Covariance Function for Shrodinger equations decision

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Introduction

It is well known that a decision of Shrodinger equations can be considered in the form of its expansion to the system of energy eigen functions. In the case of a discrete energy spectrum it has the form:

$$\Psi(x,t) = \Sigma a_i \varphi_i(x) \ \exp \ i(\frac{E_i}{h}t + \theta_i), \tag{1}$$

where x is a vector, in a co-ordinate space of arbitrary dimension; coefficients a_i and phases θ_i are real constants, depending on initial conditions; and real energy eigen values E_i and eigen functions $\varphi_i(x)$ (which also may be chosen as real) depend only on Hamiltonian expression. Further, we denote $\frac{E_i}{h}$ as ω_i.

In general, the sum is infinite, but we limit ourselves to the case of a finite sum. Generalization to the case of an infinite number of energy eigen values is evident, though some problems of convergence may arise. We remember that probability density over the space, at any moment, t, is defined as

$$P(x,t) = \Psi(x,t)\Psi^*(x,t).$$

It is known that if there is a set of independent oscillations, the frequency ratio of which is irrational, then pahses obey ergodic theorem, and their final distribution may be considered as a product of independent uniform distributions over $[0, 2\pi)$. This is a heuristic basis for the following definition:

We define a random process in time and space as

$$P(x,t) = \Psi(x,t)\Psi^*(x,t), \tag{2}$$

where

$$\Psi(x,t) = \Sigma a_i \varphi_i(x) \ \exp \ i(\omega_i t + \theta_i$$

(2a)

a_i, ω_i and $\varphi_i(x)$ are correspondingly fixed real numbers and functions; θ_i are random real values, independently and uniformly distributed over $[0, 2\pi)$. We consider ω_i and $\varphi_i(x)$ as not random because they depend only on Hamiltonian, and not initial conditions. Values a_i depend on initial conditions, but they are "remembered" by the process (some form of energy conservation law). The process defined is stationary by definition, because any shift in time corresponds to the shift of phases, and they are distributed uniformly.

Our goal is to find the main characteristics of this process, i.e., it's expectation, variance, and covariance function in space and time.

I Expectation

Before making any further calculations, we transform our definition (2),(2a) to the real form:

$$P(x,t) = \Psi(x,t)\Psi^*(x,t) =$$

$$= [\Sigma a_i \varphi_i(x) \text{ exp } i(\omega_i t + \theta_i)][\Sigma a_i \varphi_i(x) \text{ exp } - i(\omega_i t + \theta_i)] =$$

$$= \Sigma\Sigma a_i a_j \varphi_i(x)\varphi_j(x) \text{ exp } i((\omega_i - \omega_j)t + (\theta_i - \theta_j)).$$

Further, we denote $\Delta\omega_{ij} = (\omega_i - \omega_j)$, $\Delta\theta_{ij} = (\theta_i - \theta_j))$. If $i = j$, then evidently, $\Delta\omega_{ij} = 0$ and $\Delta\theta_{ij} = 0$.

Now we separate the last double sum to diagonal and non-diagonal parts:

$$P(x,t) = \Sigma a_i^2 \varphi_i^2(x) +$$

$$+\Sigma\Sigma a_i a_j \varphi_i(x)\varphi_j(x)[\text{exp } i(\Delta\omega ijt + \theta ij) + \text{exp } - i(\Delta\omega ijt + \theta ij)],$$

(the last double sum is over $j > i$), and finally

$$P(x,t) = \Sigma a_i^2 \varphi_i^2(x) + 2\Sigma\Sigma a_i a_j \varphi_i(x)\varphi_j(x) \text{ cos } (\Delta\omega_{ij} t + \Delta\theta_{ij}),\ (j > i) \qquad (3)$$

The phase difference distribution may be considered also as uniform over $[0, 2\pi)$ and for any triple i, j, k of unequal indices, the values $\Delta\theta_{ij}$ and $\Delta\theta_{jk}$ are independent. Averaging over possible phase shifts we get

$$EP(x,t) = \Sigma a_i^2 \varphi_i^2(x),$$

as far as averaged cos is equal to zero. The result does not depend on time (the process is stationary in time) but depends on spatial coordinates. Further we shall denote

$$M(x) = EP(x,t) = \Sigma a_i^2 \varphi_i^2(x). \qquad (4)$$

II Variance

In order to calculate variance we first estimate the second moment:

$$M_2(x) = EP^2(x,t) = E[\Sigma a_i^2\varphi_i^2(x) + s\Sigma\Sigma = E[M^2(x) + 4M(x)\Sigma\Sigma + 4(\Sigma\Sigma)^2].$$

Here we denote by $\Sigma\Sigma$ the double sum $(j > i)$ in expression (3). After averaging over phase shift, the middle term vanishes (as inthe case of expectation), and we have:

$$M_2(x) = M^2(x) + 4E(\Sigma\Sigma)^2 =$$

$$M^2(x) + 4E\Sigma\Sigma\Sigma\Sigma a_i a_j a_{i'} a_{j'} \varphi_i(x)\varphi_j(x)\varphi_{i'}(x)\varphi_{j'}(x) *$$

$$* \cos(\Delta\omega_{ij}t + \Delta\theta_{ij}) \cos(\Delta\omega_{i'j'}t + \Delta\theta_{i'j'}), \qquad (j > i, j' > i')$$

If not true that $i = i'$ and $j = j'$, then expectation of cosine production vanishes due to the independence of pahse shifts. Then

$$M_2(x) = M^2(x) + 4\Sigma\Sigma a_i^2 a_j^2 \varphi_i^2(x)\varphi_j^2(x)\mathrm{E}\cos^2(\Delta\omega_{ij}t + \Delta\theta_{ij}).$$

Being averaged over phase shifts $\cos^2$ gives $\frac{1}{2}$. So, we have

$$M_2(x) = M^2(x) + 2\Sigma\Sigma a_i^2 a_j^2 \varphi_i^2(x)\varphi_j^2(x), \quad (j > i) \tag{5}$$

Now to calculate the variance $D(x)$ we subtract square of expectation from the second moment and get

$$D(x) = 2\Sigma\Sigma a_i^2 a_j^2 \varphi_i^2(x)\varphi_j^2(x), \quad (j > i). \tag{6}$$

The result again does not depend on time. It is interesting that in the case whenonly one a_i differs from zero (energy is strictly defined) variance vanishes (because if $i \neq j$ then $a_i^2 a_j^2 = 0$). in this case probability distribution in space does not change in time. Otherwise variance is not zero and the distribution does permanently (eternally) change in time.

III Covariance

Covariance calculations are carried out in similar fashion to those of variance. Again we calculate first the second moment

$$M_2(x,y,t,u) = E(P(x,t)P(y,u)) = E[(\Sigma a_i^2\varphi_i^2(x)+2\Sigma\Sigma(x,t))(\Sigma a_i^2\varphi_i^2(y)+2\Sigma\Sigma(y,v))] =$$

$$= M(x)M(y) + 2M(x)E\Sigma\Sigma(y,v) + 2M(y)E\Sigma\Sigma(x,t) + 4E(\Sigma\Sigma(x,t)\Sigma\Sigma(y,v)).$$

Middle terms vanish due to averaging over phase shifts, and we get

$$M_2(x,y,t,u) = M(x)M(y) + 4E\Sigma\Sigma\Sigma\Sigma a_i a_j a_{i'} a_{j'} \varphi_i(x)\varphi_j(x)\varphi_{i'}(y)\varphi_{j'}(y) \ast$$

$$\ast \cos(\Delta\omega_{ij}t + \Delta\theta_{ij}) \cos(\Delta\omega_{i'j'}u + \Delta\theta_{i'j'}), \quad (j > i, j' > i').$$

Again, only the terms with $i = i'$ and $j = j'$ do not vanish in averaging and

$$M_2(x,y,t,u) = M(x)M(y) + 4\Sigma\Sigma a_i^2 a_j^2 \varphi_i(x)\varphi_j(x)\varphi_i(y)\varphi_j(y) \ast$$

$$\ast \ \mathrm{E}\cos(\Delta\omega_{ij}t + \Delta\theta_{ij}) \cos(\Delta\omega_{ij}u + \Delta\theta_{ij}).$$

Now let us denote $R_{ij} = (\Delta\omega_{ij}t + \Delta\theta_{ij})$, $\Delta t = y - t$. Then $(\Delta\omega_{ij}u + \Delta\theta_{ij}) = R_{ij} + \Delta\omega_{ij}\Delta t$. Now

$$\cos(\Delta\omega_{ij}t + \Delta\theta_{ij}) \cos(\Delta\omega_{ij}u + \Delta\theta_{ij}) = \cos R_{ij} \cos(R_{ij} + \Delta\omega_{ij}\Delta t) =$$

$$= \cos R_{ij}(\cos R_{ij}\cos\Delta\omega_{ij}\Delta t + \sin R_{ij}\sin\Delta\omega_{ij}\Delta t) =$$

$$= \cos^2 R_{ij}\cos\Delta\omega_{ij}\Delta t + \cos R_{ij}\sin R_{ij}\sin\Delta\omega_{ij}\Delta t.$$

Here, only terms depending on R_{ij} are random. R_{ij} may also be considered as uniformly distributed on $[0, 2\pi)$. After averaging $\cos R_{ij}\sin R_{ij}$ vanishes, and $\cos^2 R_{ij}$ gives $\frac{1}{2}$. At last we get

$$M_2(x,y,u,t) = M(x)M(y) + 2\Sigma\Sigma a_i^2 a_j^2 \varphi_i(x)\varphi_j(x)\varphi_i(y)\varphi_j(y)\cos\Delta\omega_{ij}\Delta t, \quad (j > i)$$

Subtracting the production of expectations we receive

$$\mathrm{Cov}\ (x,y,\Delta t) = 2\Sigma\Sigma a_i^2 a_j^2 \varphi_i(x)\varphi_j(x)\varphi_i(y)\varphi_j(y)\cos(\Delta\omega_{ij}\Delta t), \quad (j > i). \qquad (7)$$

In time the result depends only on time shift Δt. "Long" terms correspond to small energy difference (small $\Delta\omega_{ij}$).

It is interesting also to look at a correlation function in space for a fixed moment. To do this, we have to put into expression (7) $\Delta t = 0$ and divide it by the square root of variances in the points x and y:

$$\operatorname{Cor}(x,y)=\frac{(\Sigma\Sigma a_i^2 a_j^2 \varphi_i(x)\varphi_j(x)\varphi_i(y)\varphi_j(y))}{\sqrt{\Sigma\Sigma a_i^2 a_j^2 \varphi_i^2(x)\varphi_j^2(x)\Sigma\Sigma a_i^2 a_j^2 \varphi_i^2(y)\varphi_j^2(y)}}. \quad (j>i)$$

In the case when only two coefficients a_1 and a_2 differ from zero, we have

$$\operatorname{Cor}(x,y)=\frac{a_1^2 a_2^2 \varphi_1(x)\varphi_2(x)\varphi_1(y)\varphi_2(y)}{|a_1^2 a_2^2 \varphi_1(x)\varphi_2(x)\varphi_1(y)\varphi_2(y)|}.$$

The function gives $\operatorname{Cor}(x,y)$ only two values: $+1$ and -1 depending on the signs of φ_1 and φ_2.

In the general case it is necessary to know particular energy eigen functions.