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On the normalization of continuous-spectrum eigenvectors

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ABSTRACT. The delta-function normalization of eigenvectors of continuous spectra as a limit of the normalization of eigenvectors of discrete spectra is considered in detail. Some mathematical aspects which arise in the treatment of the density of states when the volume of the system tends to infinity are fundamental in the derivation of the Golden Rule for quantum transitions, and they are not usually considered in textbooks.

RESUMEN. Se considera en detalle la normalización de autovectores del espectro continuo (usando funciones delta de Dirac) como límite de la normalización de autovectores del espectro discreto. Son discutidos algunos aspectos matemáticos del tratamiento de la densidad de estados cuando el volumen del sistema tiende a infinito. Estas consideraciones, que son fundamentales para la derivación de la regla de oro para transiciones cuánticas, no son usualmente tratadas en textos básicos.

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As the dimensions of a quantum system tend to infinity, the density of states in the eigenvalue space tends also to infinity. However, the introduction of the so-called 'delta normalization' allows one to substitute the usual density of states by a limited factor —a "new density"— in the completeness formula and in the Golden Rule for quantum transitions. In the following sections we start with a limited system with discrete spectrum and then make the volume tend to infinity.

1. PERIODIC BOUNDARY CONDITIONS

Let there be a system —one-dimensional for the time being— in a physical state $|a\rangle$, normalized to unity:

$$\langle a|a\rangle = 1.$$

Consider now a wide enough region (with length $2l$) which contains that system (see Fig. 1, in three dimensions it would correspond to a box).

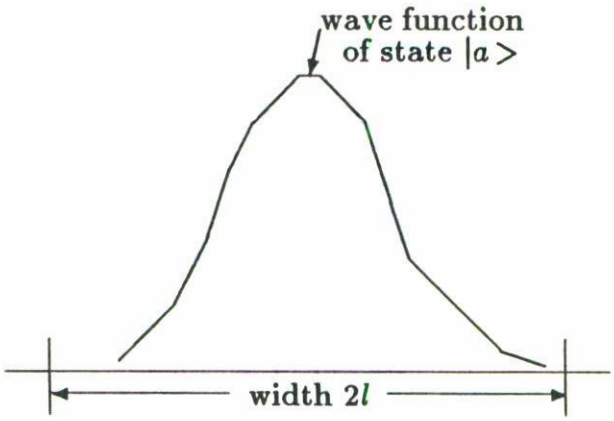

FIGURE 1. The wave function of an one-dimensional system limited in space.

Those normalized eigenvectors of the wave-number operator $\hat{k}$, denoted by $|k_n\rangle$, which obey a periodic condition at the boundaries of the region, form a complete orthonormal discrete set. We have

$$k_n = n\pi/l \qquad (n = \ldots, -2, -1, 0, 1, \ldots),$$

$$\langle k_n | k_{n'} \rangle = \delta_{n,n'} \qquad \text{(orthonormalization)}, \tag{1}$$

$$\sum_{n=k_n l/\pi=-\infty}^{+\infty} |k_n\rangle\langle k_n| = 1 \qquad \text{(completeness or closure)}. \tag{2}$$

Completeness means that any state $|a\rangle$, when written as a sum of its components in all unidimensional Hilbert subspaces defined by each of the eigenvectors $|k_n\rangle$, is still the state $|a\rangle$:

$$\sum_{n=k_n l/\pi=-\infty}^{+\infty} \langle a|k_n\rangle\langle k_n|a\rangle = 1, \tag{3}$$

or alternatively,

$$\langle a| \sum_{n=k_n l/\pi=-\infty}^{+\infty} \langle k_n|a\rangle|k_n\rangle = 1.$$

Coherently, for each one of the eigenstates $|k_{n'}\rangle$ we have Eq. (3), with use of (1), written as

$$\sum_{n=k_n l/\pi=-\infty}^{+\infty} \langle k_{n'}|k_n\rangle\langle k_n|k_{n'}\rangle = \sum_{n=k_n l/\pi=-\infty}^{+\infty} \delta_{n,n'}\delta_{n,n'} = 1. \tag{4}$$

2. A LARGE WIDTH: DISCRETE SPECTRUM

Consider now that l increases to a very large length —but not infinite— in such a way that the number of states with $|k| \leq |k_0|$ becomes very large.[1] In this case it would be possible to approximate summations over discrete states by integrals over a continuous variable k, provided we multiply each differential by the proper density of states.[2] In the next section, the limit of this possibility, as l tends to infinity, will be considered. Meanwhile, we rewrite the completeness relation as

$$\int_{-\infty}^{+\infty} \sigma(k)\langle a|k\rangle\langle k|a\rangle\, dk \simeq 1,$$

where $\sigma(k) = dn/dk = l/\pi$ (independent of k) is the number os states per unit interval of the variable k, *i.e.*, the density of states in the space k:

$$\int_{-\infty}^{+\infty} \frac{l}{\pi}\langle a|k\rangle\langle k|a\rangle\, dk \simeq 1, \tag{5}$$

or

$$\int_{-\infty}^{+\infty} \frac{l}{\pi}|k\rangle\langle k|\, dk \simeq 1 \tag{6}$$

(the similarity sign stands for the approximation considered).

Notice that the dimensions of the density and of the differential dk cancel properly. The density in k-space grows with l.

But if we try to make l tend to infinity, the density grows without limit, becoming useless. A remedy is to change the normalization of eigenstates and completeness in a convenient way.

State $|a\rangle$, as a space-limited state, remains with the same normalization prescription, *i.e.*, $\langle a|a\rangle = 1$. On the other hand, let us normalize the eigenstates $|k_n\rangle$ to

$$\langle k_n|k_{n'}\rangle = \frac{Al}{\pi}\delta_{n,n'} \tag{7}$$

(instead of expression (1)). The quantity A is a chosen constant, with the dimension of k, while the factor Al/π is dimensionless.[3]

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[1] The number of states with modulus of wave number $|k|$ less than or equal to some specified modulus $|k_0|$ is $n_{|k|\leq|k_0|} = 2l|k_0|/\pi + 1$. Frauenfelder and Henley [1] present an interpretation of this number, based on the Uncertainty Principle.

[2] Furthermore, quantities depending on the discrete wave numbers k_n, when written down as functions of the continuous variable k, must obey some rule of attribution of values. For example, they can be kept constant in each interval $k_n \leq k < k_{n+1}$; or obey some other similar choice.

[3] If we considered A as dimensionless, the normalization (7) would introduce a dimension of square root of length in each of the k–eigenstates.

So stated, the completeness relation written down for one of the eigenstates $|k_{n'}\rangle$ (corresponding to expression (4)) is

$$\sum_{n=k_n l/\pi=-\infty}^{+\infty} (\text{factor})\langle k_{n'}|k_n\rangle\langle k_n|k_{n'}\rangle = \frac{Al}{\pi}$$

(see explanation connected with expression (3)), wherefrom one deduces, by direct substitution of orthonormalization (7), that the factor is π/Al. That is, completeness is now

$$\sum_{n=k_n l/\pi=-\infty}^{+\infty} \frac{\pi}{Al}|k_n\rangle\langle k_n| = 1$$

(instead of (2)). In other words, after making the scalar product of a generic vector $|a\rangle$ with each new eigenvector, we must cancel out the factor $(Al/\pi)^{1/2}$ which has been included in it, and again cancel an other factor $(Al/\pi)^{1/2}$ that exists in the ket $|k_n\rangle$.

For a generic state $|a\rangle$ we write

$$\sum_{n=k_n l/\pi=-\infty}^{+\infty} \frac{\pi}{Al}\langle a|k_n\rangle\langle k_n|a\rangle = 1,$$

and this is now going to be rewritten as an integral expression.

The integral completeness relation (5) with the new orthonormalization condition (7) becomes

$$\int_{-\infty}^{+\infty} \frac{\not{l}}{\not{\pi}} \frac{\not{\pi}}{A\not{l}}\langle a|k\rangle\langle k|a\rangle\, dk = \int_{-\infty}^{+\infty} \frac{1}{A}\langle a|k\rangle\langle k|a\rangle\, dk \simeq 1$$

or[4]

$$\int_{-\infty}^{+\infty} \frac{1}{A}|k\rangle\langle k|\, dk \simeq 1.$$

Notice that the factor $1/A$, although it is not a real density of states in k–space, *i.e.*, a number of states per unit of k, mathematically plays such a role as in expression (5) —we could call it informally a "new density". The other factor $-Al/\pi-$ of the true density have been included in the kets and bras via the orthonormalization (7). This fact allows us to make l tend to infinity in a convenient fashion.

[4] Alternatively, we could have rewritten directly the integral completeness relation (6) with the use of orthonormalization (7).

3. THE LIMIT $l \to \infty$; CONTINUOUS SPECTRUM

Completeness relation as $l \to \infty$ is just

$$\int_{-\infty}^{+\infty} \frac{1}{A} |k\rangle\langle k| \, dk = 1. \tag{8}$$

As l goes to infinity the orthonormalization turns into

$$\begin{aligned} \langle k|k'\rangle &= \lim_{l\to\infty} \frac{Al}{\pi} \delta_{n,n'} \\ &= A \begin{cases} \lim\limits_{l\to\infty} l/\pi = \infty & \text{if } k = k', \\ 0 & \text{if } k \neq k'. \end{cases} \end{aligned} \tag{9}$$

But consider yet a further step in this limiting procedure —in order to demonstrate that this is in fact a Dirac delta function. Consider the quantity

$$\lim_{l\to\infty} \sum_{n=k_n l/\pi=-\infty}^{+\infty} \langle k_n|k_{n'}\rangle \, \Delta k,$$

where $\Delta k = k_n - k_{n-1} = \pi n/l - \pi(n-1)/l = \pi/l$. It is just the definition of an integral, which with the help of (7) becomes

$$\lim_{l\to\infty} \sum_{n=k_n l/\pi=-\infty}^{+\infty} \frac{A\not{l}}{\not{\pi}} \delta_{n,n'} \frac{\not{\pi}}{\not{l}} = \lim_{l\to\infty} A \sum_{n=k_n l/\pi=-\infty}^{+\infty} \delta_{n,n'} = A.$$

That is,

$$\int_{-\infty}^{+\infty} \langle k|k'\rangle \, dk = A.$$

An integrand which is infinite at the point $k = k'$ and null otherwise (expression (9)), and whose integral equals A, is A times the Dirac delta function:

$$\langle k|k'\rangle = A\delta(k - k'). \tag{10}$$

This is the so-called 'delta normalization' for continuous spectra (see for example Davydov [2]). Expressions (10) and (8) are respectively orthonormalization and the completeness relation for writing expansions of states over eigenvectors of a continuous spectrum.[5]

In the case of bosons, the quantity A is related to the spatial density of particles. Waves $\langle x|k\rangle = (2\pi)^{1/2}e^{ikx}$, with an (expected) particle density of $1/2\pi$ bosons per unit length ($\int_x^{x+2\pi} |\langle x|k\rangle|^2\, dx = 1$), have $A = 1$ unit of (length)$^{-1}$ [remember that $\delta(k-k') = (2\pi)^{-1}\int_{-\infty}^{+\infty} e^{i(k-k')x}\, dx$].[6] In general, the unidimensional spatial density of bosons is $A/2\pi$. For fermions there is just one particle per state, and there is no direct connection between the factor A and space density.[7]

In three dimensions, the factor A has dimension of $d^3\vec{k}$, the boson space density is $A/(2\pi)^3$, orthonormalization is $\langle\vec{k}|\vec{k}'\rangle = A\delta(\vec{k}-\vec{k}')$, and completeness is

$$\iiint_{\text{all }\vec{k}} \frac{1}{A}|\vec{k}\rangle\langle\vec{k}|\, d^3\vec{k} = 1.$$

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[5] Conversely, in order to deduce (8) from (10), we seek a quantity $\varrho(k)$ which, if included as a factor in

$$\int_{-\infty}^{+\infty} \varrho(k)|k\rangle\langle k|\, dk,$$

makes it equal to one. Applying the expression to any eigenvector $|\vec{k}'\rangle$, and by orthonormalization (10), we have

$$\int_{-\infty}^{+\infty} \varrho(k)|k\rangle\langle k|k'\rangle\, dk = \int_{-\infty}^{+\infty} \varrho(k)|k\rangle A\delta(k-k')\, dk = \varrho(k)A|k'\rangle,$$

which equals $|k'\rangle$ only if

$$\varrho(k) = \frac{1}{A}. \tag{11}$$

[6] Notice that the delta normalization for the eigenvalues of position

$$\langle r|r\rangle = \delta(r-r')$$

should strictly be read as

$$\langle r|r\rangle = 1(\text{unit of length})^{-1}\delta(r-r').$$

The factor appears for example in $\int(1/\text{unit of length})\langle b|r\rangle\langle r|a\rangle\, dr$, to yield a (dimensionless) probability.

[7] An incident beam of fermions over a target has in fact each one of them in a different k-state. In a strict sense, an interval $d^3\vec{k}_{\text{initial}}$ around a given initial state $|\vec{k}_{\text{initial}}\rangle$ and a characteristic density $\varrho_{\text{initial}}(k)$ of occupied states should be considered as the incident beam, *i.e.*, the initial condition for the problem of scattering. But nevertheless, as the interval can be narrow while the density ϱ_{initial} quite large, it is possible, in the cases where the undistinguishability of particles doesn't play a crucial role, to forget the fermionic character and also treat the fermion beam in the fashion we have just described for bosons.

4. DENSITY OF STATES AND THE GOLDEN RULE

The Golden Rule for transition rates (see for example Joachain [3]) gives the probability per unit time for transitions from an initial states $|\vec{k}_{\text{initial}}\rangle$ to a group of final states $|\vec{k}_{\text{final}}\rangle$, all with the same energy as that of $|\vec{k}_{\text{initial}}\rangle$. It is namely[8]

$$\begin{pmatrix} \text{probability} \\ \text{of transitions} \\ \text{per unit time} \end{pmatrix} = \frac{2\pi}{\hbar} |\langle \vec{k}_{\text{final}} | V | \vec{k}_{\text{initial}} \rangle|^2 \rho_{|\vec{k}_{\text{final}}\rangle}(e).$$

The quantity $\rho_{|\vec{k}_{\text{final}}\rangle}(e)$ is the density of states at that value of energy (number of states per unit interval of energy e). The formula is promptly meaningful when thought of as a calculation to a (rather dense but) discrete group of final "normalized to 1" states. On the other hand, it is specially suited for the case of a final continuous spectrum, describing systems of scattering.

For discrete plane waves normalized to one in a large box (obeying periodic boundary conditions), the absolute value of the matrix element $|\langle \vec{k}_{\text{final}} | V | \vec{k}_{\text{initial}} \rangle|$ tends to zero as the volume goes to infinity —it would correspond to quite a small incident flux; at the same time the density of final states $\rho_{|\vec{k}_{\text{final}}\rangle}(e)$ tends to infinity. On the other hand, the adoption of delta-normalized eigenfunctions makes both the matrix elements —since V is non-null in a limited region of space or, as for the coulombian potential, decays as r^{-2}— and a "new density" $\rho(e)$, well-behaved quantities.

The "new density" $\varrho(k)$, as pointed out at the end of the Section 2, does not have the meaning of a number os states per unit interval of k, or unit volume element in $\vec{k}$–space; in fact, a factor Al/π, or Al^3/π^3, has been included in kets and bras. Also the "new density" $\rho(e)$ —which also does not have the meaning of number os states per unit of energy— is calculated in the following way (θ and ϕ are angular coordinates):

$$\rho(e)\, de \sin\theta\, d\theta\, d\phi = \varrho(k) k^2\, dk \sin\theta\, d\theta\, d\phi$$

(the quantity $k^2\, dk \sin\theta\, d\theta\, d\phi$ is the volume element in $\vec{k}$–space). For plane waves we have (non-relativistically) $e = \hbar^2 k^2/2m$ and $de = (\hbar^2 k/m)\, dk$, and using expression (12) at footnote 5, we find

$$\rho(e) = \frac{1}{A} k^2 \frac{dk}{de} = \frac{mk}{A\hbar^2}, \tag{12}$$

which is the quantity to be used with the Golden Rule in the most important case of continuous spectra, with delta-normalized eigenfunctions. For that case, the Golden Rule turns into

$$\begin{pmatrix} \text{probability} \\ \text{of transitions} \\ \text{per unit time} \end{pmatrix} = \frac{2\pi}{\hbar} |\langle \vec{k}_{\text{final}} | V | \vec{k}_{\text{initial}} \rangle|^2 \frac{mk}{A\hbar^2}.$$

[8] Here, the hamiltonian is $H = H_0 + V$, the states $|\vec{k}_{\text{initial}}\rangle$ and $|\vec{k}_{\text{initial}}\rangle$ are eigenstates of H_0, and the potential V produces transitions among the eigenstates of H_0.

5. THE GOLDEN RULE AND THE CROSS SECTION

The choice of A as having dimension of dk, or $d^3\vec{k}$, makes the dimensions of the factors in the Golden Rule for continuous spectra to be the same as those for discrete spectra; the matrix elements have dimension of energy, and the quantity (11) has a dimension of number of states per unit of energy.

The transition probability to a new state, or to a set of states, is the number of particles which in average arise in that (those) new state(s).[9] In this way, the Golden Rule divided by the incident intensity yields the cross section. We have

$$\begin{aligned}\text{cross section} &= \frac{2\pi}{\hbar}|\langle\vec{k}_{\text{final}}|V|\vec{k}_{\text{initial}}\rangle|^2\frac{mk}{A\hbar^2} \\ &\quad\times(\text{density of the incident beam}\times\text{group velocity})^{-1} \\ &= \frac{2\pi}{\hbar}|\langle\vec{k}_{\text{final}}|V|\vec{k}_{\text{initial}}\rangle|^2\frac{mk}{A^2\hbar^2(2\pi)^{-3}(\hbar k/m)} \\ &= \frac{(2\pi)^4m^2}{A^2\hbar^4}|\langle\vec{k}_{\text{final}}|V|\vec{k}_{\text{initial}}\rangle|^2.\end{aligned}$$

Cross sections are in fact independent of the normalization factor A, as the matrix elements are proportional to it in view of the delta normalization, and a cancellation occurs.

The subject of normalization of continuous-spectra eigenvectors is usually considered as well-understood in most texts; it was hoped here to have contributed to the clarification of some passages which are not in fact straightforward.

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[9] For example, if the probability per unit time for a transition is one one-millionth, it means that if we prepare one million identical systems, after one second in one of them in average we will have one particle in the new states.