? An event, is it not the smashing of the material system on the screen?
Instructor: You are asking about the material system that supports the quantum state! So far focus is on quantum states. The material system certainly sustains the quantum situations but it is not described as a quantum object. Not at all!
Student: It is obvious that the material system interacts with the slit to get dispersed and finally smashes to the screen.
Instructor: Note that you are implicitly following a classical description via a trajectory the material system itself would be following. If the beam were monochromatic the interaction would be effective when the incoming system touch the slit border within a Δy variation and as the material system impinges the elements of the set will be dispersed in directions not correlated to each other…

The preceding interventions lead us to the question: what can be said on the quantum state interaction with the slit and what type of result one can expect?

Well, there are two issues here. One is the exact manner you handle the problem of solving Schrödinger eq.(8.1.7) with appropriate boundary conditions. The other point concerns the relative intensity of the material system being let through. And here comes in the unavoidable "picture" being smuggled from the dominant view gotten from our training years, namely, a particle view.

First note that at any point on the slit the incoming quantum state is the same everywhere; this is a matter of fact. Interaction at points located at equivalent positions with respect to the center will produce scattered amplitudes that can produce interference with the non-scattered component when superposed on a screen sufficiently distant from the slit.

Let us "copy" the slit shape onto the detecting surface to help discussions. A constructive interference is expected at position corresponding at the center of that virtual slit due to the superposition principle. Then, as one moves away that center, e.g. along the y-direction, intensity decreases to get at a minimum; destructive effects will be followed by another constructive interference; the amplitude being a decreasing function as one moves away the center. The picture would extend beyond the classic border of the slit.

The description quoted above comes out as a result of numeric computing with for example a Gaussian slit model. Because quantum mechanics concern *all possible* situations a material system may show, the picture just described portray all one can expect to obtain in one theoretic stroke; and this is very difficult to swallow if we are thinking in terms of trajectories, in terms of individuals.

It is interesting to remind that a diffraction where radiation impinging on the pinhole (slit in our case) is redirected in a well-defined pattern as described above. This is then a typical diffraction pattern.

Superb! There is no problem then, exclaims one of the students.
Instructor: Hold on! Your question about the material system is not to be forgotten…

Look, smashing I-frame systems one-by-one onto the detection screen produces a diffraction picture cumulatively. This is an experimental result. Can we understand this situation at the Fence?

Planck discovered that energy exchanges in lumps (Quanta) between the EM field and matter.

In general, at the Fence, energy is locally exchanged in lumps. But quantum mechanics does not describe the particles as such. It handles quantum states sustained by them: Here lies a Gordian knot.

Because the event is not included in the QM description the experimental situation contains two incommensurable elements. One is the pattern obtained from the quantum state. The other is the spot detected, namely a local event. But it is only one event versus the whole pattern derived from the wave function.

Try to gauge the difference: The pattern obtains from pure quantum mechanical elements while the event is the expression of Planck law to the extent that energy is exchanged in quanta and occurs locally. The latter is a characteristic of Fence phenomena; the former is pure Quantum Mechanics. Puzzling, is it not?

Obviously, one event is not sufficient to reconstruct the response to a quantum state. The event is collected at the detection screen and is created in such a way as to stand for the response from a local interaction. By producing a set of copies generated under identical conditions (Gibbs-ensemble) of I-frame systems one would expect under ideal conditions to reconstruct a diffraction pattern. And it does!

From the above reconstruction one cannot conclude that quantum mechanics is statistical in nature. The statistics has to do with the events. But these latter *not only* depend upon the quantum state *but also* on the material used to produce the event. These later depend upon the interactions between two systems! It elicits energy exchanges in lumps at a location. It reflects interactions in real space involving energy conservation rules and momentum conservation laws.

E&E-8.1-2. Propagating a quantum state

Let us take eq.(8.1.2) to discuss the diffraction experiment. There are many elements that must be carefully isolated. The system is prepared in the state $\Psi_o(R_i',t_o)$ that cannot change in time because it is a datum of the problem; the I-frame will move towards the screen and the quantum state propagated by $G_o(\mathbf{R},\mathbf{R}_i(t_o), t')$ until interaction with the screen takes place at t'. The quantum state produced by the generator $G(\mathbf{R},\mathbf{R}_i(t'), t)$ where

(t') is the time the slit starts scattering and the potential acts. The presentation is somewhat hasty. Observe that each time we signal a source then "propagation" is complete. This means that the initial plane wave state impinges as such and continues later on as such; the slit "starts" shinning at t' and does it as outgoing base states with specific amplitudes. Thus there are: 1) free propagation; 2) scattering quantum state from the slit. The total state at the detector is a linear superposition of these two terms. Interferences originate in this way.

8.2.2. Double-slit experiments

We have now two slits at a given distance on a screen. The source producing the quantum state is the same as in the preceding case and it is located at the antipodes of the detecting device. For the sake of discussion, the slits are assumed to be identical.

The first element to be noticed is that the quantum state $\langle \mathbf{k}|\phi\rangle$ impinging at both slits is identical to the extent it is characterized by **k**-vector. This is the key to understand what it might happen with the quantum state after interaction. As a first level of description each slit generate a quantum base state system given by $|\Psi\rangle_1$ and $|\Psi\rangle_2$ for which the origin of their sources are shifted at the center of each slit (pin-hole) but otherwise identical. The quantum state then takes on a linear superposition form:

$$|\Psi\rangle = C_1 |\Psi\rangle_1 + C_2 |\Psi\rangle_2 \qquad (8.2.2.1)$$

The labels identify the slits in their capacity of being sources. We are interested in determining the quantum state at a detecting surface so that we project over space configuration: $\langle \mathbf{r}|\Psi\rangle$ and calculate it with an external potential representing both slits included in eq.(8.1.7).

In the present context, the idea of I-frames is handy. For one now follow the quantum states $\langle \mathbf{r}|\Psi\rangle_1$ and $\langle \mathbf{r}|\Psi\rangle_2$ *as if* they were "rays" impinging at a given point of the detection-screen (D-S). We notice that the path length may differ, the choice of the point located at mid-distance from the slit transported to the D-S the path length are equal so that the phases will re-enforce: i.e. constructive interference.

What is that can be expected of the quantum state? Now, at the D-S put the origin in between the slits so that by constructive interference maximum amplitude is found. Now, moving away along the y-axis the amplitude starts diminishing until getting at a minimum. And up again; the pattern repeats for positive and negative y-directions. The result is far from being a simple sum of independent slit amplitudes. The phases here play a central role.

Once we have computed the quantum state at the surface of D-S one gets a virtual-pattern of interference; this means that at zones where no-click is detected the amplitude of the quantum state is zero, relative intensities would show up for non-zero amplitudes. And as for the preceding case, the quantum mechanical result yields in one stroke all possibilities once Axiom 4 is used to make a picture in an intensity measurement.

Student: Would you be so kind to tell me which hole the particle went through? In all what I have read there is a lot of talk about the paths and from the diffraction case the material system must go through in order to get something at the detecting surface.
Instructor: You are right concerning the fundamental role played by particle's paths in current literature. But, instead of giving "an answer" let me tell you more about experiments and the way we understand them.

It goes without saying that the material system went somehow through otherwise we would have nothing to click with, but the way it evolves in real space is not relevant to quantum behavior. But let us examine this issue a little further.

First, why do we speak of virtual-pattern of interference? If we lived in a world where the calculated pattern could be surface imprinted on one stroke then quantum mechanics would have given you that holistic answer. And for what do we know it would have been the right one. To this type of sensing we will call it a *faithful experiment*. We cannot get it in one stroke but with may be able to approach it as limit.

But we do not live in such a world. Planck discovery in the first place and many other later on clearly indicate that *exchange of energy* between systems occur locally and in energy lumps, even if these might be small. So, what the experiments can tell us?

The interference pattern emerges after a one-by-one interaction event at the screen. Let us examine this stepwise characteristic.

Consider the first spot. It is somewhere on the screen. What is this spot telling us? Answ: at that point a quantum interaction with exchange of energy took place. So the amplitude of our calculated quantum state must be different from zero there and the spot would signal that mapping. The important point for us is that no energy exchange, no spot, will show up if the amplitude were zero. It is then a first clue as to the shape the quantum state will elicit.

What happens with a second spot? Can we predict the precise point where it will be seen after the first one? To answer the first query we repeat the preceding analysis. The spot tells us that at that position the amplitude of the quantum state is different from zero. To the second query the answer is simple: we cannot predict the location of the second spot (even knowing the first). But note that

there must be a relationship because the initial quantum state is the same at both slits and these latter generate identical interactions.

We can keep adding spots, the pattern emerging will be the one associated to the quantum state at the screen.

Student: Sir, I do not understand why you cannot predict the position of one spot but you can predict the pattern of them all!
Instructor: I urge you to think about this conundrum and come up with one answer; not the answer but try to get one by yourself.
Student: Well, if we knew at least which hole the particle went through one may be able to predict the events, perhaps.

Let us see if we can do something for you now.

Whenever one writes down the equation for a quantum state the hypohesis is that such a state is sustained by a material system. It is the presence of that system which matters not its real space location. The quantum state impinging at the holes is exactly the same. Operators $\hat{V}_1$ and $\hat{V}_2$ that scatter the incoming quantum state in the same manner represent the screen and holes; only the origins are shifted. Now, assume that for whatever reasons the material system could not make it through in a systematic manner. Then, there is no forward scattered quantum state. The reason is simple to understand: there is no material support for the quantum states.

It is sufficient that the material system may go through the holes in whatever way for the forward scattered state will find its support. This is the nature of quantum physics. Classical physics requires a detailed description of trajectories and therefore the material system would make it through in a definite manner.

It is then crystal clear that one cannot impose classical physics constrints to a pure quantum mechanical phenomenon. One has to get used to this situation.

8.2.3. Event-counting and recording: Pattern reconstruction

To handle this problem we have to incorporate a new quantum layer. A two state base set $|1\rangle$ and $|0\rangle$ such that the linear superposition $D_1|1\rangle + D_0|0\rangle$ can be interpreted as follows. If the particle did not pass through the slit then $D_1=0$ and $D_0=1$; or the other way around: $D_1=1$ and $D_0=0$ a quantum of energy (I-frame carrying it) went through the slit. These are limiting situations that do not belong to Hilbert space we started with but would help us discussing some of the issues raised by our student. Now, let us construct the quantum state after interaction of the impinging quantum state with the two slits:

$$|\Psi> = C_1 |\Psi>_1 (D_{11}|1> + D_{10}|0>) + C_2 |\Psi>_2(D_{21}|1> + D_{20}|0>) \quad (8.2.2.2)$$

The quantum state (in real space now!) would discriminate any case we can think of. The term $C_1 |\Psi>_1 (D_{11}|1> + D_{10}|0>)$ concerns the quantum state originated at slit-1 including the actual I-frame state.

Thus, if $D_{11} =1$ obviously $D_{10} = D_{21} = D_{20} =0$. This results because you told me the particle went through slit (hole)-1. Then, $|\Psi> = C_1 |\Psi>_1 (D_{11}|1> = C_1 |\Psi>_1 |1>$; the amplitude C_1 is different from zero thereby making it possible for the system to exchange energy at the screen if there is a "receptor" there. You see by yourself that there is no second amplitude to interfere! Forcing the I-frame system to go though slit-1 wipe out interference. What you will get is a diffraction pattern from slit-1.

Let us analyze this by rearranging the equation above:

$$|\Psi> = \{C_1 D_{11} |\Psi>_1 + C_2 D_{21}|\Psi>_2\} |1> + \{ D_{10} C_1|\Psi>_1+ D_{20} C_2 |\Psi>_2 \}|0> \quad (8.2.3.3)$$

This quantum state can be described by using the base set $\{|1>,|0>\}$ so that if the amplitude at
$|1>$ is different from zero and the quantum state interacts with the detector screen then we have the I-frame-state ("particle") just there and a quantized energy exchange may take place.

If the amplitude at $|0>$ is different from zero the "particle"-state may receive energy from the screen but it cannot transfer energy.

Therefore, the answer to the condition put at the beginning is that only a diffraction pattern would come out slit-1.

Let us see the case $D_{11} =1$ all other amplitudes zero one gets $C_1 D_{11} |\Psi>_1$ and of course nothing new shows up besides diffraction effects.

$D_{11} = D_{10} = D_{21} = D_{20} = 1/\sqrt{2}$? Then we get the quantum state:

$$|\Psi> = 1/\sqrt{2}\{ C_1 |\Psi>_1 + C_2 |\Psi>_2\} |1> + 1/\sqrt{2} \{ C_1 |\Psi>_1+ C_2 |\Psi>_2 \}|0> \quad (8.2.3.4)$$

The possibility for an interference pattern is inscribed along both (detectors) *base states*. For the "normal" case we look at the amplitude of $|1>$; in this case destructive interference will prevent energy exchange. And *wherever the material system impinges it would carry the full interference information*. There is no collapse.

The eq.(8.2.3.3) would allow you to simulate a number of situations concerning the slits interacting with the impinging quantum state. In particular one gets an answer to the question of yours.

You can see that at this level of quantum mechanics, the particle itself is no matter of concern. For sure it has to go through! That's all.

Is it? The answer is no. So let us dig further and try to define a faithful experiment to get the pattern predicted by quantum mechanics.

A faithful experiment is the aggregate (union) of faithful events. These latter must coincide with a non-zero value of the amplitude at the space position where this event is recorded.

There are unfaithful events as well. They may be due to defaults on the D-S; insufficient granularity; too much noise, not enough energy available, etc. There can also be noise at the source and/or at the slits. The events produced under such conditions are named unfaithful events.

Let N be the number of events recorded after a given time lapse, this number can be decomposed as the sum $N_f + N_u$ of faithful and unfaithful events. A faithful experiment implies the inequality $N_f >> N_u$. Thus, for this type of experiment as N increases to a large enough value so that $N_f >> N_u$ is fulfilled one should get the quantum state pattern in the recording. An ideal faithful experiment, $N = N_f$ and on the screen you have the pattern determined by the quantum state there.

Energy exchange between the quantum state and the screen states forces a time dependent model:

$$|\Psi,t\rangle = 1/\sqrt{2}\{ C_1 |\Psi\rangle_1 + C_2 |\Psi\rangle_2\} C^1(t) |1\rangle + 1/\sqrt{2} \{ C_1 |\Psi\rangle_1 + C_2 |\Psi\rangle_2 \} C^0(t)|0\rangle \quad (8.2.3.5)$$

Normalization conditions $C^1(t)$ and $C^0(t)$ makes that at a given time $C^1(t')=1$ and $C^0(t')=0$ so that in a neighborhood of this particular time the system may act as a source of energy while no response from base state $|0\rangle$ can be expected. Of course in the next period one may have $C^1(t'')=0$ and $C^0(t'')=1$ and our quantum state might pick up one quantum of energy. The screen can be prepared so that this event wouldn't happen if one takes such a decision.

You note that eq. (8.2.3.5) is a simple product, which means that geometric and dynamic factors are separated:

$$|\Psi,t\rangle = \{C_1|\Psi\rangle_1 + C_2 |\Psi\rangle_2\} \{C^1(t) |1\rangle + C^0(t)|0\rangle\} \quad (8.2.3.5')$$

Therefore, the pattern of energy transfer is always modulated by the quantum state one is trying to experimentally get its pattern. This equation is fundamental. The first factor has to do with Hilbert space representation. The second one relates to Fence phenomena.

8.3. Mirrors and Beam Splitters

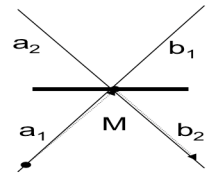
Mirrors (M) and beam-splitters (BS) are material devices at a Fence that are able to change or modulate quantum states in particular of EM (light) fields by specific interaction with. Below a scheme defines some of the basic elements to be first used in a Hilbert space representation; namely, it concerns the first factor of eq. (8.2.3.5').

The base set ($|b_1\rangle$ $|b_2\rangle$) describes outgoing states originated at cross point (vertex) and relates to the input base set ($|a_1\rangle$ $|a_2\rangle$) in manners that are characteristic for the particular device. The models assume no losses at the vertices.

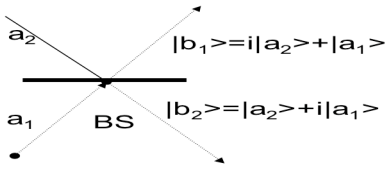
8.3.1. Mirrors

The mirror operator M can be seen as transforming base states for example: $|a_1\rangle M \rightarrow i|a_2\rangle = |b_2\rangle$; analogously, when applied along the direction $|a_2\rangle$ it will change $|a_2\rangle M$ into $i|a_1\rangle = |b_1\rangle$.

As a model for these base sets one can take the photon field state containing elements: $|0\rangle_1|0\rangle_2$, $|1\rangle_1|0\rangle_2$, $|0\rangle_1|1\rangle_2$ and $|1\rangle_1|1\rangle_2$. These base states correspond to vacuum in both channels ($|0\rangle_1|0\rangle_2$); a 1-photon in channel-1, vacuum in the other ($|1\rangle_1|0\rangle_2$); vacuum in channel-1 and 1-photon in channel-2 ($|0\rangle_1|1\rangle_2$) and finally two-photons one for each channel ($|1\rangle_1|1\rangle_2$). For the time being retain the one-photon states so that we can assign: $|a_1\rangle \rightarrow |1\rangle_1|0\rangle_2$, $|a_2\rangle \rightarrow |0\rangle_1|1\rangle_2$.



$(a_1\ a_2)M = (b_1\ b_2)$



$(a_1\ a_2)BS = (b_1\ b_2)$

With this assignment the mirror can be seen as producing a change on the base set:

$$(|a_1\rangle\ |a_2\rangle)M1 = (|1\rangle_1|0\rangle_2\ \ |0\rangle_1|1\rangle_2)M1 =$$

$$(i|0\rangle_1|1\rangle_2 \quad i|1\rangle_1|0\rangle_2)$$

If we take the separate base elements the mirror permutes $|a_1\rangle$ into $i|a_2\rangle$ or if we look at the other component the effect is analogous: $M|a_2\rangle$ into $i|a_1\rangle$.

Thus, from the scheme $|b_1\rangle$ and $|b_2\rangle$ are now rooted at the vertex acting as a source point, each one is effected by a phase indicating position of the source (vertex) and the reciprocal indicating direction: $|b_1\rangle \rightarrow i|a_1\rangle$ and $|b_2\rangle \rightarrow i|a_2\rangle$. The choice made for the present model can be changed producing new models.

In terms of quantum states one has to be careful and express them with an invariant base set. This can be done if we leave beams directions that are real space information implicit and only internal states included. In this case, the incoming state is the linear superposition

$$(|a_1\rangle \ |a_2\rangle)[1 \ \ 0] = 1|a_1\rangle + 0|a_2\rangle$$

The reflected beam is obtained as $(|b_1\rangle \ |b_2\rangle)[0 \ \ 1]$. To measure the change one expresses the result for example in the initial internal base as follows:

$$(|b_1\rangle \ |b_2\rangle) = (|1\rangle_1|0\rangle_2 \quad i|0\rangle_1|1\rangle_2) = (|a_1\rangle \ i|a_2\rangle)$$

The final state reads now:

$$(|a_1\rangle \ i|a_2\rangle)[0 \ \ 1] = (|a_1\rangle \ \ |a_2\rangle)[0 \ \ i]$$

The beam originated at the vertex has one component equal to $i|0\rangle_1|1\rangle_2$ and zero amplitude in the initial state $|1\rangle_1|0\rangle_2$. Thus, using the same base set to gauge the change introduced by the mirror the change is as follows:

$$[1 \quad 0] \rightarrow [0 \quad i]$$

or in terms of beams: $|1\rangle_1|0\rangle_2 \rightarrow \exp(i\pi/2)\ |0\rangle_1|1\rangle_2$.

With the photon field base set one can discuss elementary detection situations. Here intervenes elements that do not belong to the model Hilbert space; now one is handling a Fence situation.

By putting a detector along b_2-axis one integrates over the base function of the idle beam $\langle 0|0\rangle_1$ and the quantum state at the detector looks like $i|1\rangle_2$ so that a recording in intensity would produce $|i|^2$ at the point on the detector where the transition $|1\rangle_2 \rightarrow |0\rangle_2$ is matched by a transition involving one energy quantum so the detector itself may show a click or spot.

Note that in laboratory life, the detector may miss some physical transitions; and the mirror can show imperfections also. These fluctuations are assigned to noise and are not included in the present model. In the language developed in

previous sections, the former correspond to unfaithful events. The theoretical discussion assumes faithful events only.

Consider the case where the experimenter decides to send 1-photon beam along direction a_2 consequently the quantum state is given now by [0 1]. The beam approaches the mirror from the opposite direction compared to the previous case. The change of base set looks then as:

$$(|a_1\rangle \ |a_2\rangle)M2 = (|1\rangle_1|0\rangle_2 \ |0\rangle_1|1\rangle_2)M2 =$$
$$(\exp(+i\alpha)|1\rangle_1|0\rangle_2 \ |0\rangle_1|1\rangle_2) = (|b_1\rangle \ |b_2\rangle)$$

It is not difficult to see that the state after the mirror M2 ought to be [i 0].

The particular model handled above corresponds to $\alpha = \pi/2$. The matrix representing the effect of a mirror is given as:

$$M = \begin{pmatrix} 0 & \exp(i\alpha) \\ \exp(i\alpha) & 0 \end{pmatrix}$$

The labels must consistently be respected according to the scheme above. The correspondence is simply given by $|b_2\rangle = i|a_1\rangle$ and $|b_1\rangle = i|a_2\rangle$.

E&E-8.3.1 Give a matrix representation to the mirror effect

Consider the input quantum state $(|a_1\rangle \ |a_2\rangle)[\ \alpha_1 \ \alpha_2]$ the effect of M2 is given by:

$(|a_1\rangle \ |a_2\rangle)[\ \alpha_1 \ \alpha_2]\ M = (|a_1\rangle \ |a_2\rangle)M\ [\ \alpha_1 \ \alpha_2] = (|a_1\rangle \ |a_2\rangle)\ [\ \alpha_2\exp(\alpha) \ \alpha_1 \exp(\alpha)]$

For $\alpha=\pi/2$ one gets The product $(|a_1\rangle \ |a_2\rangle)M = (i|a_2\rangle \ i|a_1\rangle)\ [\ \alpha_1 \ \alpha_2]$. The input state chosen corresponds to the column vector [1 0] so that after the mirror the state

$(i|a_2\rangle \ i|a_1\rangle)\ [\ 1 \ 0] = i|a_2\rangle + 0i|a_1\rangle = i|a_2\rangle$

In the base set $(|b_1\rangle \ |b_2\rangle)$ the quantum state looks like [0 1] and the only thing we have to do is to revert to the original base set to sense the change. If you do this, the result reads: [0 i].

Thus the change of quantum state produced by the mirror can be cast in the form:

$$[1 \ \ 0] \rightarrow [0 \ \ i]$$

If you carefully examine the scheme above you can confirm the result by inspection.

In one word: it is the quantum state that determines the result. The base set must be first transformed with matrix M. It is the quantum state vector (amplitudes) that controls the possibility for energy exchange.

8.3.2. Beam splitters

The beam splitter generates at the vertex two linear superpositions for each b_1 and b_2 directions. If there are two beams each one can be acted independently. First

one establishes a relationship between the base sets; details are as follows. Keep the model with only one photon in the system. The change produced by the beam splitter consist in the production of a linear superposition of the kind:

$$|b_1\rangle = (1/\sqrt{2})\,(\,|a_1\rangle + i\,|a_2\rangle\,) = (1/\sqrt{2})\,(\,|1\rangle_1|0\rangle_2 + i\,|0\rangle_1|1\rangle_2\,)$$
$$|b_2\rangle = (1/\sqrt{2})\,(\,i|a_1\rangle + |a_2\rangle\,) = (1/\sqrt{2})\,(i\,|1\rangle_1|0\rangle_2 + |0\rangle_1|1\rangle_2\,)$$

or

$$(|b_1\rangle\ |b_2\rangle) = (|a_1\rangle\ |a_2\rangle)\,BS$$

where

$$(BS) = \begin{pmatrix} 1/\sqrt{2} & i/\sqrt{2} \\ i/\sqrt{2} & 1/\sqrt{2} \end{pmatrix}$$

It is sufficient to get the complex conjugate (BS)* to obtain the inverse transformation:

$$(|b_1\rangle\ |b_2\rangle)\,(BS)^* = (|a_1\rangle\ |a_2\rangle)\,(BS)(BS)^* = (|a_1\rangle\ |a_2\rangle).$$

You can check that (BS)(BS)* is a unit matrix.

The initial base set elements are then given as:

$$|a_1\rangle = (1/\sqrt{2})\,(\,|b_1\rangle - i|b_2\rangle\,)$$
$$|a_2\rangle = (1/\sqrt{2})\,(-i|b_1\rangle + |b_2\rangle\,)$$

The quantum state in the b-base once the input state is known is given by:

$$(|a_1\rangle\ |a_2\rangle) \begin{pmatrix} 1/\sqrt{2} & -i/\sqrt{2} \\ -i/\sqrt{2} & 1/\sqrt{2} \end{pmatrix} [\,\alpha_1\ \ \alpha_2] =$$
$$(1/\sqrt{2})\,(|a_1\rangle - i|a_2\rangle)\alpha_1 + (1/\sqrt{2})\,(-i|a_1\rangle + i\,|a_2\rangle)\alpha_2 =$$
$$|a_1\rangle\,(\alpha_1 - i\,\alpha_2)\,(1/\sqrt{2}) + |a_2\rangle\,(\alpha_2 - i\,\alpha_1)\,(1/\sqrt{2})$$

Thus, for a one beam coming to the vertex, $[\alpha_1\ \ 0]$, the quantum state after the BS reads:

$$|a_1\rangle\,(\alpha_1)\,(1/\sqrt{2}) + |a_2\rangle\,(-\,i\,\alpha_1)\,(1/\sqrt{2})$$

For a one-photon field $\alpha_1=1$; the quantum state after BS is the linear superposition:

$$\{|a_1\rangle - i\,|a_2\rangle\}(1/\sqrt{2})$$

Thus the name: the initial beam is split in two. The photon field still corresponds to one quantum of energy available.

If we look now to the effect a mirror does one can see the superposition of the incoming beam with a mirror-state. The amplitudes are reorganized so that the state is normalized to one.

The key to retain is that, once a quantum state enters along one direction to the beam-splitter a two component states will be emerging from the vertex; each one being a linear superposition as described above.

8.3.3. Phase shifters

This device changed one of the components of a quantum state only by a factor $\exp(-i\alpha)$. Consider the quantum state $(|k_1\rangle\ |k_2\rangle)\ [a\ \ b]$ and put a phase shifter interposed before coming to a vertex along the direction of the base state $|k_2\rangle$ one would get:

$$(|k_1\rangle\ |k_2\rangle)\ [a\ \ b] \rightarrow \text{PShifter}(-\alpha)\rightarrow (|k_1\rangle\ |k_2\rangle)\ [a\ \ \exp(-i\alpha)\ b]$$

If you put the shifter along the direction of $|k_1\rangle$ then:

$$(|k_1\rangle\ |k_2\rangle)\ [a\ \ b] \rightarrow \text{PShifter}(-\alpha)\rightarrow (|k_1\rangle\ |k_2\rangle)\ [\exp(-i\alpha)a\ \ b]$$

The geometry of the phase shifter determines the outcome. It definitely changes *locally* a given quantum state.

8.4. Mach-Zender interferometer

The Mach-Zender device discussed here includes two BSs and two mirrors intercalated between them as the scheme below shows; so that the quantum states generated at the vertex of the mirrors converge to the same point of the second beam-splitter (BS_2); the quantum states are generated at BS_1. Consider the input quantum state say [1 0]; the light ray comes from the upper left side in the X-form. In Figure 5-1 a schematic description includes detectors as well.

The present Mach-Zender interferometer permits mapping directly the input base set $(|a_1\rangle\ |a_2\rangle)$ to the output base set $(|b_1'\rangle\ |b_2'\rangle)$. Thus, by preparing a quantum state [1 0] the one-to-one map yields the result $(|b_1'\rangle\ |b_2'\rangle)\ [1\ \ 0] = |b_1'\rangle + 0\ |b_2'\rangle$. Only the detector D_1 can be activated while D_2 stay idle.

The present Mach-Zender interferometer permits mapping directly the input base set $(|a_1\rangle\ |a_2\rangle)$ to the output base set $(|b_1'\rangle\ |b_2'\rangle)$. Thus, by preparing a quantum state [1 0] the one-to-one map yields the result $(|b_1'\rangle\ |b_2'\rangle)\ [1\ \ 0] = |b_1'\rangle + 0\ |b_2'\rangle$. Only the detector D_1 can be activated while D_2 stay idle.

For a standard linear superposition state input, $[\alpha_1 \ \alpha_2]$ with $|\alpha_1|^2 + |\alpha_2|^2=1$ the detectors can respond as indicated by Axiom 4* with relative intensities $|\alpha_1|^2$ for detector D_1 and $|\alpha_2|^2$ for detector D_2.

Thus, for $\alpha_1 = 1/\sqrt{2}$ and $\alpha_2= 1/\sqrt{2}$ with a linear superposition prepared with one-photon the detectors respond by capturing the energy of one photon each time. The full pattern elicited by the quantum state indicates that half of the count should emerge on each counter.

E&E.8.4-1 Calculate amplitudes at detector channels

The quantum state at detectors according to the scheme corresponds to the linear superposition

$$\delta_1|b'_1> + \delta_2|b'_2>$$

The faithful events at detectors are modulated by the modulus square of the amplitudes. The input quantum state is taken to be [1 0] in the base set $(|a_1> \ |a_2>)$. In order to get a more general result let us take the input state $[\alpha_1 \ \alpha_2]$ as we did for the beam splitter model.

Start from the input quantum state: $(|a_1> \ |a_2>) \ [\alpha_1 \ \alpha_2]$. First apply BS_1:

$$(|a_1> \ |a_2>)(BS)_1 = (|b_1> \ |b_2>)$$

Thus

$$(|b_1> \ |b_2>) \ (BS)_1{}^* = (|a_1> \ |a_2>)$$

Operates the left hand side until we get a connection to the base set input to $(BS)_2$. First there is a mirror along each path. So that

$$(|a'_1> \ |a'_2>) = (|b_1> \ |b_2>)M=i \ (|b_2> \ |b_1>)$$

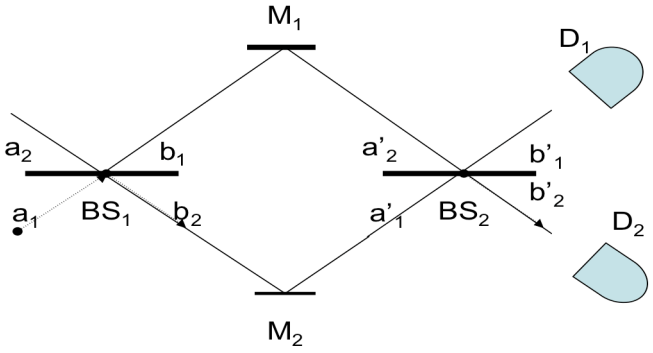
Now,

$$(|b'_1> \ |b'_2>) = (|a'_1> \ |a'_2>) \ (BS)_2$$

$$(|b'_1> \ |b'_2>) = (|b_1> \ |b_2>)M \ (BS)_2 = (|a_1> \ |a_2>)(BS)_1 \ M \ (BS)_2$$

$$(|a_1> \ |a_2>)= (|b'_1> \ |b'_2>)((BS)_1 \ M \ (BS)_2)^{-1}$$

Taking into account normalization factors the inverse of product is a negative unit matrix. This means that except for the sign, the input and the output base set for the present device are identical to within a numeric factor. Including the factor the input quantum state [1 0] is changed into [-1 0] which means that only the detector D_1 will register faithful events. D_2 detector stays idle.



The Mach-Zender discussed here serves to disentangle quantum evolution in Hilbert space from faithful events that would take place at the detectors. In few words, the whereabouts of the energy quantum (photon) within the network of beam splitters and mirrors are not the taken into account as if it were a particle. The quantum states given by the varied connecting zones, e.g. from BS_1 to M_1 and from here to BS_2 can be calculated and the final amplitudes at the detectors obtained. It is at this latter point where events (faithful and unfaithful) will show up. The symmetry forces base vector $|b_2>$ to interact with mirror M_2. So the matrix calculation is warranted.

One question we can investigate is the nature of events that can be induced by interposing measuring devices along specific paths. Let us discuss some specific situations:

1) Introduce a detector D_3 between BS_1 and M_1. We assume faithful events situation at all relevant places.
    a) Whenever an event is detected at D_3 the energy corresponds to the photon introduced in the system as input.
    b) A full event can be detected at any one of the detectors D_1 and D_2 while no-event shows up at D_3.
    c) From a total of N possible events N/2 are detected at D_3.
    d) Detectors D_1 and D_2 get N/4 each in the limit of very large N.
2) Introduce a detector D_3 between M_1 and BS_2. You can easily see that the counting pattern wouldn't change.

We can safely conclude that given the experimental set explored the photon energy (quantum) is never divided along different sections of these devices. But there are no elements allowing us to conclude that one photon is "traveling" as it were along different pathways. Information about the path is gathered *after* the faithful event took place *not before*.

Faithful events do not belong to Hilbert space. One has to be very careful if patterns of faithful events are decomposed into local subsets and use them to

reconstruct quantum states that belong to Hilbert space. One would be skating on very thin ice!

E&E-8.4-2 Neutron interferometry

We approach here a domain considered to be example of experimental quantum mechanics. Let examine some aspects of thermal neutron interferometry. The word thermal implies Boltzmann constant energy gauge: $k_BT = E_T$. Useful conversion factors are:

$$E \Leftrightarrow (\hbar^2/2m)\mathbf{k}^2 \Leftrightarrow (h^2/2m\lambda^2) \Leftrightarrow h\nu \Leftrightarrow (1/2)\, m\, \mathbf{v}^2 \Leftrightarrow$$
$$(1/2)\, m\, (d/t)^2 \Leftrightarrow k_BT$$

The base states of neutron systems $|\mathbf{k}>$ can be identified with the energy in any form that might be appropriate to the mounted device. Observe de Broglie relation: $mv \Leftrightarrow h/\lambda \Leftrightarrow \hbar k$. de Broglie wave length:

$$\lambda_{dB}=h/mv= h/\sqrt{(2mk_BT)}$$

It is widely believed that a fundamental dual nature of thermal and cold neutrons; Sometimes a particle, specially at detection, and sometimes a wave when traversing the interferometer is beautifully manifested by the highly non-local effects observed in neutron interferometry. For us, it is just a quantum physical manifestation of the material system. Quantum state propagation when traversing the interferometer (G(R,R',t) propagator), event production with an external system when detected. The nature of the event is not commensurate to the quantum system under study so that discussing such issues is not free from logical pitfalls. The concepts of particles and waves belong to classical physics. Quantum physics is another layer required to describe behavior of material systems including electromagnetic radiation.

8.5. Quantum states for periodic potentials

At the Fence one encounters crystalline potentials $W(R_i)$ sharing the periodicity of a crystal structure. One can imagine an I-frame system periodically repeated along the three space directions. We are back to the case examined in Sec.3.2.4-5 but this time the "length" L of the box correspond to $L_1L_2L_3$. The material system is "repeated" so that local quantum states can be manipulated. The question now is to study the collective quantum states if we admit that no material diffusion is allowed for.

Consider the internal quantum state for which the total mass of the material system can be taken to be located at the the respective I-frame. The boxes are periodically repeated; a new I-frame permits defining their origin coordinates. Do not mix this system with the internal states that are not coupled to the collective.

This must be done if one wants to build a framework where base states can be obtained.

Material systems such as atoms and molecules present some peculiarities. Let us mention a few of them. The nuclear quantum states depend upon the electronic state and for lowest base states of the latter the nuclear system can be taken at an average (fixed) position. This configuration can be periodically repeated so that one may have a periodic ionic background or it may simply be a neutral electronuclear state. The latter model may correspond to molecular/atom crystals while the former may produce ionic crystals. Another situation would correspond to an ionic background potential with collective electronic states such as in metals.

The simplest case corresponds to a box material system with global spin state S=0. These systems show a so-called closed electronic shell structure. One simple case: $Na^{+}(S=0)\ Cl^{-}(S=0)$.

A more interesting case occurs for a "box" system that shows unpaired state electrons ($S\neq0$). The core is taken to have a closed shell structure for simplicity so that it will constitute a crystal ionic potential for the electronic part. There will be two classes of extreme situations. In the first, the quantum states belonging to each box do not interact with the neighbors. This may correspond to a Mott-insulator state. The second extreme will be the equivalent to "free-electron-states" with quantum states extending over the whole crystal. All envisageable cases can be found for real systems. In particular there is a set where only nearest neighbor interactions are sufficient to describe electronic properties (Hubbard model). Here, focus is first put on recent developments.

8.5.1. Cooling and Trapping

Cooling and trapping of atoms is a current field of development: Bose-Einstein condensates are the starting points for the study of the so-called many-body physics. Molecular and fermionic super fluids are a hot research topic. Order can be induced in such systems with the help crossed laser beams. Recently, a trapped Yterbium atom cloud condensate was placed at the crossing point of three mutually perpendicular laser standing waves; these waves form a kind of optical lattice leading to a periodic potential for the atoms that has a simple cubic symmetry. This symmetry is superposed to harmonic confinement of the trap. Physicists can play now so as to move the quantum state from an ordered crystal-like to a super fluid (disordered-like). The quantum phase transition was experimentally detected (Cf.Moritz & Esslinger, Physics **2**, (2009)31 and references therein).

8.5.2 Building crystals from I-frame systems

Crystals are objects found in real space; these are solids displaying specific types of symmetry. The model of an ideal crystal obtains by infinite repetition of identical structural units in real space. Symmetry is related to geometry (symmetry groups), structural units to specific material systems and crystal properties to collective quantum states.

First, consider geometric aspects. Each structural unit, a Bravais cell, is made of finite number elements. The structural unit is called a (crystal) basis in solid-state language. Repeating this basis in space a Bravais lattice obtains.

The elements of structural units are represented by I-frame systems. Thus, from the very beginning real and quantum spaces are brought together. The corresponding I-frame origin and orientation are planted in real space as we discussed in Chapter 4. The fundamental model of a Bravais lattice is an infinite arrangement of I-frame quantum systems (I-F-QS); the material composition of each I-frame is kept fixed, quantum states are the variable elements.

In the business of constructing base sets, again, the quantum base states for I-frames are kept without mixing. Crystal properties would emerge once interactions are allowed for letting the I-F-QS to mix according to the cases under study. In this broad perspective, band structures develop and can be organized with the quantum numbers associated to base sets of the I-frames. Also, new phenomena can be described, e.g. solid state chemical reactions, but for now we consider a series of models starting from the simplest case to fix linguistic issues and following more complex cases later on. But first a simple illustration to guide this abstract discussion that is based on General Chemistry material.

E&E.8.5.1-1. Discuss possible states of a crystal formed with one sodium atom and one chlorine atom

Dispense yourself from the detailed electronic states for the time being. The base states of each I-frame system contains elements such as:

Na: $|$(Ne-core)3s$>$, … , $|$(Ne-core)$3s^0\ k_{3p}>$,…,etc.

Cl: $|$(Ne-core)$3s^2 3p^5>$,…, $|$(Ne-core)$3s^2 3p^4\ k_{3s}>$…,etc.

The symbols k_{3p} and k_{3s} stand for base states at the continuum just above the ionization limit of corresponding parent and holes at $3s^0$ and $3p^0$, respectively. For chlorine, without external sources there is no way to create a negative ion structure as it is possible to obtain positive ions. The crystal basis must be extended to treat the two I-frame systems as if they were a “supermolecule” by including quantum states of the negative ion:

Cl^{-1}: $|$(Ne-core)$3s^2 3p^6\ k_{3s}{}^0>$,…,$|$(Ne-core)$3s^2 3p^5\ k_{3s}>$

The states in the continuum including explicitly the holes read:

Na: $|$(Ne-core)3s $k_{3p}{}^0>$, …,$|$(Ne-core)$3s^0\ k_{3p}>$,…

Cl: $|$(Ne-core)$3s^2 3p^5\ k_{3s}{}^0>$,…,$|$(Ne-core)$3s^2 3p^4\ k_{3s}>$

Form the new base states:

$|\Phi_1\rangle = |(\text{Ne-core})3s\ k_{3p}{}^0\rangle \otimes |(\text{Ne-core})3s^2 3p^5\ k_{3s}{}^0\rangle \rightarrow$ Na Cl

$|\Phi_2\rangle = |(\text{Ne-core})3s^0\ k_{3p}\rangle \otimes |(\text{Ne-core})3s^2 3p^5\ k_{3s}{}^0\rangle \rightarrow$ Na* Cl

$|\Phi_3\rangle = |(\text{Ne-core})3s^0\ k_{3p}{}^0\rangle \otimes |(\text{Ne-core})3s^2 3p^5\ k_{3s}\rangle \rightarrow$ $Na^+ Cl^-$*

$|\Phi_4\rangle = |(\text{Ne-core})3s^0\ k_{3p}{}^0\rangle \otimes |(\text{Ne-core})3s^2 3p^6\ k_{3s}{}^0\rangle \rightarrow$ $Na^+ Cl^-$

The base functions Φ_1 and Φ_2 belong to the initial atomic I-frames while Φ_3 and Φ_4 belong to the super-molecule, which includes new states related to the negative and positive ions; here, sodium system acts as a source of electrons for the chlorine system; $|\Phi_4\rangle$ contains a hole state at sodium frame and this is another way to signal a positive charge state.

The crystal basis has quantum states where, for the time being, interactions with the remaining crystal are suppressed. These states map to the linear superpositions:

$$|\Psi\rangle = C_1|\Phi_1\rangle + C_2|\Phi_2\rangle + C_3|\Phi_3\rangle + C_4|\Phi_4\rangle =$$
$$(C_1\ C_2\ C_3\ C_4) \bullet [|\Phi_1\rangle\ |\Phi_2\rangle\ |\Phi_3\rangle\ |\Phi_4\rangle]$$

Since the initial point is a pair of atoms, the quantum state looks like the row (1 0 0 0). There is amplitude at the lowest energy base state.

The point is that the energy of base states for the ionic forms must be sensitive to external electric field interactions. Thus, switching on the interactions with the whole crystal the energy level of the ionic form $|\Phi_4\rangle$ becomes lower than the neutral pair; remember that we handle quantum base states not objects. Therefore, in the crystal including Coulomb interactions the quantum state would look like (0 0 0 1), in other words crystal effects would induce the ionic form amplitudes in the present approach. In the standard theory, this corresponds to Madelung's potential effect.

Note that by increasing the base states including electron transfer base states (e,g, $|\Phi_4\rangle$), a large number of physical and chemical states can be examined from a unified viewpoint.

Because the material systems entering the Bravais cell presents a constitution of, say, n-electrons and m-nuclei, permutation symmetry that could be imposed among the elements of repeating basis, or inside the elements included in the crystal basis, is not taken into account yet; this symmetry is to be considered on a case-by-case only. If the elements of the crystal basis are distinguishable, as a first step, the system state taken as simple product base sets without permutation symmetry.

By taking I-frame systems as models, the assumption is that base state allows for a clear mass distribution of the total mass sustaining the I-Frame QState so that a geometric arrangement would make sense to start building crystal base sets.

Why would it be possible to postpone symmetrization? The reason is simple. We are not handling the systems as collection of particles but treating collections of base states in view of determining quantum states amplitudes of linear superpositions; these base states may well be properly symmetrized.

Now, the form of the Hamiltonian, as far interactions between I-frame systems are concerned, is left unspecified except for crystal symmetry invariance;

interactions are included at places where their role might be more clearly perceived.

The zero-order model starts from the set of *non-interacting* I-frames. Thus, there are by construction all those sets of complete base functions the I-frame systems contribute including electron transfer base states; particular total mass distributions associated to the real space I-frames are implicit, the crystal basis in Bravais cells takes the place of equilibrium geometry.

The geometric elements required to construct a language and characteristic of solid-state physics are summarized in what follows.

Identical structural units, the primitive unit cell, are translated in space with the help of three linearly independent vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$; i.e., they are not collinear, the product $|\mathbf{a}_1 \cdot \mathbf{a}_2 \wedge \mathbf{a}_3| = V^{PUC}$ yields the volume of the primitive unit cell (PUC); these are the *primitive vectors*.

The lattice is defined with these primitive vectors; in a model crystal, a point in real space, say $\mathbf{x}'$ by definition must exactly have the same surrounding that the point $\mathbf{x}$ obtained after adding the vector $\mathbf{X}(n_1, n_2, n_3) = \mathbf{X}(\mathbf{n})$ according to:

$$\mathbf{x} = \mathbf{x}' + n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3 = \mathbf{x}' + \mathbf{X}(n_1, n_2, n_3) = \mathbf{x}' + \mathbf{X}(\mathbf{n}) \qquad (8.5.1.1)$$

The selection of three integers n_1, n_2, n_3 is arbitrary.

Thus, *lattice plus basis* generate the crystal structure. This is purely geometric except that now the basis would contain a great deal of quantum information via the I-frame. This is a typical example of Fence system.

Consider a basis with a finite number of I-frames (equal or different). Two indices are required to signal the position of an I-frame belonging to the n-th PUC and being the ℓ-th I-frame in the crystal basis: $\mathbf{X}(n, \ell)$. Thus,

$$\mathbf{X}(n, \ell) = \mathbf{X}(n_1, n_2, n_3) + \mathbf{X}(\ell_1, \ell_2, \ell_3) = \mathbf{X}(\mathbf{n}) + \mathbf{X}(\ell) \qquad (8.5.1.2)$$

The origin is given by $\mathbf{X}(\mathbf{n}=\mathbf{0}) = \mathbf{0}$ and the position of the j-th I-frame by $X(\mathbf{0}, \mathbf{j})$ in the crystal basis. The first index labels a given PUC origin; the second does it for the I-frame origin. The system has discrete translational symmetry; hence reciprocal spaces can be constructed.

The reciprocal primitive lattice vectors are: $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$. They are given by:

$$\mathbf{b}_1 = 2\pi\ \mathbf{a}_2 \wedge \mathbf{a}_3 / V^{PUC};\ \mathbf{b}_2 = 2\pi\ \mathbf{a}_3 \wedge \mathbf{a}_1 / V^{PUC};$$
$$\mathbf{b}_3 = 2\pi\ \mathbf{a}_1 \wedge \mathbf{a}_2 / V^{PUC} \qquad .(8.5.1.3)$$

The sets of $\mathbf{a}$ and $\mathbf{b}$ are orthogonal:

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\, \delta_{ij} \qquad (8.5.1.4)$$

Equivalent points in reciprocal space are defined with a vector simply given as:

$$\mathbf{G}(m_1,m_2,m_3) = m_1\mathbf{b}_1 + m_2\mathbf{b}_2 + m_3\mathbf{b}_3 = \mathbf{G}(\mathbf{m}).$$

The triad m_1, m_2, m_3 are integers defining the **G**-vectors. The scalar product $\mathbf{X}\cdot\mathbf{G}$ can easily be calculated resulting in an integer multiplied by the factor 2π that comes from the definition (8.5.1.3). Thus, $\mathbf{G}(\mathbf{m}) \cdot \mathbf{X}(\mathbf{n}) = 2\pi\, p$, where p equals the integer $n_1m_1 + n_2m_2 + n_3m_3$. It follows that

$$\exp(i\, \mathbf{G}(\mathbf{m}) \cdot \mathbf{X}(\mathbf{n})) = \exp(i\, 2\pi\, p) = \cos(2\pi p) + i \sin(2\pi\, p) = 1 \qquad (8.5.1.5)$$

There is nothing more than the properties of circular functions.

Consider functions $f(\mathbf{x})$ that have the periodicity of the lattice. They can be written as linear superposition of functions in the reciprocal space $f(\mathbf{G})$:

$$f(\mathbf{x}) = \Sigma_{\mathbf{G}} \exp(i\, \mathbf{G} \cdot \mathbf{x})\, f(\mathbf{G}) \qquad (8.5.1.6)$$

The function $f(\mathbf{x})$ is left unspecified; it may correspond to a global state assigned to the I-frame; eq.(8.5.1.6) elicits a general property of periodic functions.

The zero-model puts at our disposal three Cartesian displacement vectors for each I-frame and possible global angular momentum of the rigid I-frame. Thus, a quantum system of 3s degrees of freedom with respect to a laboratory frame would express 3s-6 degrees of freedom in the I-frame (3s-5 for linear cases); thus, when defined with respect to an I-frame the system's 3s degrees of freedom contains a redundant subset and appropriate changes of variables may help eliciting those 6 degrees of freedom belonging to the global I-frame (e.g. centre of mass, inertia tensor). At the Fence, a free I-frame may behave as a classical mechanics system (Cf.Chapt.4) but it can also cloak itself as a quantum system; actually, this latter statement is not accurate because it will depend whether a measuring device is set up that responds to the quantum state of the I-frame or another sensing the global mass state, but this is an experimental planning decision belonging to a social determination.

Let $\mathbf{x}(\mathbf{n}, \ell)$ be a displacement of the ℓ-th I-frame origin in the n-th Bravais cell that plays the role of fixed geometry. It is apparent that after a displacement of the PUC origin by a vector **L** one should have the equality:

$$\mathbf{x}(\mathbf{n}+\mathbf{L}, \ell) = \mathbf{x}(\mathbf{n}, \ell) \qquad (8.5.1.7)$$

Consider an infinitely extended crystal which is partitioned into units containing $L_1xL_2xL_3 = N$ unit cells. By construction, these new units, sub-crystals as it were, fill all space; these parallelepipeds have edges defined by the vector $L_1\mathbf{a}_1$, $L_2\mathbf{a}_2$, $L_3\mathbf{a}_3$. Any one of these sub-crystals can play the role of a physical crystal.

We sketch the study of vibration properties of systems submitted to these periodic boundary conditions also known as Born-von Karman boundary conditions.

Applied to the components of the displacement vector eq.(8.5.1.7) lead to:

$$\exp(2\pi i\, \mathbf{K} \cdot L_1\mathbf{a}_1) = \exp(2\pi i\, \mathbf{K} \cdot L_2\mathbf{a}_2) = \exp(2\pi i\, \mathbf{K} \cdot L_3\mathbf{a}_3) = 1 \qquad (8.5.1.8)$$

The vector **K** fulfilling these equalities can be written with the help of **G**(**m**) as:

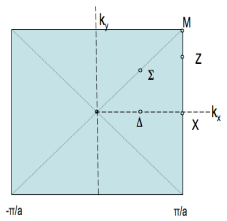
$$\mathbf{K} = (1/L)\, \mathbf{G}(\mathbf{m}) = (m_1/L_1)\, \mathbf{b}_1 + (m_2/L_2)\, \mathbf{b}_2 + (m_3/L_3)\, \mathbf{b}_3 \qquad (8.5.19)$$

This construction permits moving from the basic case $L_1xL_2xL_3 = N = 1$ to situations where the number of unit cells N can be a large number.

8.5.2. Brillouin zone and Wigner-Seitz primitive cell

The continuous translation group in real space was examined in Chapt.2, conservation of linear momentum **p** results from space homogeneity; here translations are discrete thereby entailing a specific reciprocal space representation: **k**-space.

E&E-8.5.2.2-2. Brillouin zones for linear and square lattices



Caption: The center of Brillouin Zone (BZ) is label with Γ; symmetry operations permit identifying some critical points. Along the k_x-axis there is the intersection X with the square edge and the mid point Δ. On the diagonal there is the point M and halfway Σ, these points are on a symmetry axis. The points at the limit of the BZ that do not coincide with X and M is denoted Z. The four vertices are equivalent points. There is degeneracy associated to points transforming into equivalent ones under symmetry operations. For X and M there are four operations leading to equivalent points: the axis C_4 applied twice (C_4^2) perpendicular to the plane (k_x,k_y);The interior points do not have any singularity.

One can restrict the values of **k** to one reciprocal lattice cell. The reason to do this is that for any point outside that cell, there exists a point inside within the cell connected to it by a reciprocal lattice vector that we call **K**; this is related to **G**-vectors as seen in eq. (8.5.1.9). Thus, there is a map between the primitive unit cell and the corresponding reciprocal lattice cell. For practical considerations one can define equivalent regions in both **k**-space and direct space that show a greater geometric symmetry. The constraint in **k**-space is that a reciprocal lattice vector cannot relate two points inside the chosen region; this is the first Brillouin cell. In direct space, the corresponding space is known as Wigner-Seitz primitive cell.

For the simplest cubic case, a Wigner-Seitz primitive cell obtains whenever in a Bravais lattice nearest neighbors surrounding each I-frame are used to define a polyhedral figure. Draw mid-planes perpendicular to the straight lines drawn between the neighbors and the origin the volume enclosed defines this primitive cell. This cell displays the symmetry of the Bravais lattice. The cell includes a complete crystal basis in a closed volume. The pictorial appearance of a unit cell and a Wigner-Seitz cell is different.

If we perform the above operations in reciprocal space the Brillouin zone obtains around **k=0**. The Wigner-Seitz primitive cell mapped into reciprocal space is the first Brillouin zone.

8.5.3. Lattice planes

For a particular Bravais lattice, any plane defined by three non-collinear points corresponds to a lattice plane. By translational symmetry of the Bravais lattice, any such plane contains infinite many lattice points that form a 2-D Bravais lattice. Designate the shortest distance between the planes belonging to a given family by d. For any reciprocal vector **K**, there is a family of lattice planes; the planes being at distance d; the length of the shortest reciprocal lattice vector parallel to **K** is $2\pi/d$.

The Miller indices of a lattice plane are the coordinates of the shortest reciprocal vector normal to the plane referred to a specified set of primitive reciprocal lattice vectors. In short, a lattice plane with Miller indices h,k,l is perpendicular to the reciprocal vector $\mathbf{K}= h\mathbf{b}_1+k\mathbf{b}_2+l\mathbf{b}_3$ so it is contained in the plane $\mathbf{K}\cdot\mathbf{r}$=constant. Let this plane intersect the axes at the points $x_1\mathbf{a}_1$, $x_2\mathbf{a}_2$, $x_3\mathbf{a}_3$ so that $\mathbf{K}\cdot\mathbf{r}$=constant=F is fulfilled with $\mathbf{r}= x_1\mathbf{a}_1+ x_2\mathbf{a}_2+ x_3\mathbf{a}_3$. Then $x_1= F/2\pi h$, $x_2= F/2\pi k$ and $x_3= F/2\pi l$; the 2π factor comes from eq.(8.5.14). Thus, the intercepts of a lattice plane with the crystal axes are inversely proportional to the Miller indices.

Consider a plane with intercepts $[x_1\ x_2\ x_3]$ with the cubic axes and calculate the Miller indices. Take the example $[1\ \ \bar{2}\ \ 4]$ where $\bar{2} = -2$, the reciprocal numbers required to get Miller indices yield $1,\ \ \bar{1}/2,\ \ 1/4$, by definition the indices are integers so that now multiply by 4 to get the indices $(4\ \ \bar{2}\ \ 1)$ that are Miller indices sought.

8.5.4. Lattice translation symmetry and band structure

Consider a **k**-vector defined as: $\mathbf{k} = \kappa_1\ \mathbf{b}_1+ \kappa_2\ \mathbf{b}_2+ \kappa_3\ \mathbf{b}_3$, as discussed above, take a crystal composed of a large number of unit cells, N_j in the direction $\mathbf{a}_j$ (j=1,2,3). Then $N= N_1\ N_2\ N_3$ stands for the total number of unit cells that can be of order 10^{23}. Born-von Karman boundary conditions are appropriate to examine periodicity, they are defined by:

$$f_{\mathbf{k}}(\mathbf{x}) \ = \ f_{\mathbf{k}}(\mathbf{x} + N_j\ \mathbf{a}_j). \qquad (8.5.4.1)$$

We examine now the translation symmetry as applied to the base vectors $|\mathbf{x}\rangle$ by the operator $\hat{T}(N_j\ \mathbf{a}_j)$. From eq.(8.5.13.1) we can see that:

$$\hat{T}(N_j\ \mathbf{a}_j)\ |\mathbf{x}\rangle = |\ \mathbf{x} + N_j\ \mathbf{a}_j\ \rangle \qquad (8.5.4.2a)$$

This is a translation of the origin belonging to an I-frame.

The effect translation symmetry has on the energy levels of the zero-model is the issue. Take a primitive unit cell with one I-frame that seen from the laboratory has a mass M at the origin.

For a higher level model, the remaining I-frames systems are interacting with the one selected by us; assume that such effect can be model with an external potential V(**x**). Together with $\hat{K} = (\hbar\nabla_{\mathbf{x}})^2/2M$, the kinetic energy operator, define the Hamiltonian: $\hat{H} = (\hat{K} + V) = (\hbar/i)\nabla_{\mathbf{x}})^2/2M + V(\mathbf{x}) = \hat{H}(\mathbf{x})$. The potential has the crystal symmetry by fulfilling an equation similar to (8.5.13.1). We are in the business of constructing base state for the I-frame as such.

The operators $\hat{H}(\mathbf{x})$ and $\hat{T}(N_j\ \mathbf{a}_j)$ commute and, consequently can be simultaneously brought to a diagonal form. The problem is to find simultaneous eigenvectors. To extract basic aspect to this problem let us consider a 1D model.

Consider one I-frame per Bravais lattice model by a 1D array separated by a distance a: V(x±a) = V(x). Take the base ket |x> and define the unitary translation operator $\hat{T}(a)$ by:

$$\hat{T}(a)\,|x\rangle = |x+a\rangle \qquad (8.5.4.2b)$$

The Hamiltonian is invariant under the translation, i.e. $\hat{T}\,\hat{H} = \hat{H}\,\hat{T}$. Note that because $\hat{T}$ is unitary (not hermitean) the eigenvalues are complex numbers of unit modulus.

The energy eigenvectors for the I-frame origin located at position n is indicated by |n>. The operator $\hat{T}(+a)|n\rangle$ shifts the origin to |n+1>, while $\hat{T}(-a)|n\rangle = |n-1\rangle$. Note that $\hat{T}(na)|0\rangle = |n\rangle$, the base vector |0> is not the vacuum but the system at the origin. Remind that with or without interaction, an identical system is found at each location the energy of them is independent from the location.

We take now the I-frame at its ground state energy E_o and take again the zero order case such as each I-frame system has no interaction with the surrounding, namely, V=0. Naturally, all positions along the line have the same energy E_o. Thus, $\hat{H}|n\rangle = E_o\,|n\rangle$ but $\hat{T}(+a)|n\rangle = |n+1\rangle$. In words, the vector |n> is not a simultaneous eigenvector of these two operators. The issue is the construction of such a vector. One way to do this is to construct a linear combination via a parameter w:

$$|w\rangle = \sum_{n=-\infty}^{\infty} \exp(inw)\,|n\rangle \qquad (8.5.4.3)$$

The parameter w is real and must vary between $-\pi \le w \le \pi$. This is a quantum state over the complete base set of crystal positions; all base states have the same energy E_o. Let us apply $\hat{T}(+a)$ to this ket and obtain the new vector $\hat{T}(+a)|w\rangle$:

$$\hat{T}(+a)|w> = \hat{T}(+a) \sum_{n=-\infty}^{\infty} \exp(inw)\ |n> =$$

$$\sum_{n=-\infty}^{\infty} \exp(inw)\ \hat{T}(+a)|n> = \sum_{n=-\infty}^{\infty} \exp(inw)\ |n+1>.$$

At this point replace n by n-1 in the last equality. You can do this because n is a dummy index. Rearrange the sum; you get: $\sum_{n=-\infty}^{\infty} \exp(i(n-1)w)\ |n>$. A simple trick permits rewriting this as $\exp(iw) \sum_{n=-\infty}^{\infty} \exp(inw)\ |n>$ so the final result is that |w> is eigenvector of the translation operator with eigenvalue exp(iw):

$$\hat{T}(+a)|w> = \exp(iw)\ |w> \qquad (8.5.4.4)$$

Besides, this equation confirms that the operator $\hat{T}(+a)$ is unitary.

Calculate now the energy associated to this linear superposition engaging all sites in an infinite linear lattice:

$$\hat{H}|w> = \hat{H} \sum_{n=-\infty}^{\infty} \exp(inw)\ |n> = \sum_{n=-\infty}^{\infty} \exp(inw)\ \hat{H}|n>.$$

Because all elements have amplitudes at the ground state only the result is:

$$\hat{H}|w> = E_o \sum_{n=-\infty}^{\infty} \exp(inw)\ |n> =$$

$$E_o\ |w> \qquad (8.5.4.5)$$

Therefore, the linear superposition eq. (8.5.4.3) is a common eigenvector for the operators $\hat{H}$ and $\hat{T}(+a)$.

The model Hamiltonian expressed in the base {|n>} at the site n simply reads as $E_o|n><n|$ that is our zero-model for a linear chain. Unless the site elements interact among themselves the base functions are of no interest.

Let us introduce interactions between nearest neighbors and check the resulting energy spectra. Now, the Hamiltonian has off-diagonal elements: $<n|\hat{H}|n\pm1> = -\Delta$. The interaction parameter Δ will be used to represent varied situations of interest. Thus, with this new Hamiltonian one gets:

$$\hat{H}|n> = \Sigma_m <m|\hat{H}|n>|m> =$$

$$E_o\ |n> - \Delta|n+1> - \Delta\ |n-1> \qquad (8.5.4.6)$$

The model implies that matrix elements <n±m| $\hat{H}$ |n> are all zero except when m equals ±1 or zero. Now we need calculate $\hat{H}$|w>. This is done in E&E-8.5.4-3 below.

E&E-8.5.4-3 Explicit calculation of $\hat{H}$|w>
This calculations use the properties associated to linear operators (Cf.Chapt.1). Thus, for a Hamiltonian like the one introduced in (8.5.4.6) transform eq.(8.5.4.5):

$$\hat{H}|\mathbf{w}\rangle = \sum_{n=-\infty}^{\infty} \exp(inw)\ \hat{H}|n\rangle =$$
$$\sum_{n=-\infty}^{\infty} \exp(inw)\ \Sigma_m \langle m|\hat{H}|n\rangle\ |m\rangle.$$

The sum over m is zero except for the nearest neighbour terms:

$$\{\exp(inw)\langle n|\hat{H}|n\rangle|n\rangle + \exp(i(nw)\langle n+1|\hat{H}|n\rangle|n+1\rangle +$$
$$\exp(inw)\langle n-1|\hat{H}|n\rangle|n-1\rangle\} =$$
$$\{\exp(inw)\ E_o\ |n\rangle - \exp(i(n)w)\ \Delta\ |n+1\rangle - \exp(i(n)w)\ \Delta\ |n-1\rangle\}.$$

Now, inserting this equality one gets

$$\hat{H}|\mathbf{w}\rangle = \sum_{n=-\infty}^{\infty} \exp(inw)\ E_o\ |n\rangle -$$
$$\sum_{n=-\infty}^{\infty} \exp(i(n)w)\ \Delta\ |n+1\rangle - \sum_{n=-\infty}^{\infty} \exp(i(n-1)w)\ \Delta\ |n-1\rangle\}$$

The second and third sums are reshuffled by changing the index n by n-1 in the second and n by n+1 in the third because they are dummy indices, the result is

$$\sum_{n=-\infty}^{\infty} \exp(inw)\ \{E_o - \Delta\exp(-iw) - \Delta\exp(+iw)\}\ |n\rangle =$$
$$E(w)\ |w\rangle$$

The term in curly brackets does not depend upon n and is taken outside the sum symbol:

$$\{E_o - \Delta(\exp(-iw) + \exp(+iw))\} \sum_{n=-\infty}^{\infty} \exp(inw)\ |n\rangle =$$
$$E(w)\ |w\rangle$$

Calculate the term (exp(-iw) + exp(+iw)= cos(iw)-isin(w) + cos(w)+isin(w) = 2 cos(w) to get the equation below. Thus,

$$\hat{H}|w\rangle = E(w)\ |w\rangle = (E_o - 2\Delta\cos(w))\ |w\rangle.$$

The energy as a function of w reads:

$$E(w) = (E_o - 2\Delta \cos(w)) \qquad (8.5.4.7)$$

As this parameter w changes from π to $-\pi$ we obtain an energy band varying between $E_o - 2\Delta$ and $E_o + 2\Delta$.

This is a remarkable result depending upon the translation symmetry where the interaction Δ actually defines the splitting width. But there is more.

Equate now the parameter w=ka to get the final link with lattices. The range where k can vary is $-\pi \leq ka \leq \pi$ or $-\pi/a \leq k \leq \pi/a$. This corresponds to the first Brillouin zone. We have then a *dispersion relation* or energy as a function of k:

$$E(k) = E_o - 2\Delta \cos(ka) \qquad (8.5.4.8)$$

The allowed energy values form a band. Also, there is a cut-off $|k|=\pi/a$.

The effect of translational symmetry for interacting I-frames systems is to produce the rupture of energy degeneracy leading to a *band structure* at the first Brillouin zone. The width of this band is 4Δ. This type of splitting applies to any energy level of the isolated I-frame system where now the internal (quantum) structure is about to play a central role.

The band structure is sometimes referred to as lattice energy levels. A narrow band, e.g. Δ very small, the system would correspond to I-frames states fully degenerate. A model situation where the I-frame systems are at infinite distance would show no interactions and the spectra will correspond to the spectra of the isolated I-frames quantum systems. Thus, in a crystal one would expect band structures whenever the matrix elements $<n \pm 1|H|n>$ are different from zero.

The crystal base function reads now as:

$$|k> = \sum_{n=-\infty}^{\infty} \exp(inka)\, |n> \qquad (8.5.4.3')$$

This is a Fourier transform that can be inverted to get the site base functions |n> as linear combinations over the k-waves.

The I-frame concept is extremely general. The fundamental band structure imposed by translation symmetry is hence valid for mass fluctuations (vibrations) about the rigid Bravais lattice structure as well as for the quantum systems associated to the I-frames. Unfortunately, here is not the place for extensive solid-state physics discussions; however, a couple of issues that are central to the study of quantum technologic systems are to be examined.

8.5.5. Phonons

The model is adapted by introducing the vector **u**(**n**,**l**) describing displacements of the l-th I-frame from the n-th cell; the crystal structure provides a fixed framework. Consider the case of one I-frame by Bravais cell; thus, **u**(**n**,**l**) simplifies into **u**(**n**) that stands for a displacement coordinate associated to the mass M. The zero-order model corresponds to a set of harmonic oscillator fluctuating independently from each other. This is Einstein model for a crystal.

The coordinate vectors $\mathbf{u}(\mathbf{n})=u_n$ for a model with one I-frame per unit cell is transformed into a collective (phonon) coordinates Q_k using the lattice ansatz equivalent to eq. (8.5.4.3'):

$$u_n = (N)^{-1/2} \Sigma_k Q_k \exp(ikna) \qquad (8.5.5.1a)$$

The inverse relation reads:

$$Q_k = (N)^{-1/2} \Sigma_n u_n \exp(-ikna) \qquad (8.5.5.1b)$$

Periodic boundary conditions $u_n = u_{n+N}$ lead to N allowed values for the wave vector k, the distance between two nearest neighbours is indicated by a. Thus,

$$k= 2\pi n/Na;$$
$$n= 0, \pm1, \pm2, \ldots,\pm(N/2 -1), +N/2 \qquad (8.5.5.2)$$

The limit values of k being $\pm(N/2)\ 2\pi/aN$ they correspond well to the first Brillouin zone. The dynamical part requires the introduction of linear momenta with transformation property:

$$p_n = (N)^{-1/2} \Sigma_k P_k \exp(-ikna)$$
$$P_k = (N)^{-1/2} \Sigma_n p_n \exp(ikna) \qquad (8.5.5.3)$$

E&E-5.5.2-4. Find an expression to the commutator [Q_k, $P_{k'}$]
Introducing the definitions with adapted indexes one obtains:

$$[Q_k, P_{k'}] = N^{-1} [\Sigma_n u_n \exp(-ikna), \Sigma_{n'} p_{n'} \exp(ik'n'a)] =$$
$$N^{-1} \Sigma_n \Sigma_{n'} [u_n, p_{n'}] \exp(-ikna)\exp(ik'n'a) =$$
$$N^{-1} \Sigma_n \Sigma_{n'} [u_n, p_{n'}] \exp(-i(kn-k'n')a).$$

The commutator $[Q_k, P_{k'}]$ is thus expressed as linear superpositions over local commutators $[u_n, p_{n'}]$.

The quantization rules require that:

$$[u_n, p_{n'}] = i\hbar\, \delta(n,n') \qquad (8.5.5.4)$$

Then:

$$[Q_k, P_{k'}] = N^{-1}\, i\hbar\, \Sigma_n \exp(-i(k-k')na) = i\hbar\, \delta(k,k') \qquad (8.5.5.5)$$

The Hamiltonian for the linear chain motif in k-space is given in the form:

$$H = \Sigma_k\, H_k = \Sigma_k\, \{(1/2M)\, P_k\, P_{-k} + (1/2)M\omega_k^2\, Q_k\, Q_{-k}\} \qquad (8.5.5.6)$$

The equation of motion read:

$$\ddot{Q}_k + M\omega_k^2\, Q_k = 0 \qquad (8.5.5.7)$$

Observe that the operator symbol (a caret ˆ) is removed to simplify the discussion. But they are operators so that we need base states to construct the quantum states to sense the crystal response. Actually, what is relevant now is the state of excitation the system can be, and for that we need a Fock space similar to the one used in quantizing the electromagnetic field. We know that the energy is quantized according to:

$$\varepsilon_k = (n_k + \tfrac{1}{2})\, \hbar\, \omega_k \qquad (8.5.5.8)$$

Fock space is hence constructed along lines similar to those found in Sect.6.2. Here, operators for creation and annihilation of energy quanta are designated as $\hat{b}$ and $\hat{b}^\dagger$ instead of $\hat{a}$ and $\hat{a}^\dagger$ used for the electromagnetic field. All equations derived there have the same form here. In particular the phonon Hamiltonian takes on the form:

$$\hat{H}_{ph} = \Sigma_k\, (\hbar\, \omega_k)(\hat{b}_k^\dagger \hat{b}_k + \tfrac{1}{2}) \qquad (8.5.5.9)$$

The fundamental thing now is the construction of a base set. This is given as direct products of base states for each k-level, although now a simplified notation is used if many modes are present. Again, zero available excitation at a given frequency is named the vacuum with the property: $\hat{b}_k|0_k\rangle = 0$. The number of excitations of a given frequency is represented by the base vector $|n_k\rangle$:

$$(1/\sqrt{n_k!})\, (\hat{b}_k^\dagger)^n\, |0_k\rangle = |n_k\rangle \qquad (8.5.5.10)$$

An arbitrary quantum state for the transverse phonon field, say $|\Xi>$, is represented by a row vector of complex numbers: $<n_k|\Xi>$:

$$|\Xi> = \Sigma_k <n_k |\Xi> |n_k > \qquad (8.5.5.11)$$

The average energy for this state is given by $<\Xi| \hat{H}_{ph}|\Xi>$. The result is:

$$<\Xi| \hat{H}_{ph}|\Xi> = <\Xi| \Sigma_j (\hbar \omega_j)(\hat{b}_j^{\dagger} \hat{b}_j + ½)|\Xi> =$$
$$\Sigma_{jkl} <n_l|\Xi>^*<n_k|\Xi>(\hbar\omega_j)<n_l|(\hat{b}_j^{\dagger} \hat{b}_j +1/2)|n_k> \qquad (8.5.5.12)$$

The constant term: $<n_l|(1/2)|n_k> = (1/2)\delta_{lk}$; and $<n_l| (\hat{b}_j^{\dagger} \hat{b}_j) |n_k>$ the occupation number equals $<n_l| \hat{N}_j|n_k > = n_j <n_l|n_k> \delta_{jk}$, thus there are two Kronecker delta, δ_{jk} $\delta_{nl,nk}$ eliminating two sum signs to get the average energy for the quantum state $|\Xi>$ given by:

$$<\Xi| \hat{H}_{ph} |\Xi> =$$
$$\Sigma_j |<n_j|\Xi>|^2(\hbar\omega_j)(n_j+1/2) \qquad (8.5.5.13)$$

The running index j indicates the k-states intervening in the quantum state. *Only those base states showing non-zero amplitude contribute to the total energy*.

It would be adequate to go back and read **E&E-5.2-2** concerning field magnitudes for defined quantum states.

The average energy depends upon those amplitudes that are different from zero in the quantum state via $|<n_j|\Xi>|^2$, the squared amplitudes. The energy that can be exchanged at the Fence amounts to: $n_j(\hbar\omega_j)$. But, in the expression for the average energy this degree of freedom contributes only a fraction $|<n_j |\Xi>|^2 (\hbar \omega_j) n_j$. Caution is required because one may mix up two different things: $n_j(\hbar\omega_j)$ is a quantity characteristic of Fock space while $|<n_j |\Xi>|^2$ tells what the relative response intensity the quantum state show if a probe were used to measure the quantum state. Intensity response belongs to real space or Fence space. As a rule of thumb, keep yourself handling thing in one domain without mixing theoretical magnitudes belonging to another realm, unless you do it with full control.

The similarities between a phonon field and the t-EM field stop when we look at the nature of fluctuations. Remember that at the bottom it is the material displacement field u_n that sustain the vibration modes. The Fourier transform, $u_n = (N)^{-1/2} \Sigma_k Q_k \exp(ikna)$, allowed the introduction of collective coordinates $\{Q_k\}$ and boundary conditions defining allowed values for k, namely, $-\pi/a< k \leq \pi/a$; this range of allowed k-values is the first Brillouin zone of the linear lattice. These coordinates and the conjugated moments $\{P_k\}$ taken as operators (we know their commutation relations) can be cast in terms of Fock operators:

$$Q_k = (\hbar/2M\omega_k)^{1/2} [\hat{b}_k + \hat{b}_{-k}^{\dagger}] \quad (8.5.5.14a)$$

$$P_k = i(\hbar M\omega_k/2)^{1/2} [\hat{b}_k - \hat{b}_{-k}^{\dagger}] \quad (8.5.5.14b)$$

Also,

$$\hat{b}_k=(2\hbar)^{-1/2}[(M\omega_k)^{1/2}Q_{+k}+i(M\omega_k)^{-1/2}P_{-k}] \quad (8.5.5.15a)$$

$$\hat{b}_k^{\dagger}=(2\hbar)^{-1/2}[(M\omega_k)^{1/2}Q_{-k}+i(M\omega_k)^{-1/2}P_{+k}] \quad (8.5.5.15b)$$

Thus, the fluctuation field operator

$$u_n=\Sigma_k(\hbar/2NM\omega_k)^{+1/2}[\hat{b}_k\exp(ikn)+\hat{b}_k^{\dagger}\exp(-ikn)] \quad (8.5.5.16)$$

This equation relates the I-frame displacement operator to phonon creation and annihilation operators in Fock space. The commutation relations between these Fock space operators read:

$$[\hat{b}_k, \hat{b}_{k'}^{\dagger}] = \delta(k,k') \quad (8.5.5.17)$$

The time dependence is constructed by replacing $\hat{b}_k$ by $\hat{b}_k \exp(-i\omega_k t)$ in (8.5.5.16) to get:

$$u_n(t)= \Sigma_k (\hbar/2NM\omega_k)^{+1/2} [\hat{b}_k \exp(i(kn-\omega_k t)) + \hat{b}_k^{\dagger} \exp(-i(kn-\omega_k t))] \quad (8.5.5.18)$$

Take a quantum state of type: $|\Psi\rangle=C(n_k)|n_k\rangle + C(n_k-1)|n_k-1\rangle + C(n_k+1)|n_k+1\rangle$. In the average value one can check that $\langle n_k|\hat{b}_k^{\dagger}|n_k-1\rangle$ and $\langle n_k+1|\hat{b}_k^{\dagger}|n_k\rangle$ are different from zero.

Thus, somehow we got a nearest neighbour interactions built in the formalism. In fact, it is eq.(8.5.5.6) defining the Hamiltonian that hides the dispersion relation that is related to $M\omega_k^2$. This point is disentangled below in E&E.

E&E.5.5.5-5

Let us restate the mechanical model underlying the phonon approach. This is a set of N masses (M) that are connected by springs of force constant Δ forming a ring (to simulate the Born-von Karman boundary conditions); with respect to the ring plane, the masses perform a transverse displacements. For a mass with position label s let the displacement be u_s and the associated momentum be p_s. The Hamiltonian is:

$$H = \Sigma_{s=1}^{N} (p_s^2/2M + \Delta (u_{s+1} - u_s)^2 /2) \quad (8.5.5.19)$$

Let us transform p_s^2 and $(u_{s+1} - u_s)^2$ in term of k-space base functions, namely, eq.(8.5.5.x) and eq. (8.5.5.1a):

$$\Sigma_s\, p_s^2 = (N)^{-1} \Sigma_s \{\Sigma_k P_k \exp(-iksa)\}\{\Sigma_{k'} P_{k'} \exp(-ik'sa)\} =$$
$$(N)^{-1} \{\Sigma_k \Sigma_{k'} P_k P_{k'} \Sigma_s \exp(-i(k+k')sa)\} =$$
$$\Sigma_k \Sigma_{k'} P_k P_{k'} \delta(-k,k') = \Sigma_k P_k P_{-k} \Sigma_s (u_{s+1} - u_s)^2 =$$
$$(N)^{-1} \Sigma_s \Sigma_k \Sigma_{k'} \{ Q_k \exp(ik(s+1)a) - Q_k \exp(iksa)\}$$
$$\{ Q_{k'} \exp(ik'(s+1)a) - Q_{k'} \exp(ik'sa)\} =$$
$$(N)^{-1} \Sigma_s \Sigma_k \Sigma_{k'} \{ Q_k \exp(iksa) (\exp(ika) -1)\}$$
$$\{ Q_{k'} \exp(ik'sa)(\exp(ik'a) -1)\} =$$
$$\{\Sigma_k \Sigma_{k'} (N)^{-1} \{\Sigma_s \exp(iksa) \exp(ik'sa)\}$$
$$Q_k Q_{k'}(\exp(ika) -1)(\exp(ik'a) -1)\} =$$
$$\Sigma_k \Sigma_{k'} Q_k Q_{k'}(\exp(ika) -1)(\exp(ik'a) -1)\, \delta(-k,k')\} =$$
$$\Sigma_k Q_k Q_{-k}(\exp(ika) -1)(\exp(-ika) -1) =$$
$$\Sigma_k Q_k Q_{-k}(1 - \exp(-ika) - \exp(ika) +1) =$$
$$\Sigma_k Q_k Q_{-k}\, 2(1-\cos ka)$$

In crystal coordinates the Hamiltonian takes on the form:

$$H = \Sigma_k \ (1/2M)\, P_k P_{-k} + Q_k Q_{-k}\, \Delta(1-\cos(ka))$$

Defining the dispersion relation as:

$$\omega_k = (2\Delta/M)^{1/2} (1-\cos(ka))^{1/2}$$

the Hamiltonian transform into a well known form:

$$H = \Sigma_k \ (1/2M)\, P_k P_{-k} + (1/2)\, M\, \omega_k^2\, Q_k Q_{-k}$$

This is eq. (8.5.5.6).

Now we have the dispersion relation between frequency and wave vector **k**:

$$\omega^2 = (2\Delta/M)\,(1-\cos(ka)) \qquad (8.5.5.20a)$$

The boundary of the first Brillouin zone is $ka = \pm\pi$. Calculating now $d\omega^2/dK$ one gets $(2\Delta/M)\, d(1-\cos(Ka))/dK$ that equals $(2\Delta/M)a \sin(Ka)$. At the boundaries one obtains $\sin(\pm a\pi/a) = \sin(\pm\pi/)$ so that the first derivative is always zero there. Finally, the factor $(1-\cos(Ka))$ can be rewritten with the help of a trigonometric identity as:

$$\omega^2 = 4(\Delta/M)\, \sin^2(Ka/2) \qquad (8.5.5.20b)$$

Taking square root and changing notation so that three dimensional vectors comes in we get:

$$\Omega(\mathbf{k}) = \Omega(-\mathbf{k}) = 2(\Delta/M)^{1/2} |\sin(\mathbf{ka}/2)| \qquad (8.5.5.21)$$

The allowed values of k are given by eq.(8.5.5.2), namely, k= 2πn/Na; n= 0, ±1, ±2, …,±(N/2 -1), +N/2.

For a given number of phonons at the **k**-th state, $|n_{\mathbf{k}}>$ permits calculating the average value of the displacement operator $u_n(t)$ given in eq.(8.5.5.18). Obviously, $<n_{\mathbf{k}}| u_n(t)|n_{\mathbf{k}}>$ is zero; in a stationary state there is no motion! We calculate instead $u_n(t)^2$:

$$<n_{\mathbf{k}}| u_n(t)^2|n_{\mathbf{k}}> = (\hbar\, n_{\mathbf{k}}/MN\, \Omega(\mathbf{k})) +$$

$$\Sigma_{k'\neq 0}\, \hbar\, (2MN\, \Omega(k'))^{-1}$$

The second term represent zero-point vibration contributions when all $n_{\mathbf{k}}$=0. The case **k**=0 describes the global motion of the crystal. The masses for **k**=0 do not vibrate. In the second term, the values of |**k**| are equal or larger than 2π/N|**a**| meaning with this that the frequencies $\Omega \geq (2\pi/N)\,(\Delta/M)^{1/2}$.

The excited base states are determined by a wave vector **k**, a quasi impulsion ħ**k** and energy E(**k**)= ħΩ(**k**). These excited states are phonons. If we know phonon frequencies as a function of vector **k** then phase (V_p) and group (V_g) velocities can be calculated. V_p is defined as Ω(**k**) /|**k**| and V_g=dΩ(|**k**|)/d|**k**|. For the present model we get:

$$V_p = \Omega(\mathbf{k})\,/|\mathbf{k}| = 2(\Delta/M)^{1/2}\,|\sin(\mathbf{ka}/2)|\,/|\mathbf{k}|\,;$$
$$V_g=(\Delta/M)^{1/2}\,|\mathbf{a}|\,|\cos(\mathbf{ka}/2)| \qquad (8.5.5.22)$$

For very long wave length excitations, ka=2πa/λ <<1, then sin(ka/2) is approximated by the linear term ka/2 and

$$\Omega(\mathbf{k}) \sim |\mathbf{k}||\mathbf{a}|\,(\Delta/M)^{1/2} \qquad (8.5.5.23)$$

While the term cos(ka/2) is approximately equal to 1 so that $V_p \sim 2(\Delta/M)^{1/2}\ |\mathbf{ka}|/2\,/|\mathbf{k}|$ that equals to $(\Delta/M)^{1/2}\ |\mathbf{a}|$; and $V_g \sim (\Delta/M)^{1/2}\,|\mathbf{a}|$ showing that the system at very long wave length excitations behaves as elastic waves, i.e. V_p=V_g. These elementary excitations correspond to *acoustic phonons*.

For the opposite limit of the Brillouin zone, ka→π or λ→ 2a the group velocity tends towards zero and the phase velocity to $(2|\mathbf{a}|/\pi)\,(\Delta/M)^{1/2}$.

The model used so far seems to be too simple. If the interaction between two sites located at n and n-l is specific, we can put a label to the interaction parameter Δ that now should read Δ_l and the interaction potential takes on the form of a sum over two indices: $\Delta_l(u_n-u_{n-l})^2$. The expression for the frequency is now:

$$M\Omega^2(\mathbf{k}) = 4\Sigma_{\boldsymbol{\ell}}\, \Delta_{\boldsymbol{\ell}}\, \sin 2(\mathbf{k}\boldsymbol{\ell})/2 \;;$$

$$\boldsymbol{\ell} = \ell\mathbf{a} \text{ and } \ell=1,2,\ldots,N\ell \qquad (8.5.5.24)$$

The analysis continues in the same manner as for the simple case.

The displacements in a linear model can be transversal (two) and longitudinal. The phonons related to the long wavelength are hence named transverse acoustic (TA) and longitudinal acoustic (LA) modes. For these modes energy increases linearly is a neighbourhood of $\mathbf{k}$=0, they have zero slope at the limit of the Brillouin zone.

Consider now systems having at least two I-frames per crystal basis. Take the case of two I-frames. If the distance between these I-frames were frozen then nothing new concerning phonon spectra would be found, as the entity would behave as an effective "atom". However, if these two I-frames were vibrating against each other optical phonons representing this type of fluctuation would appear. The acoustic phonons present transverse and longitudinal degrees of freedom.

There are then transverse optic (TO), longitudinal optic (LO) phonons and for acoustic modes there are TA and LA phonons. This completes the qualitative classification of this type of quantized excitations.

I-frames vibrations in the crystal are elicited by a number of phenomena: Crystal infrared absorption/emission processes; inelastic light diffusion (e.g. Raman effect); inelastic neutron scattering. These are ranged as linear-response effects to the extent the external probe is weak enough. There are a host of non-linear effects involving phonon-phonon interactions.

So far, I-frame systems have been considered as classical to the extent that the internal quantum state is thought as glue producing a definite total mass distribution. In the same spirit, I-frames endowed with an internal total angular momentum can be discussed with just the models discussed above, namely, linear arrays of "spins". The case of interest is one for which s=1/2.

5.5.6. Spin waves

I-frame systems showing spin S and disposed in a crystal can form several types of magnetic systems. Following with the simple linear crystal model we will sketch the study of collective fluctuations: the magnons.

A *magnon* is a quantized spin wave or collective excitation of I-frames systems showing a total spin S.

The quantum state of each spin I-frame is controlled by the complex amplitudes over the relevant base set noted as: $|S,M_S;i\rangle$ or simply $|S_i,M_{Si}\rangle$ where the index concerns a given Wigner-Seitz cell or a Bravais lattice.

Take the one dimensional space model where the amplitudes giving the specific quantum state with respect to the spin operators; the dimension includes the base states M_{Si}, M_{Si}-1,…, -M_{Si}+1, -M_{Si}. There are $2S_i$+1 terms that are degenerate in absence of interactions. In what follow, all N-sites of a linear array will show the same spin S. The ground state for non-interacting I-frame (separated) systems the ground state will be $(2S+1)^N$-fold degenerate. The interaction between two spin is indicated by Δ_{ij}; in the literature it is usually designated as J_{ij}, the exchange coupling constant. The model spin Hamiltonian is given as a sum over all pair of I-frames:

$$H_{spin} = - \Sigma_{ij} \ \Delta_{ij} \ S_i \cdot S_j \qquad (8.5.6.1)$$

This operator is known as Heisenberg Hamiltonian. What we need now are the base sets required to construct spin quantum states.

Base states at each site are label as $|S,\{M_S\};i\rangle$ the symbol designates the subspace 2S+1-fold degenerate at each site and the global base set is designated as: $[|S,\{M_S\};1\rangle,\ldots,|S,\{M_S\};N\rangle]$. The base element at site-1, for example, $|S,S;1\rangle$ stands for $|S,M_S=S;1\rangle$ corresponding to the maximum value M_S can take. Similarly, $|S,-S;1\rangle$ designates $|S,M_S=-S;1\rangle$. It is certainly not an easy task to lay down the complete base set for the model. We go for the simplest case S=1/2 for which $M_S=\pm 1/2$. The site base state is a 2-spinor: $|S=1/2,\{M_S\};j\rangle = [\alpha \ \beta]^j$. The spin quantum state for the j-th site is given by the linear superposition:

$$|S; j> = C_\alpha(j)\ \alpha + C_\beta(j)\ \alpha =$$

$$C_\alpha(j)\ |1/2,+1/2; j> + C_\beta(j)\ |1/2,-1/2; j> =$$

$$(C_\alpha(j)\quad C_\beta(j))\ [\ \alpha \quad \beta] \qquad (8.5.6.2)$$

Note that one can eliminate the supra index in the spin base; they are independent from the site label. The quantum state at the j-site is simply given the row vector $(C_\alpha(j)\ C_\beta(j))$.

The special case $(C_\alpha(j)=1\ C_\beta(j)=0)$ we call it state +1 and $(C_\alpha(j)=0\ C_\beta(j)=1)$ corresponds to state -1; these states are used now to designate site spin state. For a row vector $(1,1,\ldots,1_j,\ldots 1_N)$ the linear chain has been prepared with spin state $(1\ 0)=\alpha$ at all sites. Similarly, $(-1,-1,\ldots,-1_j,\ldots,-1_N)$ the 1D crystal has been prepared in the spin state $(0\ \ 1)=b$ at all sites.

Consider the case where at the j-site the label is -1 while all other have a +1; the initial state corresponds to a ferromagnetic material. One can think of the sequential process at the Fence:

Initial state:	$(1,1,\ldots,1_j,\ldots 1_N)$	Ferromagnetic state
Inject spin β-state at j=1:	$(-1,1,\ldots,1_j,\ldots 1_N)$	
Make the system drift:	$(1,-1,\ldots,1_j,\ldots 1_N)$	

Propagation	$(1,1,\ldots,-1_j,\ldots 1_N)$	

Probe at site N:	$(1,1,\ldots,1_j,\ldots,-1_N)$	

As the state -1 is changing position in a sequential manner we can see the process as a prototype spin wave. For this spin wave there is spin transport but not I-frame (electron) transport. Observe that the energy is constant once the spin β-state was injected.

Look at the drifting system when $(1,1,\ldots,-1_j,\ldots 1_N)$, the time dependent Schrödinger equation in the nearest neighbor model has the form:

$$i\hbar\, dC_j(t)/dt = E_o\, C_j(t) - \Delta C_{j+1}(t) - \Delta C_{j-1}(t) \qquad (8.5.6.3)$$

There are similar equations for $i\hbar\, dC_{j-1}(t)/dt$ and $i\hbar\, dC_{j+1}(t)/dt$. But, for the present model it is enough to solve the equation for the j-th case.

The energy is fixed, say E, and we look at solutions having the form

$$C_j(t) = a_j \exp(-iEt/\hbar) \qquad (8.5.6.4)$$

Introducing (8.5.6.4) into (8.5.6.3) one gets:

$$E\, a_j \exp(-iEt/\hbar) =$$

$$(E_o\, a_j - \Delta\, a_{j+1} - \Delta\, a_{j-1}) \exp(-iEt/\hbar) \qquad (8.5.6.5)$$

Simplifying the exponential $\exp(-iEt/\hbar)$ one gets: $E\, a_j = (E_o\, a_j - \Delta\, a_{j+1} - \Delta\, a_{j-1})$. The sub indices identify a place on the linear chain, e.g. $a_j = a(x_j)$ and we can write the simplified eq.5.5.6.5) as: $E\, a(x_j) = E_o\, a(x_j) - \Delta\, a(x_{j+1}) - \Delta\, a(x_{j-1})$. Use now the relationships: $x_{j+1} = x_j + b$, where b is the I-frame spacing. Try now the form: $a(x_j) = \exp(ikx_j)$. Then one gets: $E \exp(ikx_j) = E_o \exp(ikx_j) - \Delta \exp(ik(x_{j+1}+b)) - \Delta \exp(ik(x_{j+1}-b))$. Divide by the common factor to obtain the dispersion relation:

$$E = E_o - \Delta \exp(ikb)) - \Delta \exp(-ik\, b)) =$$

$$E_o - 2\Delta \cos(kb) \qquad (8.5.6.6)$$

The amplitudes a_j are given by: $a_j = \exp(ikx_j) \exp(-iEt/\hbar) = \exp(i(kx_j - Et/\hbar)$. The energy E is given by a dispersion relation $E(\Omega) = \hbar\, \Omega$ and can be used to express the amplitudes as:

$$a_j = \exp(i(kx_j - \Omega\, t)) \qquad (8.5.6.7)$$

The spin excitation propagating along the linear chain receives the name magnon.

The state of motion for a magnon can be altered by interactions with a phonon field. Magnons can interact among themselves also. The quantization of the magnon field can be done without further problems, creation operators ($\hat{\mu}^{\dagger}$) and annihilation operators ($\hat{\mu}$) operate on a vacuum of zero available excitations (magnons).

Spin waves in anti-ferromagnetic materials will not be discussed here. The reader is kindly asked to examine a good Solid State Physics textbook.